State-Sum Models of Piecewise Linear Quantum Gravity

This book gives a description of state-sum quantum gravity models which are based on triangulations of a smooth spacetime manifold. It contains detailed descriptions of Regge quantum gravity, spin-foam models and spin-cube models. Some other similar models, like the dynamical triangulations models, are only briefly described, since the sum over the spacetime triangulations is outside the scope of this book.

The book also contains a detailed description of the approach where the piecewise linear (PL) manifold corresponding to a smooth manifold triangulation is considered as the basic structure of the spacetime. Hence the PL structure is not an auxiliary tool used to define the gravitational path integral for a smooth spacetime, but it is taken as a physical property of the spacetime. Consequently, it is straightforward to construct a finite gravitational path integral. Another consequence is that the problems of determination of the classical limit and how to calculate the quantum corrections can be solved by using the effective action method. The smooth manifold limit problem is then replaced by the problem of a smooth manifold approximation for the effective action, which can be obtained by using the standard quantum field theory with a physical cutoff.

Some physical effects of a PL spacetime quantum gravity theory are also described, one of which is that the cosmological constant spectrum contains the observed value.

A short exposition of higher gauge theory is also given, which is a promising way to generalize a gauge symmetry by using the concept of a 2-group. A 2-group is a categorical generalization of a group, and by using this approach one can construct the spin-cube models of quantum gravity.

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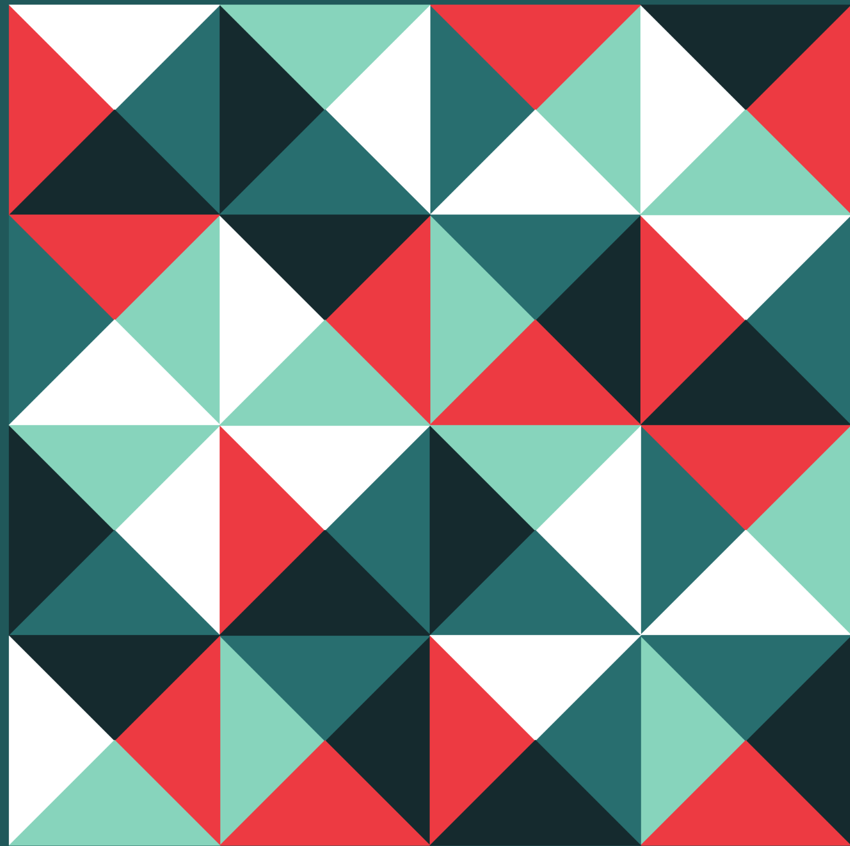

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Preface

This book describes a novel approach in the study of quantum gravity (QG) state-sum models, which is based on the application of the effective action method from quantum field theory. Related to that is a study of the effect of a non-trivial path-integral (PI) measure on the PI finiteness, as well as a study on the dependence of the semi-classical expansion of the effective action on the PI measure.

Another novelty is a detailed study of the idea that the spacetime at small distances is not a smooth manifold but a piecewise linear (PL) manifold corresponding to a triangulation of a smooth manifold. This is a radical departure from the standard approach in PLQG, where the PL structure, i.e. the triangulation, is assumed to be non-physical and an auxiliary tool serving to define a QG theory on a smooth manifold. The main advantage of this paradigm shift is that finite QG path integrals can be constructed, while the semi-classical limit can be explored by using the effective action formalism. A smooth spacetime is then interpreted as an approximation to a PL manifold when the maximal edge length is small and the number of spacetime cells is large. The corresponding effective action can be then approximated by the usual QFT effective action with a cutoff, where the cutoff is determined by the average edge length in the spacetime triangulation. A further consequences of the idea that the spacetime is a PL manifold is that the cosmological constant has a continuous spectrum, and that the spectrum contains the observed value of the cosmological constant. We also describe some implications for quantum cosmology.

A description of higher gauge theory formulation of general relativity is also given, since the corresponding state-sum models do not suffer from the problems found in the spin-foam models of QG. These new state-sum models are called spin-cube models, and they are categorical generalizations of the spin-foam models, since one labels the edges, the triangles and the tetrahedra in a triangulation with representations of a 2-group, which is a categorical generalization of a group.

A major part of the book is devoted to the results obtained by the authors in the period from 2009 to 2016, and some more recent results have been also included. The book contains descriptions of the main PLQG approaches, but the emphasis is on a more detailed description of the Regge PLQG and the corresponding effective action. Our book can serve as an introductory text for a further research, so that it can be useful for young researchers, as well as for other researchers who are interested in this area.

We would like to thank John Barrett, Louis Crane, Laurent Freidel, Renate Loll, Steven Carlip, Ignatios Antoniadis and Hermann Nicolai for conversations over the years, who helped us to clarify our ideas.

Lisbon, March 2023

Aleksandar Miković and Marko Vojinović

Contents

Causal orders, quantum circuits and spacetime: distinguishing between definite and superposed causal orders

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We study the notion of causal orders for the cases of (classical and quantum) circuits and spacetime events. We show that every circuit can be immersed into a classical spacetime, preserving the compatibility between the two causal structures. Using the process matrix formalism, we analyse the realisations of the quantum switch using 4 and 3 spacetime events in classical spacetimes with fixed causal orders, and the realisation of a gravitational switch with only 2 spacetime events that features superpositions of different gravitational field configurations and their respective causal orders. We show that the current quantum switch experimental implementations do not feature superpositions of causal orders between spacetime events, and that these superpositions can only occur in the context of superposed gravitational fields. We also discuss a recently introduced operational notion of an event, which does allow for superpositions of respective causal orders in flat spacetime quantum switch implementations. We construct two observables that can distinguish between the quantum switch realisations in classical spacetimes, and gravitational switch implementations in superposed spacetimes. Finally, we discuss our results in the light of the modern relational approach to physics.

1 Introduction

The notion of causality is one of the most prominent in science, and also in philosophy of Nature. Its treatment separates Aristotelian from the modern physics, and its *formal* meaning within the latter is likely to have played a significant role, over the past centuries since Galileo, in forming our current *everyday* understanding of the notion of causality. While in Newtonian physics the cause-effect relations were encompassed by a rather simple linear and absolute time, Einstein's analysis of causal relations was pivotal in the formulation of the theory of relativity. But it was quantum mechanics (QM) that, through the EPR argument [1], further formalised by Bell [2], showed how quantum nonlocality, rooted in the superposition principle of QM, revolutionised our everyday notion of causality. Finally, strong theoretical evidence that, when combining the two fundamental theories of the modern physics, one is to expect explicit dynamical nonlocal effects in quantum gravity (QG), shows that our basic understanding of causality and causal orders might be crucial in the development of new physics.

Recently, causal orders were, mainly within the quantum information community, discussed in the context of controlled operations. In particular, it was argued that the quantum switch, a specific controlled operation introduced in [3], exhibits superpositions of causal orders, not only in the context of quantised gravity, where genuine superpositions of different states of gravity are present, but also in the experimental realisations performed in classical spacetimes with fixed causal structure [4, 5, 6]. Note that the notion of causal order discussed in these papers is *different* from the causal order of the underlying spacetime structure. We discuss in detail the relation between the two.

In this paper, we analyse the notion of causal orders in the context of classical and quantum circuits, and relate it to the spacetime causal structures. We prove that each circuit can be

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realised in a classical spacetime, preserving the fixed causal relations of the former, with respect to the causal relations between spacetime events of the latter (see the next section for the details of the theorem). Further, we analyse possible realisations of the quantum switch, showing that those performed in everyday labs do not feature superpositions of causal orders between spacetime events (consistent with our theorem), but rather standard non-relativistic quantum mechanical (coherent) superpositions of different evolutions of a system. On the other hand, we argue that genuine superpositions of different causal orders are indeed to be expected within the QG scenario, where superpositions of different states of the gravitational field, with their corresponding causal orders, are manifestly allowed (Hardy was one of the first to discuss the notion of superpositions of causal orders in the context of QG [7]). In addition, we explicitly construct two distinct observables that can distinguish between the realisations of the quantum switch in classical spacetimes, and implementations of the gravitational switch in superposed spacetimes. This way, we show that the two notions of causal orders, namely one discussed in [4, 5, 6] and the other discussed in this paper, can be experimentally distinguished, in contrast to the opposite claim present in the literature [4]. Finally, we discuss our results in the context of the relational approach to physics.

The layout of the paper is as follows. In Section 2, we introduce the notion of causal order for circuits, and prove the Theorem of the circuit immersion in classical spacetimes. Section 3 is devoted to the analysis of the quantum switch implementations in classical spacetimes that do not feature superpositions of spacetime causal orders, as well as implementations in the context of QG. In Section 4, we compare the quantum switch implementations discussed, and introduce observables that can distinguish between those that feature superpositions of spacetime causal orders, and those that do not. Section 5 is devoted to the discussion of the superpositions of causal orders in the context of the relational approach to physics. Finally, in Section 6, we present and discuss the results, provide some final remarks, and list possible future research directions.

2 Causal orders

We begin by discussing circuits and their realisations in (classical) spacetimes with well defined fixed causal orders. Given a directional acyclic graph $G = (I, E)$, where I is the set of graph nodes, and $E = \{(u, v) \,|\, u, v \in I\}$ is the set of its directed edges (arrows pointing from u to v representing the *wires* of the circuit), a *circuit* $\mathcal{C}$ over the set of operations $\mathcal{G}$ is a pair $\mathcal{C} = (G, g)$, where the mapping $g : I \to \mathcal{G}$ assigns operations to each node. Depending on the type of the operations from $\mathcal{G}$, we will call the circuit *classical* (if the operations are, say, classical logic gates), or *quantum* (if the operations are, say, unitaries, measurements, etc.).

The fact that G is directional and acyclic allows one to define a *partial order* $\prec_I$ over the set I as

$$u \prec_I v \quad \overset{\text{def}}{\Longleftrightarrow} \quad \Big(\exists\, n \in \mathbb{N} \;\wedge\; \{u \equiv u_1, u_2, \dots, u_n \equiv v\} \subset I\Big) \; \Big(\forall\, i \in \{1, 2, \dots, n{-}1\}\Big)\; (u_i, u_{i+1}) \in E\,, \tag{1}$$

representing the causal relation between the graph nodes. Next, we define the set of *gates of the circuit* $\mathcal{C}$ as $\mathcal{G}_\mathcal{C} = \{g_u \equiv (u, g(u)) \,|\, u \in I\}$. The induced causal order between the circuit gates $\prec_\mathcal{C}$ is by definition given as

$$g_u \prec_\mathcal{C} g_v \quad \overset{\text{def}}{\Longleftrightarrow} \quad u \prec_I v\,. \tag{2}$$

Moreover, since there exists a canonical bijection between I and $\mathcal{G}_\mathcal{C}$, the order relations $\prec_I$ and $\prec_\mathcal{C}$ are *isomorphic*.

Finally, we can introduce the set $\mathcal{M}$ of all spacetime events, which is assumed to be a traditional $4D$ manifold. On this spacetime manifold we assume to have a gravitational field, described in a standard way, using a metric tensor $g_{\mu\nu}$. The metric is assumed to be of Minkowski signature, such that the metric-induced light cone structure determines a partial order relation between nearby events, denoted $\prec^g_\mathcal{M}$ (or simply $\prec_\mathcal{M}$ when the choice of the metric is implicit). Note that the causal order over the spacetime events is not an intrinsic property of the spacetime manifold itself, but rather determined by the metric, i.e., the configuration of the gravitational field living on the manifold.

One might pose a question if, given a formal circuit $\mathcal{C}$ with gates $\mathcal{G}_\mathcal{C}$, it is possible to realise it in a lab — if it is possible to "immerse" it into spacetime. More precisely, given an arbitrary spacetime manifold $\mathcal{M}$, our goal is to study if there exists an *order-preserving map* $\mathcal{P} : \mathcal{G_C} \to \mathcal{M}$, i.e., if the partial order relations satisfy

$$g_u \prec_{\mathcal{C}} g_v \implies \mathcal{P}(g_u) \prec_{\mathcal{M}} \mathcal{P}(g_v)\,, \tag{3}$$

for every $g_u, g_v \in \mathcal{G_C}$. To that end, we formulate the following theorem (the proof is given in Appendix A).

Theorem. *Any circuit $\mathcal{C}$ can be immersed into a globally hyperbolic spacetime manifold $\mathcal{M}$, such that its relation of partial order $\prec_{\mathcal{C}}$ is preserved by the relation of spacetime events $\prec_{\mathcal{M}}$.*

Regarding the physical interpretation of the Theorem, note that it assigns a spacetime point to each gate in a circuit, as opposed to a point in $3D$ space. Since each spatially localised apparatus may perform the same operation more than once, at different moments in time, it may then correspond to several different gates of the circuit, and thus several different nodes of the graph, instead of just one. In other words, a single piece of experimental equipment *does not* always correspond to a single gate of a circuit.

In addition to the above comment, note that in reality each operation actually takes place in some finite volume of both space and time. However, in theoretical arguments it is convenient to approximate this finite spacetime volume with a single point, ignoring the size and time of activity of the device performing the operation. We adopt this approximation throughout this paper.

Circuits are seen as operations acting upon certain inputs to obtain the corresponding outputs. Usually, the initial/final states (which include instructions, measurement results, etc.) are depicted by the wires. But in our approach, the input state is prepared by the "initial gate" $\mathcal{I}$, while the output state is obtained by the "final gate" $\mathcal{F}$. This way, the circuit $\mathcal{C}$ is seen as an operation $\mathcal{O_C}$ acting from $\mathcal{I}$ to $\mathcal{F}$.

Note that, given a circuit $\mathcal{C}$, the corresponding overall operation $\mathcal{O_C}$ (as well as the input and the output gates $\mathcal{I}$ and $\mathcal{F}$) is uniquely defined. The opposite is not the case: given the operation $\mathcal{O}$, one can design different circuits $\mathcal{C}, \mathcal{C}', \ldots$ that achieve it. To see this, let us consider the simplest case of the operation which satisfies $\mathcal{O} = \mathcal{O}_2 \circ \mathcal{O}_1$, where $\circ$ represents the composition of operations. This operation can be trivially achieved by the two circuits: (i) $\mathcal{C}$, which consists of three nodes — node i whose gate $\mathcal{I}$ prepares the input state, node o that applies the gate $g_o = \mathcal{O}$, and node f whose gate $\mathcal{F}$ outputs either the quantum state, the classical outcome(s), or the combination of the two; (ii) $\mathcal{C}_{12}$, which consists of four nodes — nodes i and f that perform the same operations as before, and *two* intermediate nodes o_1 and o_2 that perform $g_{o_1} = \mathcal{O}_1$ and $g_{o_2} = \mathcal{O}_2$, respectively. For simplicity, here and elsewhere in the text, by $\mathcal{O}$ we denote both the operation and the gate that implements it. The two situations are depicted in the following diagrams (see Figure 1).

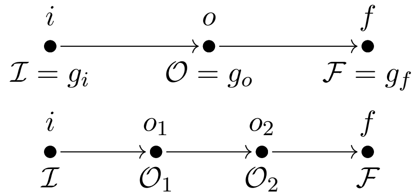

Figure 1: Implementing operation $\mathcal{O}$ with a single gate (upper diagram), and by two consecutive gates $\mathcal{O}_1$ and $\mathcal{O}_2$ (lower diagram).

Finally, in recent literature one can find a notion of an event which is different from the notion of a spacetime point [3, 4, 5, 6, 8, 9, 10, 11]. Namely, one can talk about events as interactions between the quantum system under consideration and the apparatus in the lab. This is motivated by the operational approach to physics, where the interactions between objects are taken as fundamental. Then, one can introduce the relation of partial order, which reflects the causal relationships between such events. Of course, in general, this causal order does not need to coincide with the spacetime causal order. Throughout this paper, if not explicitly stated otherwise, by causal order we mean the order between the spacetime points, which due to our Theorem can also be regarded as the order between the circuit gates. We discuss the difference between the two notions of causal orders in Section 4.

3 Quantum switch

The most prominent feature of quantum systems is that they can be found in *coherent superpositions* of states. This allows for applying the so-called *control operations*. For simplicity, let us assume that operations $\mathcal{O}$ are unitaries, denoted as U. Given a *control* system C in a superposition $|\varphi\rangle_C = a|0\rangle_C + b|1\rangle_C$ (with $\langle 0|1\rangle_C = 0$), the control operation

$$U_{CT} = |0\rangle_C\langle 0| \otimes U_0 + |1\rangle_C\langle 1| \otimes U_1 \qquad (4)$$

transforms the initial product state $|\Psi_i\rangle_{CT} = |\varphi\rangle_C \otimes |\psi_i\rangle_T$ between the control and the *target* systems into the final entangled state $|\Psi_f\rangle_{CT} = a|0\rangle_C \otimes U_0|\psi_i\rangle_T + b|1\rangle_C \otimes U_1|\psi_i\rangle_T$. A simple realisation of such operation by a circuit consisting of three gates is shown below (see Figure 2).

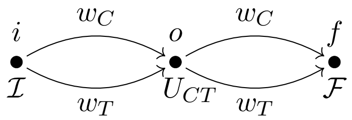

Figure 2: Controlled operation U_{CT}. Applying operation U_b on a system in the wire w_T *controlled* by the state $|b\rangle$ on a system in the wire w_C, with $b = 0, 1$.

Here, the first node and the corresponding gate prepares the initial superposition of the control system, the second implements U_{CT}, and the third is either an identity, a measurement on the two systems, or a combination (say, a measurement of the target qubit, while leaving the control intact). In order to allow for the description of quantum superpositions, we introduce the notion of a vacuum in the analysis of quantum circuits, as is done for example in [12] (for technical details, see Appendix B).

As noted above, given the operation, many different circuits can achieve it. Indeed, in standard optical implementations of the above controlled operation (4), the control qubit is spanned by two spatial modes of a photon, while the target one is its polarisation degree of freedom. The initial superposition state of the control qubit is prepared by a beam splitter, while the two operations U_0 and U_1 are implemented locally in Alice's and Bob's laboratories. Note that, since the control qubit is achieved by the means of two spatial modes of a single photon, while the target qubit is, being the photon's polarisation, "attached to" the control, the target is formally achieved by two degrees of freedom (two wires), one assigned to Alice (T_A), and the other to Bob (T_B). Thus, in such a realization, the control degree of freedom is redundant in the circuit diagram and can be omitted. Nevertheless, since we will later discuss the case of the gravitational quantum switch, in which the gravitational degree of freedom plays the role of the control, here we keep its corresponding wire and gate in the diagram, as presented below (see Figure 3).

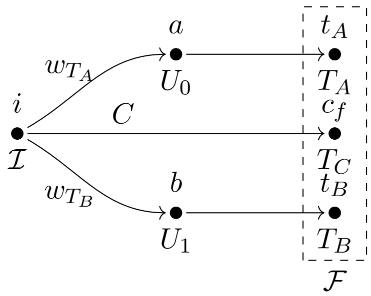

Figure 3: Implementation of the controlled operation using the spatial degree of freedom as a control.

The final gate $\mathcal{F}$ consists of three "elementary gates", represented by the circuit nodes t_A and t_B for the two target wires, and the node c_f for the final control wire.

An important instance of controlled operations is the so-called *quantum switch*, for which the two controlled operations are given by $U_0 = UV$ and $U_1 = VU$, where U and V are two arbitrary unitaries [3]. Having two pairs of equipment, one applying U and the other V, it is straightforward to implement the quantum switch through the circuit similar to the one above, which instead of two gates, one in the node a applying U_0, and another in node b applying U_1, contains four gates placed in the nodes a_U, a_V, b_V and b_U (see Figure 4).

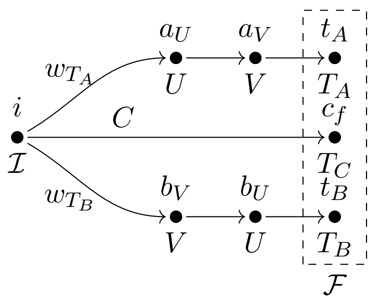

Figure 4: The quantum switch.

The question arises, is it possible to achieve the same using less resources, say, using only two such pieces of equipment, located in two different points (regions) of 3D *space*? Indeed, it is possible to do so, and recently a number of implementations of the quantum switch were performed in flat Minkowski spacetime [4, 5, 6]. Nevertheless, such implementations still correspond to circuits that implement U_0 and U_1 by four, rather than two gates. The difference is that, when immersing it in a flat spacetime, the two pairs of gates are now distinguished only by the temporal, rather than all four spacetime coordinates. Thus, one cannot talk of superpositions of causal orders between spacetime events in such implementations, as flat (indeed, any globally hyperbolic) spacetime has a manifestly fixed causal order. To implement U_0 and U_1 of the quantum switch by a circuit that consists of two gates only (and thus two corresponding spacetime points), one needs a superposition of gravitational fields with different (incompatible) causal orders. In the following two subsections, we analyse in more detail the "4-event" and the "3-event" implementations of the quantum switch, while the "2-event" case is discussed in the last subsection (the numbers 4, 3 and 2 refer to the numbers of spacetime events corresponding to distinct gates used to achieve U_0 and U_1). A detailed mathematical description using the process matrix formalism [8], is presented in the Appendices C, D and E.

Following the previously mentioned distinction between the spacetime event and the operational notion of the event, the 4-event and 3-event quantum switch implementations will have a description within the operational approach that is different from the spacetime description. In particular, in such approach these two implementations of quantum switch would feature only 2 operationally defined events, and thus the superposition of the corresponding causal orders.

3.1 4-event process

The realisations of the quantum switch are performed in table-top experiments in the gravitational field of the Earth, and can be for all practical purposes considered as being performed in flat Minkowski spacetime. In such experiments, Alice performs the unitary U in her localised laboratory, and Bob performs V in his separate localised laboratory, such that both are stationary with respect to each other and the Earth. The operations are applied on a single particle that arrives from the beam splitter, in a superposition of trajectories towards Alice and Bob, and, upon the exchange between the two agents, is finally recombined on the same beam splitter (for simplicity, we chose one beam splitter, but the whole analysis equally holds for two spatially separated beam splitters), and then measured. Below, we present a spacetime diagram of this experimental realisation of the quantum switch, which also represents a circuit of the implementation scheme (see Figure 5).

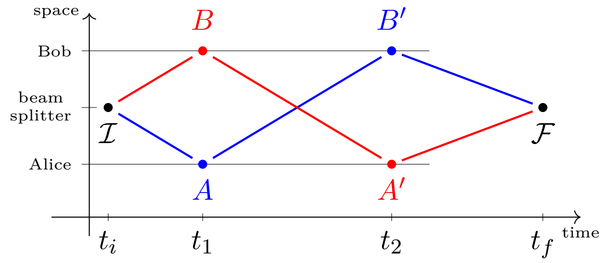

Figure 5: Spacetime diagram, as well as the circuit representation, of the 4-event implementation of the quantum switch.

Black horizontal lines represent world lines for Alice and Bob, as well as the global time coordinate line at the bottom. The black vertical line represents global space coordinate line. Quantum gates are represented by big dots. The composite gate $\mathcal{I}$ consists of the two preparation gates and the initial beam splitter gate, while $\mathcal{F}$ consists of the final beam splitter gate and the target gates that perform the final measurements (for details, see Appendix C). For simplicity, from now on we omit writing the labels of the nodes and keep only the labels of the corresponding circuit gates. The two histories of the particle exchanged between Alice and Bob, representing Alice's and Bob's wires, are full lines coloured in blue and red, respectively.

From the diagram we can see that in the blue history we have the following chain of gates

$$\mathcal{I} \prec_C A \prec_C B' \prec_C \mathcal{F}\,, \tag{5}$$

while for the red history we have

$$\mathcal{I} \prec_C B \prec_C A' \prec_C \mathcal{F}\,. \tag{6}$$

In total, there are four spacetime events involving Alice's and Bob's actions on the particle (gates), namely A, B, A' and B'. Thus, we call the above diagram the "4-event diagram". This setup was already discussed in the literature (see the very end of the Supplementary Notes of [13]).

In order to compare the cases of the quantum and the gravitational switches, it would be interesting to analyse the two examples within recently introduced powerful *process matrix* formalism [8]. To do so, one needs to formulate the formalism involving the vacuum state (see Appendix B for details). The straightforward application of the formalism to the 4-event case is in full accord with the experimental results, as demonstrated in Appendix C.

3.2 3-event process

One can imagine that instead of two, one of the agents implements only one gate. For example, by conveniently choosing the velocity of the particle along its trajectory between Alice and Bob, we can identify Bob's two gates,

$$B \equiv B' \,. \tag{7}$$

We thus arrive to the new spacetime diagram and the associated circuit, called the "3-event diagram" (see Figure 6).

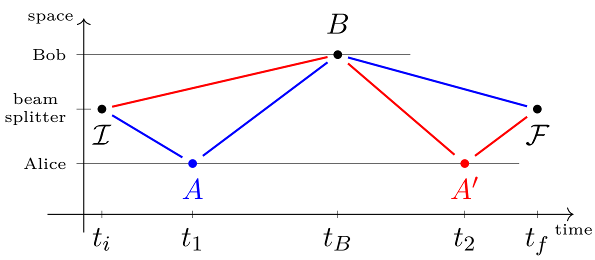

Figure 6: Spacetime diagram, as well as the circuit representation, of the 3-event implementation of the quantum switch.

Now, the obvious question is the following — can we, in addition to (7), impose also that

$$A \equiv A' \,, \tag{8}$$

i.e., also identify Alice's gates into a single spacetime event? In flat Minkowski spacetime, the answer is negative. Namely, by simply looking at the 3-event diagram one can see that the trajectory of the particle between Alice and Bob would require either superluminal speed, or backwards-in-time trajectory in at least one history (note that the diagram assumes that light propagates along the lines that form the 45° angle with the coordinate axes). This is also seen directly from inequalities (5) and (6): identifying both $A \equiv A'$ and $B \equiv B'$ would lead to requiring that *both* $A \prec_{\mathcal{C}} B$ and $B \prec_{\mathcal{C}} A$ are satisfied, i.e., $A \equiv B$. As guaranteed by our Theorem from Section 2, in a curved spacetime it is also impossible to make both identifications (7) and (8), at least if spacetime were globally hyperbolic. Finally, as in the 4-event case, here also the process matrix formalism is consistent with the experimental results, see Appendix D.

3.3 2-event process — gravitational switch

Despite the conclusion of the previous subsection, within the framework of quantum gravity one is allowed to construct superpositions of different gravitational field configurations, leading to superpositions of different causal structures for the spacetime manifold. The assumption of superpositions of different gravitational field configurations is common to all models of QG. Other than that, we will not have any additional assumptions, and thus our approach does not depend on any particular QG model.

In what follows, for the sake of concreteness, we assume the "traditional" approach to the formulation of the QG formalism. Namely, we assume that there exists a smooth $4D$ manifold, called *spacetime*, and denoted as $\mathcal{M}$. Quantum fields, including the gravitational field, live on top of $\mathcal{M}$. The gravitational field is described either via the metric or via some other degrees of freedom (for example, tetrads and spin connection), such that the metric is a function of these. We call this kind of construction "traditional" because it represents a minimal deviation from the mathematical structure of quantum field theory (QFT) in flat Minkowski spacetime, in the sense of preserving the underlying manifold structure. A QG model implementing this approach is, for example, the asymptotic safety framework [14]. Of course, we do not aim to provide a full-fledged model of QG, but rather to only specify the status of the manifold structure within it. As an alternative, in Subsection 5.2, we will discuss the relational framework of QG in which the manifold structure does not exist a priori, but is emergent from relational properties of quantum fields themselves. Finally, note that the discussion of the flat-spacetime cases in the previous sections implicitly assumes the traditional point of view on spacetime manifold. Nevertheless, it has to be compatible with the semiclassical limit of any viable QG model.

As a consequence of the superposition of causal structures in QG, it is possible to achieve a *gravitational switch*, which implements the same quantum switch as described above, with a circuit consisting (in addition to the initial and final gates $\mathcal{I}$ and $\mathcal{F}$) of only two gates: the Alice's gate A that applies U, and Bob's gate B that applies V. Superposing two gravity-matter states, such that in the first the spacetime geometry (described by the metric tensor g_0) establishes the causal structure

$$\mathcal{I} \prec^{g_0}_{\mathcal{M}} A \prec^{g_0}_{\mathcal{M}} B \prec^{g_0}_{\mathcal{M}} \mathcal{F} \,, \tag{9}$$

while in the second (described by the metric g_1) it is

$$\mathcal{I} \prec^{g_1}_{\mathcal{M}} B \prec^{g_1}_{\mathcal{M}} A \prec^{g_1}_{\mathcal{M}} \mathcal{F} \,, \tag{10}$$

the overall circuit applies operations $U_0 = UV$ and $U_1 = VU$, conditioned on the state of gravity. As a side note, it is clear from (9) and (10) that superpositions of the spacetime causal orders can occur only in the framework of quantum gravity.

Such a switch was previously introduced by Zych *et al.* [15], in the context of two spacetimes which are solutions of the Einstein equations. In their proposal, the beam splitter acted *only* on the gravitational degree of freedom (and the accompanied source, the planet), while leaving the rest of the matter, in particular the particle, Alice and Bob, unaffected. Upon the final beam splitter recombination, the matter is left in an *incoherent* mixture of two states proportional to $\{U, V\}|\Psi\rangle$ and $[U, V]|\Psi\rangle$. Subsequently, the mass (along with its gravitational degrees of freedom) is being measured in the superposition basis. Upon a post-selection conditioned on the outcome of the measurement, the matter is again in a pure state.

Another way to obtain a genuine superposition of two different causal orders is by using a spatially delocalised beam splitter, that acts on both gravitational and matter fields. This can be depicted by the following 2-event diagram (see Figure 7).

The yellow region in this diagram represents a compact piece of spacetime where the gravitational field is in a superposition of the two distinct states, and plays the role of the control degree of freedom. Along the boundary of that region, both gravitational configurations smoothly join into a single configuration outside. The boundary of the

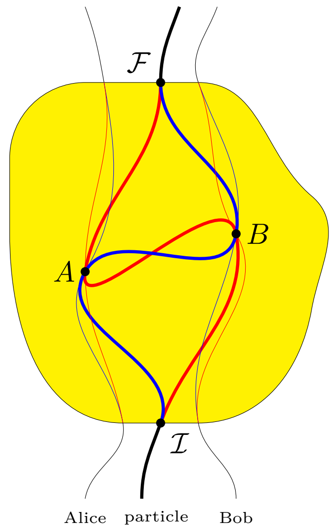

Figure 7: Spacetime diagram of the 2-event implementation of the gravitational switch. Note that formally this is not a circuit diagram, as the control wire, implemented by the state of the gravitational field in the yellow region, is missing.

yellow region thus acts as a beam splitter for anything that enters, and again (in the recombining role) for anything that exits. Therefore, all worldlines (namely, of Alice, Bob and the particle) are doubled inside the yellow region. The blue and red colours represent their spacetime trajectories in two different gravitational field backgrounds, respectively.

We model our gravitational switch such that the overall output state is the product between the state of the gravitational field and the state of the particle. The state of the particle is of the form $(\alpha UV + \beta VU)|\Psi\rangle$, obtained without performing final selective measurement. In particular, in order to compare it with the other quantum switch realizations, we choose either $\{U, V\}|\Psi\rangle$ or $[U, V]|\Psi\rangle$. In order to achieve this, the gravitational switch should act upon *all* degrees of freedom, both gravitational and matter. Note that our gravitational switch does require certain fine tuning, in the sense that the whole, delocalised beam splitter, that acts non-trivially on the whole joint gravity-matter system, is designed for the particular pair of operations applied by Alice and Bob: only for those operations, the beam splitter will output the product state between gravity and matter. Otherwise, the output will be the entangled gravity-matter state, like in the cases of the optical quantum switch and the gravitational switch introduced by Zych et al. (before the final selective measurement). Still, the process matrix describing the gravitational switch itself is independent of the choice of the gate operations of the agents. See Appendix E for details.

The question whether this kind of diagram is admissible in some theory of quantum gravity is nontrivial, and model dependent, on several grounds. First, it is impossible to construct this diagram by superposing two classical configurations of gravitational field, such that each configuration satisfies Einstein equations. The reason is simple — assuming that the gravitational field is specified outside the yellow region, Einstein equations have a unique solution (up to diffeomorphism symmetry) for the compact yellow region, given such a boundary condition. Therefore, one cannot have two different solutions to superpose inside. The only two options are to either superpose one on-shell and one off-shell configuration of gravity, or two off-shell configurations. This scenario can arguably be considered within the path integral framework for quantum gravity.

Second, the question of the particle trajectory is nontrivial. Namely, given one gravitational configuration in which the particle has the spacetime causal structure (9), corresponding to the blue history, it is not obvious that there can exist another gravitational configuration (with the same boundary conditions at the edge of the yellow region), in which the particle has the spacetime causal structure (10), corresponding to the red history. Even if one admits arbitrary off-shell configurations of gravity, it may turn out that the order of events inside the yellow region must be fixed by the boundary conditions. The only viable way to answer this question is to try and construct an explicit example of two geometries implementing (9) and (10) for the same boundary conditions. Numerical investigations are underway to explore this possibility.

4 Distinguishing 2-, 3-, and 4-event realisations of the quantum switch

In a number of both theoretical proposals [3, 8, 9, 10, 11], as well as experimental realisations [4, 5, 6] of the quantum switch, it is claimed that they feature genuine superpositions of causal orders. The reason for this is the introduction of an alternative, operational notion of the event, which differs from a spacetime point. The motivation for this lies in the claim that the individual spacetime points A and A' (and B and B') do not have an operational meaning. In words of the authors of [4] (see the Discussion section):

> *"The results of the experiment confirm that such [which way] information is not available anywhere and that the interpretation of the experiment in terms of four, causally-ordered events cannot be given any operational meaning. If, on the other hand, one requires events to be defined operationally, in terms of measurable interactions with physical systems [...], then the experiment should be described in terms of only two events — a single use of each of the two gates."*

While it is obvious that the mentioned which-way information is not available in the quantum switch experiment, in what follows we argue that this does not imply that one cannot give an operational meaning to spacetime points, even in the context of the quantum switch in classical geometries.

Below, we first present a critical analysis of the arguments behind introducing the operational notion of event. Then, we show how one can experimentally, at least in principle, distinguish 2-, 3-, and 4-event realisations of the quantum switch.

It is the operational approach to understanding spacetime, applied within the framework of relationalism (see Section 5 for a detailed discussion of the relation between the two frameworks), that is arguably the main argument for introducing the alternative notion of an event. This new notion of an event gives rise to the superposition of respective causal orders in the realisations of the quantum switch even in classical spacetimes. Assuming that the smooth (classical) spacetime is an emergent phenomenon, in the operational approach one considers "closed laboratories" [8] as the primal entities within which one can locally apply standard quantum mechanics, while their connections form the relations from which the spacetime emerges. Indeed, it seems that the process matrix formalism was developed precisely with this idea in mind: to be a mathematical tool in analysing the emergence of the spacetime through the relations between the closed laboratories. We would like to note that, as shown in Appendices C, D and E, the mentioned formalism is also fully applicable within the standard formulation of quantum mechanics in classical Minkowski spacetime.

Given that in the case of coherent superpositions of the two paths (a particle first goes to Alice, then to Bob, and vice versa) it is not possible to know which of the two has actually been taken, one may conclude that one cannot distinguish between spacetime events A and A', and that the two are operationally given by the single action of a *spatially* localised laboratory. However, this point of view is at odds with our understanding of the ordinary double slit experiment. Namely, by exchanging the roles of time and space, and following the above logic, applied to the case of the standard double slit experiment, one could analogously conclude that, since in order to obtain the interference pattern at the screen one must not (and thus cannot) learn which slit the particle went through, the two slits represent one and the same operational "lab", and one operational point (region) in space.

Let us explain our argument in slightly more detail. Consider first the optical quantum switch. Here, a particle passes through Alice's lab, described by the two spacetime points, (x_A, t) and (x_A, t'). Any attempt to distinguish the times t and t' at which the particle passes through Alice's lab would destroy the superposition. Consider now the standard double slit experiment. Here, a particle passes through the two slits, described by the two spacetime points, (x_L, t) and (x_R, t). Any attempt to distinguish the positions of the slits x_L and x_R through which the particle passes would destroy the superposition. Note that by exchanging the roles of space and time, the descriptions of the above two situations are essentially identical.

According to the operational approach, as a consequence of the above, one should describe Alice's actions in the optical quantum switch in terms of only one operational event. Thus, analogously, one should also describe the particle passing through the slits in terms of only one operational event. However, such interpretation of the double slit experiment is, to the best of our knowledge, absent from the literature.

Note also that the 3-event realisation of the quantum switch offers a natural alternative interpretation of this phenomenon, as a well known *time double slit experiment* [16]. Indeed, the two events (gates) A and A' play the role of the two time-like slits, while the event (gate) B separates the two in the same way the closed shutter separates the two time-like slits in the time double slit experiment. This comes as no surprise: quantum superpositions are in general accompanied by the interference effects, and the quantum switch is, as already emphasised in Section 3, just another instance of a superposition of two different states of the standard quantum mechanics in Minkowski spacetime.

The operational interpretation of identifying the events A and A' in the current experimental realisations of the quantum switch indeed seems to be a tempting proposal. Nevertheless, we would like to point out that in fact it does not resolve any open problem. In addition, being similar to Mach's ideas, it too may be at odds with the theory of general relativity (GR), see Subsection 5.1 for a detailed discussion.

4.1 Distinguishing by decohering the particle

In the above quote from [4], the authors claim that in order to directly distinguish points A and A' (as well as B and B'), one *must* destroy the superposition in the apparatus. Conversely, being unable to distinguish those points in any experiment that maintains superposition and realises the quantum switch, one cannot give them operational meaning. Therefore, those spacetime points are redundant in the theory, and each pair should be replaced by a single operational event. In this subsection, we discuss this type of an argument. In the next, we give an explicit example of an observable that does distinguish such spacetime points without obtaining the which way information.

Let us study one concrete way of distinguishing the mentioned pairs of points, which decoheres the particle. For simplicity, we will analyse the 4- and 2-event cases only. To this end, we will introduce a third agent, Alice's and Bob's *Friend*. At each run of the quantum switch experiment, Alice will, independently and at random, decide whether just to apply her operation onto the particle, or in addition to that, send a photon to Friend. The same holds for Bob. In 25% of the cases, both agents just perform their respective operations, thus performing the quantum switch. Next, in the 25% of the cases, both agents decide, in addition to applying their respective operations, to send the photons to Friend, who detects them in his spatially localised lab. The remaining 50% of the cases are essentially the same as the previous ones, so for simplicity we omit their analysis.

First, we present the spacetime diagram of the 4-event quantum switch for the case when the agents decide to send the photons to Friend (see Figure 8).

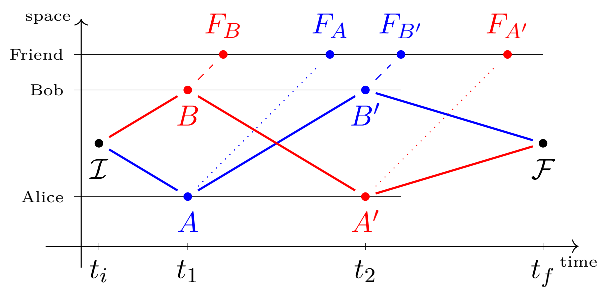

Figure 8: Distinguishing spacetime points by decohering the particle in the 4-event quantum switch. The dotted (dashed) lines represent photons sent by Alice (Bob) to Friend.

The photons coming from Alice are dotted, while the photons coming from Bob are dashed. By knowing the geometry of the whole experiment, Friend would be able to measure, in a generic setup, four *different* times of the photon arrivals: t_A and $t_{A'}$ for spacetime points F_A and $F_{A'}$, and two more for the photons sent by Bob.

On the other hand, in the case of the 2-event gravitational switch realisation, Friend would detect only two times of the photons' arrival. Below, we extend the diagram of the gravitational switch we introduced in Section 3.3, by adding the photons sent to Friend. In order to indicate the fact that the events A and A', etc., are in this setup indeed identified, we write the tilde over the corresponding letters A, B and F (see Figure 9).

Clearly, the two situations are experimentally distinguishable.

Nevertheless, as noted in [4], one might argue that, since the photons sent to Friend in the 4-event case decohere the particle in the switch, this situation does not correspond to the experiment in which the coherence is maintained. Therefore, in the latter, the pair of spacetime events A and

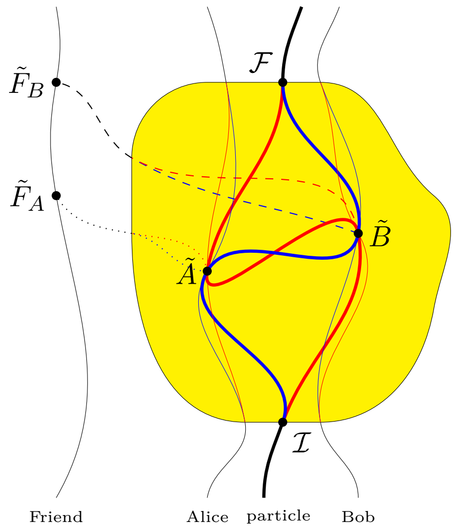

Figure 9: Distinguishing spacetime points by decohering the particle in the 2-event gravitational switch. The dotted (dashed) lines represent photons sent by Alice (Bob) to Friend.

A' still ought to be substituted with a single operational event (and analogously for B and B').

However, even if instead of spacetime points one decides to talk about operational events, such a framework should still be consistent with the experimentally tested theories, GR in particular. According to GR, in flat spacetime (or in any classical configuration of the gravitational field), regardless of whether we decohere the particle or not, both experiments feature four spacetime points, such that A and B (as well as A' and B') can be considered to be simultaneous (see Figure 8). Therefore, the time of execution of both experiments is $\delta t = t_2 - t_1 + C$, where $C \equiv (t_1 - t_i) + (t_f - t_2)$. Note that the time period $t_2 - t_1$ represents the travel time of the particle from one laboratory to the other, and is therefore strictly positive.

From the operational point of view, the decohered version of the experiment also features four operational events, and is thus manifestly consistent with the GR description. Note that a decohered version of the switch still features only two events *per run*: in a classical mixture between "Alice's event before Bob's event" and "Bob's event before Alice's event" each run features just two events, and the duration of the overall experiment in each run is the time between the two events of that run (plus the above constant C).

On the other hand, if the coherence were maintained, the operational point of view features only two operational events, one per laboratory. Then, the total time of execution of the experiment ought to be $\delta\tau = 0 + C$, which is clearly different from the GR prediction. The total time of execution of the quantum switch experiment is a measurable quantity. This means that one can easily determine whether this time is $\delta\tau$ or δt. The former outcome invalidates GR, which would necessitate the formulation of an alternative theory. Note that in this case, a sheer decision to either decohere a particle or not would allow agents to influence the time flow in their labs. Moreover, it raises the question of the time flow in nearby labs *isolated* from the experiment during its execution. The latter outcome poses the problem of the precise formulation of an *operational theory* such that the experiment which features only two operational events lasts precisely the same time as the experiment which features four operational events.

4.2 Distinguishing without decohering the particle

In addition to the above argument, supported by the experimental setup presented in the previous subsection, by erasing the which way information it *is* possible for Friend to distinguish the 4-event and the 2-event realisations even when the "full" quantum switch is executed. For that, one needs to supply Friend with a photon non-demolition measurement. This is in principle possible to construct, although in practice a bit challenging. It thus might be technically easier to use some particles other than photons for sending signals to Friend.

By agreeing in advance of the particular experimental setup, Friend would be able to predict the *distinct* times of arrival of the photons, t_{F_A}, $t_{F_{A'}}$, t_{F_B} and $t_{F_{B'}}$ in the 4-event case, and $t_{\tilde{F}_A}$, $t_{\tilde{F}_B}$ in the 2-event case, thus defining the states of the two photons that arrive to his lab: $|F_A, F_{B'}\rangle$, $|F_{A'}, F_B\rangle$, and $|\tilde{F}_A, \tilde{F}_B\rangle$, respectively. Let us define $\mathcal{H}_{A\prec B'} = \text{span}\{|F_A, F_{B'}\rangle\}$, $\mathcal{H}_{B\prec A'} = \text{span}\{|F_{A'}, F_B\rangle\}$, and $\mathcal{H}_{A\prec B \wedge B\prec A} = \text{span}\{|\tilde{F}_A, \tilde{F}_B\rangle\}$. Then, the relevant Hilbert space of the two photons is

$$\mathcal{H}_{ph} = \mathcal{H}_{A\prec B'} \oplus \mathcal{H}_{B\prec A'} \oplus \mathcal{H}_{A\prec B\wedge B\prec A}\,. \qquad (11)$$

Let us define $P_<$, $P_>$ and $P_=$ as orthogonal projectors onto $\mathcal{H}_{A\prec B'}$, $\mathcal{H}_{B\prec A'}$ and $\mathcal{H}_{A\prec B\wedge B\prec A}$, respectively. One can then define a dichotomic photon non-demolition orthogonal observable performed by Friend on the two photons in his laboratory:

$$M = 1\cdot(P_< + P_>) + 0\cdot P_=\,. \qquad (12)$$

Provided that the experimental setup is *either* that of the 4-event, or the 2-event type, such measurement would not change the state of the experimental setup (the interferometer, the particle in it, and the photons in the Friend's apparatus), while still leaking the information to Friend (via the measurement outcome) about the type of the quantum switch realisation. Finally, by performing the *quantum erasing* procedure [17, 18], the which way information is lost, and the final state of the particle is restored to a coherent superposition.

Let us examine this more formally. Let the two states of the particle in the quantum switch be $|R\rangle$ and $|B\rangle$, corresponding to the red and the blue trajectory, respectively. After $\mathcal{I}$, the state of the particle in the quantum switch is $\frac{1}{\sqrt{2}}(|R\rangle + |B\rangle)$. As the particle passes through Alice's and Bob's labs, two photons are emitted, which arrive at the Friend's lab. The overall state of the particle and the two photons in the 2-event quantum switch is then

$$\frac{1}{\sqrt{2}}\Big(|R\rangle + |B\rangle\Big)|\tilde{F}_A, \tilde{F}_B\rangle. \qquad (13)$$

The particle in the quantum switch is in superposition of the two paths, and it stays so upon measuring M and obtaining the result 0.

On the other hand, the overall state of the particle and the two photons in the 4-event quantum switch is, upon the photons' arrival in the Friend's lab, given by

$$\frac{1}{\sqrt{2}}\Big(|R\rangle|F_{A'}, F_B\rangle + |B\rangle|F_A, F_{B'}\rangle\Big) \qquad (14)$$

$$= \frac{1}{2\sqrt{2}}\Big[\Big(|R\rangle + |B\rangle\Big)\Big(|F_{A'}, F_B\rangle + |F_A, F_{B'}\rangle\Big) + \Big(|R\rangle - |B\rangle\Big)\Big(|F_{A'}, F_B\rangle - |F_A, F_{B'}\rangle\Big)\Big].$$

The particle is now decohered by the two photons, and it remains so upon measuring M and obtaining 1 as the result. Therefore, to erase the which way information, Friend has to perform an additional measurement in the basis

$$|\pm\rangle = \frac{1}{\sqrt{2}}\Big(|F_{A'}, F_B\rangle \pm |F_A, F_{B'}\rangle\Big), \qquad (15)$$

thus collapsing the state of the particle in one of the two pure states

$$\frac{1}{\sqrt{2}}\Big(|R\rangle \pm |B\rangle\Big). \qquad (16)$$

Knowing the outcome of the measurement of M, Friend can post-select the output of the particle coming out of the quantum switch. Alternatively, in the case of obtaining the $|-\rangle$ result, Friend can change the relative phase between the two of the particle's superposed states.

4.3 Other types of gravitational switches

It is important to note that the framework of QG also allows for the construction of 3- and 4-event switches, in addition to the 2-event one. This is straightforward to see, for example by immersing the above 3- or 4-event spacetime diagram into a superposition of different geometries.

Moreover, all of these gravitational switches may give different outcomes when measuring the observable M, given by (12), followed by the quantum erasing procedure (15). The criteria to necessarily obtain the outcome 0 are: (i) that the photons in red and blue histories meet at the boundary of the yellow region, and (ii) from that point on they recombine into a single photon history. Depending on the details of their construction, all gravitational switches either may or may not satisfy the criteria (i) and (ii). On the other hand, no quantum switch realisations in classical spacetimes with definite causal order could ever yield result 0. Finally, we note that even though some of 2-event gravitational switches may give the outcome 1 when measuring M, it does not necessarily mean that there exist no other observable that could distinguish them from the 4-event quantum switches in a classical geometry. This is a matter for further research.

Detailed graphical visualisations of various gravitational switches are presented in the Appendix F.

5 Relational approach to physics

In the light of the operational framework, which suggests the substitution of the spacetime events A and A' with a single operational event (and analogously for B and B'), it is important to comment on one different but related approach to understanding spacetime, called relationalism. Note that by this promotion of operational events as fundamental entities that ought to replace and play the role of the spacetime events, effectively means the identification of A with A', and B with B'. In this section, we first present a historical review of the relational approach to physics. Then, we discuss the operational framework within the context of the modern approach to relationalism.

5.1 Mach principle and the history of relationalism

The idea of relationalism is an old one, it traces back at least as far as Decartes, and is very important in human thought, in particular in the history of physics. It was brought back to science by Mach in the second half of the XIX century (for an overview and history of the Mach principle and the relational approach to space, from its origins in ancient Greece, see for example [19] and the references therein). Based on the Leibniz ideas of a relational world, Mach formulated his famous Mach principle, an intuitively reasonable approach in analysing physics, and space(time) relations in particular. One of the main characteristics of the Mach principle is that (see [20], page 17):

> *"Space as such plays no role in physics; it is merely an abstraction from the totality of spatial relations between material objects."*

The same formulation can be found in [21], slightly re-phrased as *"Mach7: If you take away all matter, there is no more space."* It is interesting to note that the authors attribute this formulation to A. S. Eddington [22], page 164.

As discussed at the beginning of Section 4, in the operational approach one attributes the ultimate existence to the "closed laboratories" only, while their mutual relations, epitomised by the process matrix, are then giving rise to higher level emergent entities. This clearly shows striking similarities between the Mach's and the operational approaches to space(time).

Mach's ideas were crucial for Einstein in formulating the theory of relativity. And while many of Mach's predictions were indeed realised in the new theory, some of them were not. Mach's idea that the matter is the basic entity, and that by abstracting the relations between the objects the space emerges, led him to the following statement: if the matter in the universe were finite and had 3D rotational symmetry, it would be impossible to determine its angular momentum (indeed, even talking about it would have no meaning). This is a plausible idea. Nevertheless, it does not hold in general relativity (GR), where one can find two solutions of the Einstein equations for the isolated black hole (the stationary Schwarzschild solution and the rotating Kerr solution [23]). Moreover, while according to the Mach principle the matter completely determines the space, this is not the case in GR: not only that there exists a solution for the gravitational field in the absence of matter (when the stress-energy tensor T is identically zero), but the solution is not unique, as it depends on the boundary conditions as well (i.e., flat Minkowski spacetime is not the only solution — gravitational waves being a possible alternative [23]). This also holds for the general $T \neq 0$ case, as there too boundary conditions play an important role. Thus, matter does not fully determine the inertia, as should according to Mach principle, which states that the inertia of a massive body is given solely in terms of its relations with the other massive bodies.

Motivated by giving the ultimate reality to material objects only (closed laboratories in the case of the operational approach), Mach formulated the above list of claims. Nevertheless, they were later shown not to hold in GR. Provided the similarities between the Mach ideas and the operational approach, the latter might face similar problems as well. We thus believe that introducing the operationalist notion of an event should be accompanied by more elaborate proposals of new physical hypotheses and theories. We hope that our discussion may serve as a small step towards achieving this goal.

5.2 Modern approach to relationalism

In contrast to the historical approach to relationalism and Mach's ideas, that sounded plausible at the time but ultimately failed with the development of GR, the more elaborate modern approach to relationalism is epitomised in the words of Carlo Rovelli (see Section 2.3 of [24]):

> *"The world is made up of fields. Physically, these do not live on spacetime. They live, so to say, on one another. No more fields on spacetime, just fields on fields."*

In particular, the modern relational approach to spacetime defines a particular spacetime point by the physical processes that are "happening at that point". More technically, given an ordered set of classical fields $\phi \equiv (\phi_1, \dots, \phi_n)$ used to describe physics in a given classical theoretical framework, one traditionally starts from some spacetime point $\tilde{x}$ and evaluates the fields at that point, $\tilde{\phi}_i = \phi_i(\tilde{x})$, obtaining an n-tuple of numbers $(\tilde{\phi}_1, \dots, \tilde{\phi}_n)$. The idea of relationalism does the opposite — one starts from n-tuples of field values, and then defines a spacetime point using an n-tuple, $\tilde{x} \equiv (\tilde{\phi}_1, \dots, \tilde{\phi}_n)$, so that the same equation $\tilde{\phi}_i = \phi_i(\tilde{x})$ holds. The question of how to operationally relate values of different fields, and assign and distribute them into n-tuples, is a matter of a separate study [25]. In this work, we assume that this problem is already solved. Moreover, note that fields ϕ need not be observable, due to potential gauge symmetries (for example, the electromagnetic potential A_μ and the metric $g_{\mu\nu}$). To that end, we introduce an ordered set of gauge invariant functions $\mathcal{O}(\phi) \equiv (\mathcal{O}_1(\phi), \dots, \mathcal{O}_m(\phi))$, where $m \geq n$ (for example, the electromagnetic field strength $F_{\mu\nu}$ and the curvature $R^\lambda{}_{\mu\nu\rho}$), and *define a spacetime point* as an m-tuple of their values $\tilde{\mathcal{O}}$.

Unless the physical system features some global symmetry, each m-tuple $\tilde{\mathcal{O}}$ defines a unique point in spacetime. Note that, in the context of GR, the absence of global symmetries is actually the generic case. Thus, the essential feature of this definition is that it does not make sense to say that the same m-tuple of field strengths can occur in two different spacetime points, since "both" spacetime points in question are defined in terms of the one and the same m-tuple, and therefore represent a *single* point.

Moving from classical to the quantum framework, where no system has predetermined physical properties independent of observation, one needs to talk about observables. Given an ordered set of quantum fields $\phi \equiv (\phi_1, \dots, \phi_n)$, one constructs one *specific* complete set of compatible observables $\mathcal{O} \equiv (\mathcal{O}_1(\phi), \dots . \mathcal{O}_m(\phi))$, where

- *compatible* means that all observables mutually commute, $[\mathcal{O}_i, \mathcal{O}_j] = 0$ for every i and j, while

- *complete* means that the eigenspaces common for all these observables are nondegenerate, i.e., they are one-dimensional subspaces of the total Hilbert space.

Here, by "specific" we mean the set of observables which depend *only* on fields ϕ, but *not* on their conjugated momenta. This fixes the coordinate representation, such that each common eigenvector corresponds to one classical configuration of fields. The outcomes of the measurements of these observables can then be grouped into m-tuples and used to *define individual spacetime points*, as in the classical case above, thus giving rise to an emergent classical spacetime. On the other hand, if the state is not an eigenvector of $\mathcal{O}$, one cannot speak of a single classical configuration of fields, and thus the notion of emergent spacetime and its points ceases to make sense globally, according to the relational approach. At most, one could speak of a superposition of classical configurations and corresponding emergent spacetimes, but without any natural way to relate spacetime points across different branches in the superposition. Nevertheless, this does not mean that establishing such a relation is impossible for certain subregions of spacetime. Indeed, the whole non-yellow "outside" part of the gravitational switch picture from Subsection 3.3 represents a subregion with a locally classical configuration and thus well defined spacetime points.

In order to better appreciate the relational definition of spacetime points given above, it is instructive to look at the realisation of spacetime in the context of a relational quantum gravity model, such as a spinfoam model in the Loop Quantum Gravity (LQG) framework [24, 26]. There, the spacetime is "built" out of the spin foam — a lattice-like structure with vertices, edges and faces, each labeled by the eigenvalues of particular field operators that "live" on these structures, depicted as follows (see Figure 10):

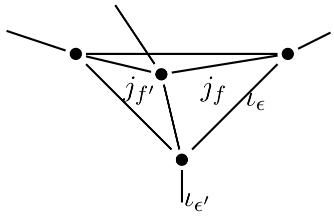

Figure 10: A piece of a spin foam diagram. The field j labels the faces $f, f', \dots$, while the field ι labels the edges $\epsilon, \epsilon', \dots$, of the diagram.

For example, the *area operator*, which is a function of the gravitational field, has eigenvalues determined by a half-integer label $j \in \mathbb{N}/2$, and each face of the spin foam carries one such label, specifying the area of the surface dual to that face. In particular, the spectrum of the area operator is given as

$$A(j) = 8\pi\gamma l_p^2 \sum_f \sqrt{j_f(j_f+1)}\,, \tag{17}$$

where l_p is the Planck length, γ is the Barbero-Immirzi parameter, while the sum goes over all faces f of the spin foam that intersect the surface whose area we are interested in, see [24, 26] for details. All other physical observables similarly provide appropriate labels for each vertex, edge and face of the spin foam. Since edges and faces meet at vertices, a given vertex carries labels of all observables of all edges and faces that are connected to that vertex. These observables form the complete set of compatible observables $\mathcal{O}$, and their eigenvalues label each vertex, determining the identity of that vertex. In other words, each labeled vertex of a spin foam defines a "spacetime point", and if two vertices have completely identical properties in the sense of their labels and their connectedness to neighbouring objects, they actually represent the one and the same vertex.

At first sight, it is tempting to apply the ideas of relational spacetime to the case of the quantum switch, as follows. At the spacetime event A, Alice interacts with the particle as it enters and exits her lab, while at the spacetime event A' Alice also interacts (in exactly the same way) with the same particle. The idea of relational spacetime then might suggest that one should *define* the spacetime events A and A' by the physical event of interaction between Alice and the particle. Since this interaction is the same in both cases, one ought to identify the two points, $A \equiv A'$, and claim that both of these correspond to the same spacetime event, defined by the interaction between Alice and the particle. The same argument applies to Bob, and events B and B'.

Unfortunately, this argument is not fully in line with relationalism. The reason lies in the fact that the interaction between Alice and the particle (and also between Bob and the particle) does not meet the criteria given in the above relational definition of a spacetime point. Namely, neither Alice, nor Bob, performs a measurement of a *complete set of compatible observables* $\mathcal{O}$. The mentioned interaction with the particle is merely a subset of this. In particular, the interaction of Alice with the particle does not uniquely fix the state of, say, the gravitational field, or the electromagnetic field, or the Higgs field, etc. Therefore, it may happen that the measurement outcomes of the whole set of observables $\mathcal{O}$ at spacetime events A and A' are still mutually distinct, thereby defining the events A and A' as two distinguishable spacetime points. In order to be certain that A and A' are really the same spacetime event, Alice would need to measure the complete set of observables $\mathcal{O}$, and convince herself that the results of all those measurements at A and at A' are identical. The mere interaction with the particle is not enough to achieve this, and the experimental setups such as [4, 5, 6] obviously fall short of accounting for the state of all other possible physical fields that Alice and Bob can interact with, in addition to the interaction with the particle.

We see that, when applied to the case of the quantum switch in classical gravitational field, the relational framework is at odds with the operational approach — the former distinguishes A and A' while the latter regards them as identical. This is because the matter fields of the particle are in a superposition of two classical configurations. Similarly, in the case of the 2-event gravitational switch introduced in Subsection 3.3, the overall state of gravity and matter is a superposition of two distinct classical configurations. Therefore, within the relational framework, it is not possible to talk about a single emergent spacetime, nor to compare the points that belong to different branches. This is different from the operational approach, which aims to identify points from different branches. It is also different from the traditional approach, since the latter postulates a unique classical spacetime manifold.

Note that, if understood as an *interpretation*, relational framework ought to have all experimental predictions the same as those from the traditional approach. Thus, the observable constructed in Subsection 4.2 should distinguish the quantum from the gravitational switch, in the same way as in the traditional approach. On the other hand, potential new physics formulated based on the relational framework might, or might not, feature different experimental predictions.

It is important to emphasise that, as discussed in Subsection 4.3, various realisations of the quantum switch are possible by superposing different causal orders in the framework of QG. In particular, regarding the 2-event realisations, one can consider the following diagram (see Figure 11):

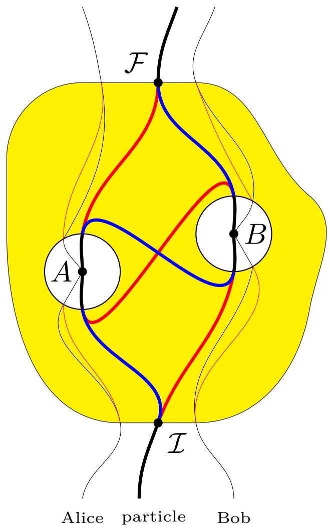

Figure 11: Spacetime diagram of a version of a 2-event gravitational switch, in which Alice and Bob perform their respective operations in the regions of spacetime with a single gravitational configuration.

This diagram features two *classical* spacetime subregions surrounding Alice's and Bob's laboratories. As such, Alice and Bob can measure the complete set of compatible observables within their laboratories, without obtaining which-way information and destroying the superposition. Therefore, even from the relational point of view, this represents an implementation of a 2-event gravitational switch. Note that in this case Alice and Bob do not even need Friend in order to verify the 2-event nature of their gravitational switch.

It is interesting to observe that this realisation of the quantum switch implements the operational idea of a 2-event quantum switch, in terms of closed laboratories. However, to achieve such an implementation, it is necessary to have a genuine superposition of metric-induced spacetime causal orders in the yellow region of spacetime, which does not feature in experimental realisations [4, 5, 6].

6 Conclusions

In this paper, we analysed the notion of causal orders both in classical and quantum worlds, with the emphasis on the latter. We defined the notion of the causal order for the case of (classical and quantum) circuits, in terms of partial ordering between the nodes of the circuit's underlying graph that defines the cause-effect structure. We discussed the possibility of implementing an abstract circuit in the real world, showing that it is always possible to do so for the case of a globally hyperbolic (classical) spacetime, in which the circuit's causal order is preserved by the metric-induced relation between the spacetime events.

The superposition principle of quantum mechanics offers the possibility of controlled operations, in particular the quantum switch, whose experimental realisations have been claimed to present genuine superpositions of causal orders. Within the process matrix formalism, we have analysed the 4- and 3-event realisations of the quantum switch in classical spacetimes with fixed spacetime causal orders, and the 2-event realisation of a gravitational switch that features superpositions of different gravitational field configurations and their respective spacetime causal orders. To that end, we have extended the process matrix formalism, by introducing the notion of a vacuum state. Our analysis shows that the process matrix formalism can explain the quantum switch realisations within the standard physics, and is thus consistent with it.

Thus, as a consequence of our Theorem, and the analysis of the quantum switch implementations, we argued that, in contrast to the gravitational switch, the current experimental implementations do not feature superpositions of spacetime causal orders, and that they are variants of the time double slit experiment. Moreover, by explicitly constructing two different observables, presented in Sections 4.1 and 4.2, respectively, we showed that it is possible to experimentally distinguish between different realisations of the quantum switch.

Finally, in Section 5, we analysed the relation among the traditional QFT approach to QG (used throughout this paper), the operational point of view, and the relational framework of QG. On the example of the quantum switch, we showed that the operational viewpoint, while consistent with the approach advocated by Mach, is nevertheless at odds with the modern relational framework. On the other hand, the traditional QFT approach and the relational framework may or may not be compatible, depending on the concrete realisation of the quantum switch. In particular, for the specific realisation of the gravitational switch given in Subsection 5.2, the two frameworks are compatible in the prediction that Alice and Bob can locally (without the help of Friend) verify that the switch is implemented on 2 events.

In a recent work [27], the authors report on a violation of the causal inequality [8] in flat Minkowski spacetime with a definite causal order. To achieve it, they consider laboratories that are localised in space only, while delocalised in time. Therefore, their alternative notion of a "closed laboratory", and that considered in [8], do not coincide, this way manifestly violating the conditions necessary for the causal inequality to hold. For the same reason, the scenario considered in [27] falls out of the scope of the current work as well. Additionally, in another recent work [28], the author discusses the quantum switch in terms of the time-delocalised quantum subsystems and operations, and generalises it to more complex quantum circuits and processes. The results of these two papers deserve further analysis and remain to be a subject of future research.

Exploring possible generalisations of our Theorem, as suggested at the end of Appendix A, presents a straightforward future line of research. Also, one could further analyse the process matrix formalism, in particular by exploring the situations in which the operational approach interpretation fails to describe the known processes. Or, to search for the opposite — the instances of physical processes that cannot be explained by the process matrix formalism, when applied within the standard physics. In order to show that the process matrix formalism is perfectly suitable for describing the quantum switch implementations within the standard physics, we formulated its version that features the vacuum state. One can thus further study possible generalisations of this formalism and its applications to the cases that go beyond simple non-relativistic mechanics. Finally, motivated by our analysis and discussion from Subsections 4.1 and 5.1, one can try to formulate alternative theories that would be consistent with the experimentally tested known physics (GR in particular), while at the same time substituting the spacetime events A and A', from the quantum switch realisations in classical spacetimes, with a single operational event (and analogously for B and B').

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A Proof of the Theorem

Here we give an explicit constructive proof of the Theorem from the main text.

Given the graph G, we begin the proof by partitioning its set of nodes I into disjoint subsets, in the following way. Since the graph is finite, we introduce the subset $M_1 \subset I$ which consists of all minimal nodes of the graph G:

$$M_1 = \{ u \in I \,|\, (\neg \exists v \in I) \, v \prec_I u \} \,. \tag{18}$$

Since all nodes in M_1 are minimal, there is no order relation $\prec_I$ between any two of them. Therefore, we can intuitively understand them as "simultaneous". As a next step, we remove these nodes and the corresponding edges from G, reducing it to a subgraph $G_2 = (I_2, E_2)$, where

$$I_2 = I \backslash N_1 \,, \qquad E_2 = \{ (u,v) \,|\, u, v \in I_2 \,,\, (u,v) \in E \} \,. \tag{19}$$

Then we repeat the construction for the graph G_2, obtaining the new minimal set M_2, and the next subgraph G_3, in an analogous way. Since the graph G is finite, after a certain finite number of steps we will exhaust all nodes in I, ending up with a partition of "simultaneous" subsets $M_1, \dots, M_m$ ($m \in \mathbb{N}$), such that

$$(\forall i \neq j) \quad M_i \cap M_j = \emptyset \,, \qquad \bigcup_{i=1}^{m} M_i = I \,. \tag{20}$$

Once we have partitioned the set of nodes I into subsets, we turn to the construction of the immersing map $P : I \to \mathcal{M}$, in the following way. Since spacetime is globally hyperbolic, we can write $\mathcal{M} = \Sigma \times \mathbb{R}$, where Σ is a spatial 3-dimensional hypersurface, and $\mathbb{R}$ is timelike. Without loss of generality, one can then introduce a foliation of spacetime into a family of such hypersurfaces, denoted Σ_t and labeled by a parameter $t \in \mathbb{R}$. Start from some initial parameter t_1, and choose a compact subset $S_{t_1} \subset \Sigma_{t_1}$. Denoting the number of elements in the partition M_i as $\|M_i\|$, we pick in an arbitrary way the set of $\|M_1\|$ points $\vec{x}_k \in S_{t_1}$ (here, $k = 1, \dots, \|M_1\|$), and define the map P to assign a node from M_1 to each point $\vec{x}_k$ in a one-to-one fashion:

$$P(u_k) = (t_1, \vec{x}_k) \in \mathcal{M} \,, \qquad k = 1, \dots, \|M_1\| \,. \tag{21}$$

Once this assignment has been defined, construct a future-pointing light cone from each spacetime point $(t_1, \vec{x}_k)$. Then we find a new hypersurface, Σ_{t_2}, which contains a common intersection with all constructed light cones, and denote this intersection $S_{t_2} \subset \Sigma_{t_2}$. In this way, by construction, all points $(t_1, \vec{x}_k)$ are in the past of all points in S_{t_2},

$$(t_1, \vec{x}_k) \prec_{\mathcal{M}} S_{t_2} \,, \qquad k = 1, \dots, \|M_1\| \,. \tag{22}$$

Now extend the definition of P such that it assigns the nodes from the next partition, M_2, to a randomly chosen set of points in S_{t_2} in a similar way as before, then construct a set of light cones from them, and repeat the construction for all partitions M_i. Constructed in this way, the map P ensures that for every pair of nodes $u, v \in I$, we have

$$u \prec_I v \quad \Longrightarrow \quad P(u) \prec_{\mathcal{M}} P(v) \,, \qquad \forall u, v \in I \,. \tag{23}$$

Once we have constructed the map $P : I \to \mathcal{M}$ satisfying (23), using the definition (2), it induces the map $\mathcal{P} : \mathcal{G}_{\mathcal{C}} \to \mathcal{M}$, which satisfies the required statement (3).

This completes the proof. □

Note that, while the causal order $\prec_{\mathcal{M}}$ indeed preserves the causal order $\prec_{\mathcal{C}}$, it is "stronger" in the sense that it may introduce additional relations between the images of nodes, which do not hold in the graph itself. Indeed, the construction of the map P in the above proof is such that *each* image of a node from some given partition M_i is in the causal past of *all* images from the previous partition M_{i-1}, which is not necessarily the case for the nodes themselves. One might study if the causal orders over the set of nodes and over the set of its images can be equivalent, i.e., if the opposite implication from equation (23) also holds (in this case the immersion P is called an *embedding* of G into $\mathcal{M}$). Whether such an embedding exists for all hyperbolic spacetimes, or at least for some, is an open question.

Next, one could also discuss the generalisation of the above theorem to the case of countably infinite graphs G. However, for our purposes, the existence of a partially ordered map $\mathcal{P}$ over the set of finite graphs will suffice.

Regarding the proof itself, one can formulate an alternative (and simpler) approach to the proof of the theorem. Namely, one can first prove that every circuit can be immersed into the flat Minkowski spacetime. Then, knowing that the sufficiently small neighbourhood of every spacetime point in an arbitrary manifold $\mathcal{M}$ can be well approximated with its tangent space, one can always immerse the whole circuit into this small neighbourhood. However, this implies that the geometric size of the circuit can be considered negligible compared to the curvature scale of the manifold, which may render such implementation practically unfeasible. Moreover, this alternative approach does not cover the cases where one actually wants the scale of the circuit to be comparable to the curvature scale. Specifically, if one wishes to employ the circuit to study gravitational phenomena, its gates must be distributed across spacetime precisely in a way that is sensitive to curvature. Therefore, the construction of the map P used in the proof of the theorem is more general than the construction in this alternative approach.

Finally, given the construction in the proof, the gates of the set of minimal nodes M_1 define the initial gate $\mathcal{I}$, the set of maximal nodes M_m define the final gate $\mathcal{F}$, while the the gates of the remaining intermediary sets of nodes $M_2, \dots M_{m-1}$ define the operation $\mathcal{O}_\mathcal{C}$. This is illustrated in the diagram below (see Figure 12).

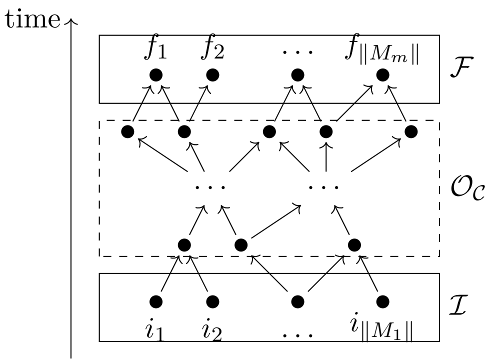


Figure 12: The spacetime diagram of the circuit $\mathcal{C}$, with the initial gate $\mathcal{I}$, the operation gate $\mathcal{O}_\mathcal{C}$, and the final gate $\mathcal{F}$.

B Qutrit states, operators and bases

The notion of a qubit can be generalised from a 2-dimensional Hilbert space to a d-dimensional Hilbert space. The generalised object is called "qudit" in d dimensions [29]. Since we are interested in describing ordinary 2-dimensional qubits with an additional vacuum state, it is natural to consider qudits in $d = 3$, called "qutrits". We introduce the following notation for the basis states of a qutrit in $\mathcal{H}_3 = \mathbb{C}^3$:

$$|0\rangle \equiv \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \qquad |1\rangle \equiv \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \qquad |v\rangle \equiv \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{24}$$

The states $|0\rangle$ and $|1\rangle$ will be understood as the usual computational basis for a 2-dimensional qubit, while the state $|v\rangle$ will represent the vacuum, i.e., the "absence of a qubit". In cases when we take sums over the basis vectors, we will assume that the vacuum state carries the index 2, i.e., $|v\rangle \equiv |2\rangle$, so that we can write

$$\sum_{i=0}^{2} |i\rangle = |0\rangle + |1\rangle + |v\rangle\,, \qquad \text{and} \qquad \sum_{i=0}^{1} |i\rangle = |0\rangle + |1\rangle\,. \tag{25}$$

Using this notation, we write the unnormalised maximally correlated states for the qutrit and the qubit as

$$|\mathbb{1}\rangle\!\rangle = \sum_{i=0}^{2} |i\rangle|i\rangle = |0\rangle|0\rangle + |1\rangle|1\rangle + |v\rangle|v\rangle \in \mathcal{H}_3 \otimes \mathcal{H}_3\,, \qquad |1\rangle\!\rangle = \sum_{i=0}^{1} |i\rangle|i\rangle = |0\rangle|0\rangle + |1\rangle|1\rangle \in \mathcal{H}_2 \otimes \mathcal{H}_2\,, \tag{26}$$

so that

$$|\mathbb{1}\rangle\!\rangle = |1\rangle\!\rangle + |v\rangle|v\rangle\,. \tag{27}$$

One can also introduce the standard Hilbert-Schmidt basis in the space $\mathcal{L}(\mathcal{H}_3)$ of linear operators on $\mathcal{H}_3$. This basis consists of 9 matrices 3×3, labeled as $\lambda_0, \dots, \lambda_8$, as follows:

- the three symmetric matrices

$$\lambda_1 = \sqrt{\frac{3}{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \lambda_2 = \sqrt{\frac{3}{2}} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \qquad \lambda_3 = \sqrt{\frac{3}{2}} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \tag{28}$$

- the three antisymmetric matrices

$$\lambda_4 = \sqrt{\frac{3}{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \lambda_5 = \sqrt{\frac{3}{2}} \begin{bmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{bmatrix}, \qquad \lambda_6 = \sqrt{\frac{3}{2}} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \tag{29}$$

- and the three diagonal matrices

$$\lambda_7 = \sqrt{\frac{3}{2}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \lambda_8 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}, \qquad \lambda_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{30}$$

The matrix λ_0 is the unit matrix, while $\lambda_1, \dots, \lambda_8$ are self-adjoint, traceless, and orthogonal with respect to the standard scalar product:

$$\lambda_i^\dagger = \lambda_i\,, \qquad \operatorname{Tr} \lambda_i = 0\,, \qquad \operatorname{Tr} \lambda_i^\dagger \lambda_j = 3\delta_{ij}\,, \qquad i = 1, \dots, 8\,. \tag{31}$$

They represent the generators of the $SU(3)$ group, and are known as the Gell-Mann matrices (up to a normalisation factor $\sqrt{3/2}$).

If we denote $\mathcal{H}_v$ as the 1-dimensional vacuum-spanned subspace of $\mathcal{H}_3$, one can see that $\mathcal{L}(\mathcal{H}_2) \oplus \mathcal{L}(\mathcal{H}_v) \subset \mathcal{L}(\mathcal{H}_3)$. In particular, if we denote the standard Pauli matrices as $\sigma_x, \sigma_y, \sigma_z$ and the unit 2×2 matrix as I_2, they form the basis in $\mathcal{L}(\mathcal{H}_2)$, and the qubit basis can thus be constructed as

$$\sqrt{\frac{2}{3}}\lambda_1 = \left[\begin{array}{cc|c} \multicolumn{2}{c|}{\sigma_x} & 0 \\ & & 0 \\ \hline 0 & 0 & 0 \end{array}\right], \qquad \sqrt{\frac{2}{3}}\lambda_4 = \left[\begin{array}{cc|c} \multicolumn{2}{c|}{\sigma_y} & 0 \\ & & 0 \\ \hline 0 & 0 & 0 \end{array}\right], \qquad \sqrt{\frac{2}{3}}\lambda_7 = \left[\begin{array}{cc|c} \multicolumn{2}{c|}{\sigma_z} & 0 \\ & & 0 \\ \hline 0 & 0 & 0 \end{array}\right], \tag{32}$$

along with

$$\frac{2}{3}\lambda_0 + \frac{\sqrt{2}}{3}\lambda_8 = \left[\begin{array}{cc|c} \multicolumn{2}{c|}{I_2} & 0 \\ & & 0 \\ \hline 0 & 0 & 0 \end{array}\right]. \tag{33}$$

Also, the vacuum space $\mathcal{L}(\mathcal{H}_v)$ is one-dimensional, and the basis is

$$\frac{1}{3}\lambda_0 - \frac{\sqrt{2}}{3}\lambda_8 = \left[\begin{array}{cc|c} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right]. \tag{34}$$

C Process matrix evaluation

Let us give an explicit step by step evaluation of the probability distribution for the 4-event process discussed in the text, using the process matrix formalism. The complete spacetime diagram of the process is given as (see Figure 13):

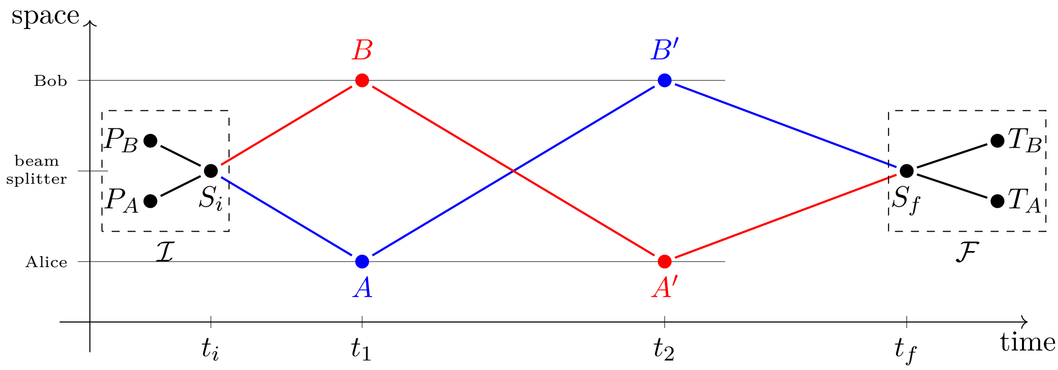


Figure 13: Spacetime diagram of the 4-event implementation of the quantum switch. The internal structures of the composite gates $\mathcal{I}$ and $\mathcal{F}$ are explicitly depicted.

The composite event $\mathcal{I}$ consists of the two preparation events P_A, P_B, and the initial beam splitting event S_i, while $\mathcal{F}$ consists of the recombination event S_f and the measurement events T_A and T_B.

The corresponding circuit diagram is obtained from the above one by promoting each event of interaction to a gate, and the propagation of each particle to a channel. This leads to the following circuit diagram (see Figure 14):

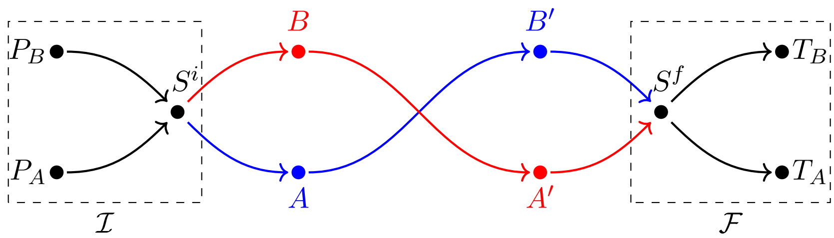


Figure 14: Circuit diagram of the 4-event implementation of the quantum switch. The internal structures of the composite gates $\mathcal{I}$ and $\mathcal{F}$ are explicitly depicted.

Its structure is in one-to-one correspondence with the spacetime diagram for the 4-event process, where the preparation and measurement spacetime events $\mathcal{I}$ and $\mathcal{F}$ have been split into three sub-gates each, for clarity.

The operations on each of the gates are given as follows. The preparation gate P_A maps from the input Hilbert space P_{A_I} to the output Hilbert space P_{A_O}, and analogously for gate P_B. The input spaces are trivial, $\dim P_{A_I} = \dim P_{B_I} = 1$, while each output space is spanned by vectors $|0\rangle$, $|1\rangle$ and $|v\rangle$. Here, $|0\rangle$ and $|1\rangle$ represent the two orthogonal qubit states (say, vertical and horizontal polarisations along certain axis in 3D space), while $|v\rangle$ is the vacuum state, representing the absence of particles in the corresponding arm of the interferometer. The operations performed at these gates, $P_A = |\Psi\rangle$ and $P_B = |v\rangle$, specify the initial conditions for the rest of the circuit diagram, and are described by the Choi-Jamiołkowski (CJ) states as

$$|P_A^*\rangle\!\rangle^{P_{A_I} P_{A_O}} = |\Psi^*\rangle^{P_{A_O}} , \qquad |P_B^*\rangle\!\rangle^{P_{B_I} P_{B_O}} = |v\rangle^{P_{B_O}} . \tag{35}$$

Here, $*$ denotes the complex conjugation.

Analogously, the target gates T_A and T_B facilitate the final measurement outcomes of the circuit diagram. The input spaces T_{A_I} and T_{B_I} are three-dimensional, spanned over the two qubit states and the vacuum, while the output spaces are one-dimensional. The operations performed at these gates, $T_\alpha = \langle\alpha|$ and $T_\beta = \langle\beta|$, read out the measurement results $\alpha, \beta \in \{0, 1, v\}$. The corresponding CJ states are given as

$$|T_\alpha^*\rangle\rangle^{T_{A_I}T_{A_O}} = |\alpha\rangle^{T_{A_I}} , \qquad |T_\beta^*\rangle\rangle^{T_{B_I}T_{B_O}} = |\beta\rangle^{T_{B_I}} . \tag{36}$$

The gates A, A', B and B' perform the unitaries U and V. The input and output spaces A_I and A_O of the Alice's gate A are both spanned by vectors $|0\rangle$, $|1\rangle$ and $|v\rangle$, and analogously for the input and output spaces of the remaining three gates. Assuming that in her (spatially) local laboratory Alice performs the unitary U on the particle's internal degree of freedom, the induced operation between the three-dimensional spaces A_I and A_O that include the vacuum states is given by

$$\tilde{U}^{A_O A_I} = U^{A_O A_I} P_{01}^{A_I A_I} + I^{A_O A_I} P_v^{A_I A_I} , \tag{37}$$

where $P_{01}^{A_I A_I} = |0\rangle^{A_I}\langle 0|^{A_I} + |1\rangle^{A_I}\langle 1|^{A_I}$, $P_v^{A_I A_I} = |v\rangle^{A_I}\langle v|^{A_I}$, and $I^{A_O A_I}$ represents the identity map between the Hilbert spaces A_O and A_I. The analogous construction also holds for the gate A', so the respective CJ states for the gates A and A' are then given by:

$$\begin{aligned} |\tilde{U}^*\rangle\rangle^{A_I A_O} &= \left[I^{A_I A_I} \otimes (\tilde{U}^*)^{A_O A_I} \right] |\mathbb{1}\rangle\rangle^{A_I A_I} , \\ |\tilde{U}^*\rangle\rangle^{A'_I A'_O} &= \left[I^{A'_I A'_I} \otimes (\tilde{U}^*)^{A'_O A'_I} \right] |\mathbb{1}\rangle\rangle^{A'_I A'_I} . \end{aligned} \tag{38}$$

Here, the "transport vector" is given by (for details of the process matrix formalism for the case of three-dimensional spaces — qutrits, see Appendix B):

$$|\mathbb{1}\rangle\rangle = |0\rangle|0\rangle + |1\rangle|1\rangle + |v\rangle|v\rangle . \tag{39}$$

Bob performs V in his (spatially) local laboratory, and therefore the CJ states for the gates B and B' are given as:

$$\begin{aligned} |\tilde{V}^*\rangle\rangle^{B_I B_O} &= \left[I^{B_I B_I} \otimes (\tilde{V}^*)^{B_O B_I} \right] |\mathbb{1}\rangle\rangle^{B_I B_I} , \\ |\tilde{V}^*\rangle\rangle^{B'_I B'_O} &= \left[I^{B'_I B'_I} \otimes (\tilde{V}^*)^{B'_O B'_I} \right] |\mathbb{1}\rangle\rangle^{B'_I B'_I} . \end{aligned} \tag{40}$$

The gates S^i and S^f act as beam splitters, i.e., they both perform the same Hadamard operation H, given as follows. The beam splitter input and output spaces consist of the Alice's and Bob's factor spaces. For the case of the Alice's input space, we have $S_{A_I} = \text{span}\{|0\rangle^{S_{A_I}}, |1\rangle^{S_{A_I}}, |v\rangle^{S_{A_I}}\}$, and analogously for the output space, as well as for Bob's factor spaces. The overall input and output beam splitter spaces are therefore defined as $S_I = S_{(AB)_I} = S_{A_I} \otimes S_{B_I}$ and $S_O = S_{(AB)_O} = S_{A_O} \otimes S_{B_O}$. Finally, the unitary matrix associated to gate S representing the action of the balanced Hadamard beam splitter is given by:

$$\begin{aligned} H^{S_O S_I} = \; & \frac{1}{\sqrt{2}} \left(|0\rangle^{S_{A_O}} |v\rangle^{S_{B_O}} + |v\rangle^{S_{A_O}} |0\rangle^{S_{B_O}} \right) \langle 0|^{S_{A_I}} \langle v|^{S_{B_I}} \\ & + \frac{1}{\sqrt{2}} \left(|1\rangle^{S_{A_O}} |v\rangle^{S_{B_O}} + |v\rangle^{S_{A_O}} |1\rangle^{S_{B_O}} \right) \langle 1|^{S_{A_I}} \langle v|^{S_{B_I}} \\ & + \frac{1}{\sqrt{2}} \left(|0\rangle^{S_{A_O}} |v\rangle^{S_{B_O}} - |v\rangle^{S_{A_O}} |0\rangle^{S_{B_O}} \right) \langle v|^{S_{A_I}} \langle 0|^{S_{B_I}} \\ & + \frac{1}{\sqrt{2}} \left(|1\rangle^{S_{A_O}} |v\rangle^{S_{B_O}} - |v\rangle^{S_{A_O}} |1\rangle^{S_{B_O}} \right) \langle v|^{S_{A_I}} \langle 1|^{S_{B_I}} . \end{aligned} \tag{41}$$

The beam splitter acts such that the system coming from the Alice's side comes into an equal superposition of the two output spatial modes coming to Alice and Bob, with zero relative phase, while the system coming from the Bob's side (blue line) comes into an equal superposition of the two output spatial modes with relative phase π. Thus, in the output space the correlation between the Alice's and Bob's vacuum state is the opposite as in the input case. The corresponding CJ state is then

$$|H^*\rangle\rangle^{S_I S_O} = \left[I^{S_I S_I} \otimes (H^*)^{S_O S_I} \right] |\mathbb{1}\rangle\rangle^{S_I S_I} \,, \tag{42}$$

where the transport vector $|\mathbb{1}\rangle\rangle$ for the beam splitter, when projected to a single-particle subspace, is given by

$$|\mathbb{1}\rangle\rangle = |0v\rangle|0v\rangle + |1v\rangle|1v\rangle + |v0\rangle|v0\rangle + |v1\rangle|v1\rangle \,. \tag{43}$$

Note that the full transport vector contains nine terms instead of the above four, but for the purpose of this paper, we do not need those five additional terms.

The process vector encodes the wires between the gates, and it is being constructed by taking the tensor product over appropriate transport vectors $|\mathbb{1}\rangle\rangle$ for Alice's and Bob's qutrits, see equations (26) and (27), such that each transport vector corresponds to one wire in the circuit diagram, connecting the output of the source gate to the input of the target gate. The process vector is thus given as:

$$\begin{aligned} |W_{\text{4-event}}\rangle\rangle \;=\; & \underbrace{|\mathbb{1}\rangle\rangle^{P_{A_O} S^i_{A_I}} |\mathbb{1}\rangle\rangle^{P_{B_O} S^i_{B_I}}}_{\text{initial}} \underbrace{|\mathbb{1}\rangle\rangle^{S^i_{A_O} A_I} |\mathbb{1}\rangle\rangle^{A_O B'_I} |\mathbb{1}\rangle\rangle^{B'_O S^f_{B_I}}}_{\text{blue}} \\ & \underbrace{|\mathbb{1}\rangle\rangle^{S^i_{B_O} B_I} |\mathbb{1}\rangle\rangle^{B_O A'_I} |\mathbb{1}\rangle\rangle^{A'_O S^f_{A_I}}}_{\text{red}} \underbrace{|\mathbb{1}\rangle\rangle^{S^f_{A_O} T_{A_I}} |\mathbb{1}\rangle\rangle^{S^f_{B_O} T_{B_I}}}_{\text{final}} \,. \end{aligned} \tag{44}$$

One can now evaluate the probability distribution

$$p(\alpha, \beta) = \left\| \mathcal{M}(\alpha, \beta) \right\|^2 \,, \tag{45}$$

where the probability amplitude $\mathcal{M}(\alpha, \beta)$ is constructed by acting with the tensor product of all gate operations (35), (42), (38), (40), (42) and (36), on the process vector (44). Since each of the gate operations acts in its own part of the total Hilbert space, the order of application of these operations is immaterial, and we are free to choose the most convenient one.

To see what happens when the operations (35) of the preparation gates act on the process vector, let us evaluate the action of $|P^*_A\rangle\rangle^{P_{A_I} P_{A_O}}$ on $|\mathbb{1}\rangle\rangle^{P_{A_O} S^i_{A_I}}$:

$$\langle\langle P^*_A|^{P_{A_I} P_{A_O}} |\mathbb{1}\rangle\rangle^{P_{A_O} S^i_{A_I}} = \langle \Psi^*|^{P_{A_O}} \sum_{k=0}^{2} |k\rangle^{P_{A_O}} |k\rangle^{S^i_{A_I}} = \sum_{k=0}^{2} \Big(\langle \Psi | k \rangle \Big)^* |k\rangle^{S^i_{A_I}} = |\Psi\rangle^{S^i_{A_I}} \,. \tag{46}$$

An analogous calculation can be performed for $|P^*_B\rangle\rangle^{P_{B_I} P_{B_O}}$, so the action of both preparation operations (35) on the process vector (44) evaluates to:

$$\begin{aligned} & \Big(\langle\langle P^*_A|^{P_{A_I} P_{A_O}} \otimes \langle\langle P^*_B|^{P_{B_I} P_{B_O}} \Big) |W_{\text{4-event}}\rangle\rangle = \\ & |\Psi\rangle^{S^i_{A_I}} |v\rangle^{S^i_{B_I}} \underbrace{|\mathbb{1}\rangle\rangle^{S^i_{A_O} A_I} |\mathbb{1}\rangle\rangle^{A_O B'_I} |\mathbb{1}\rangle\rangle^{B'_O S^f_{B_I}}}_{\text{blue}} \\ & \underbrace{|\mathbb{1}\rangle\rangle^{S^i_{B_O} B_I} |\mathbb{1}\rangle\rangle^{B_O A'_I} |\mathbb{1}\rangle\rangle^{A'_O S^f_{A_I}}}_{\text{red}} \underbrace{|\mathbb{1}\rangle\rangle^{S^f_{A_O} T_{A_I}} |\mathbb{1}\rangle\rangle^{S^f_{B_O} T_{B_I}}}_{\text{final}} \,. \end{aligned} \tag{47}$$

Next one acts with the initial Hadamard operation (42) on this process vector, transforming it into

$$\begin{aligned} & \left(\langle\langle P^*_A|^{P_{A_I} P_{A_O}} \otimes \langle\langle P^*_B|^{P_{B_I} P_{B_O}} \otimes \langle\langle S^*|^{S^i_{(AB)_I} S^i_{(AB)_O}} \right) |W_{\text{4-event}}\rangle\rangle = \\ & \frac{1}{\sqrt{2}} \Big(|\Psi\rangle^{A_I} |v\rangle^{B_I} + |v\rangle^{A_I} |\Psi\rangle^{B_I} \Big) \underbrace{|\mathbb{1}\rangle\rangle^{A_O B'_I} |\mathbb{1}\rangle\rangle^{B'_O S^f_{B_I}}}_{\text{blue}} \\ & \underbrace{|\mathbb{1}\rangle\rangle^{B_O A'_I} |\mathbb{1}\rangle\rangle^{A'_O S^f_{A_I}}}_{\text{red}} \underbrace{|\mathbb{1}\rangle\rangle^{S^f_{A_O} T_{A_I}} |\mathbb{1}\rangle\rangle^{S^f_{B_O} T_{B_I}}}_{\text{final}} \equiv |W_{QS_4}\rangle\rangle \,. \end{aligned} \tag{48}$$

The resulting process vector is the outcome of the action of the composite gate $\mathcal{I}$ on (44), before the actions of Alice and Bob (note that often in the literature this is taken as the initial process vector in the analysis):

$$|W_{QS_4}\rangle\!\rangle = \frac{1}{\sqrt{2}}\left(|\Psi\rangle^{A_I}|v\rangle^{B_I} + |v\rangle^{A_I}|\Psi\rangle^{B_I}\right)|\mathbb{1}\rangle\!\rangle^{A_O B'_I}|\mathbb{1}\rangle\!\rangle^{B_O A'_I}|\mathbb{1}\rangle\!\rangle^{(A'_O B'_O)S_{(AB)_I}}|\mathbb{1}\rangle\!\rangle^{S_{(AB)_O}T_{(AB)_I}}\,. \quad (49)$$

Continuing the computation, the action of the remaining gate operations (38), (40), (36) and (42) on the process vector (49) gives us the probability amplitude,

$$\mathcal{M}(\alpha,\beta) \equiv$$
$$\left(\langle\!\langle\tilde{U}^*|^{A_I A_O} \otimes \langle\!\langle\tilde{U}^*|^{A'_I A'_O} \otimes \langle\!\langle\tilde{V}^*|^{B_I B_O} \otimes \langle\!\langle\tilde{V}^*|^{B'_I B'_O} \otimes \langle\!\langle H^*|^{S_I S_O} \otimes \langle\!\langle T^*_\alpha|^{T_{A_I}T_{A_O}} \otimes \langle\!\langle T^*_\beta|^{T_{B_I}T_{B_O}}\right)|W_{QS_4}\rangle\!\rangle\,. \quad (50)$$

Let us now calculate the action of $\langle\!\langle\tilde{U}^*|^{A_I A_O}$ on (49):

$$\langle\!\langle\tilde{U}^*|^{A_I A_O}|W_{QS_4}\rangle\!\rangle = \langle\!\langle\mathbb{1}|^{A_I A_I}\left[I^{A_I A_I}\otimes(\tilde{U}^T)^{A_O A_I}\right]|W_{QS_4}\rangle\!\rangle\,. \quad (51)$$

Looking at the structure of the process vector, one sees that the resulting new process vector will have the form

$$\langle\!\langle\tilde{U}^*|^{A_I A_O}|W_{QS_4}\rangle\!\rangle = \frac{1}{\sqrt{2}}\left(|X\rangle^{B'_I}|v\rangle^{B_I} + |Y\rangle^{B'_I}|\Psi\rangle^{B_I}\right)|\mathbb{1}\rangle\!\rangle^{B_O A'_I}|\mathbb{1}\rangle\!\rangle^{(A'_O B'_O)S_{(AB)_I}}|\mathbb{1}\rangle\!\rangle^{S_{(AB)_O}T_{(AB)_I}}\,, \quad (52)$$

where $|X\rangle^{B'_I}$ and $|Y\rangle^{B'_I}$ are shorthands for the expressions

$$|X\rangle^{B'_I} \equiv \langle\!\langle\mathbb{1}|^{A_I A_I}\left[I^{A_I A_I}\otimes(\tilde{U}^T)^{A_O A_I}\right]|\Psi\rangle^{A_I}|\mathbb{1}\rangle\!\rangle^{A_O B'_I} \quad (53)$$

and

$$|Y\rangle^{B'_I} \equiv \langle\!\langle\mathbb{1}|^{A_I A_I}\left[I^{A_I A_I}\otimes(\tilde{U}^T)^{A_O A_I}\right]|v\rangle^{A_I}|\mathbb{1}\rangle\!\rangle^{A_O B'_I}\,, \quad (54)$$

which need to be evaluated. The explicit computation of the first expression goes as follows:

$$\begin{aligned}
|X\rangle^{B'_I} &= \langle\!\langle\mathbb{1}|^{A_I A_I}\left[I^{A_I A_I}\otimes(\tilde{U}^T)^{A_O A_I}\right]|\Psi\rangle^{A_I}|\mathbb{1}\rangle\!\rangle^{A_O B'_I} \\
&= \sum_{k=0}^{2}\langle k|^{A_I}\langle k|^{A_I}\left[I^{A_I A_I}\otimes(\tilde{U}^T)^{A_O A_I}\right]|\Psi\rangle^{A_I}\sum_{m=0}^{2}|m\rangle^{A_O}|m\rangle^{B'_I} \\
&= \sum_{m=0}^{2}\left[\sum_{k=0}^{2}\left(\langle k|^{A_I}I^{A_I A_I}|\Psi\rangle^{A_I}\right)\left(\langle k|^{A_I}(\tilde{U}^T)^{A_O A_I}|m\rangle^{A_O}\right)\right]|m\rangle^{B'_I} \\
&= \sum_{m=0}^{2}\left[\sum_{k=0}^{2}\langle k|\Psi\rangle^{A_I}\;\langle m|^{A_O}\tilde{U}^{A_O A_I}|k\rangle^{A_I}\right]|m\rangle^{B'_I} \\
&= \sum_{m=0}^{2}\left[\langle m|^{A_O}\tilde{U}^{A_O A_I}|\Psi\rangle^{A_I}\right]|m\rangle^{B'_I}\,.
\end{aligned} \quad (55)$$

Using (37), the coefficient in the brackets can be evaluated as

$$\langle m|^{A_O}\tilde{U}^{A_O A_I}|\Psi\rangle^{A_I} = \langle m|^{A_O}\left(U^{A_O A_I}P_{01}^{A_I A_I} + I^{A_O A_I}P_v^{A_I A_I}\right)|\Psi\rangle^{A_I} = \langle m|U|\Psi\rangle\,, \quad (56)$$

since $P_{01}^{A_I A_I}|\Psi\rangle^{A_I} = |\Psi\rangle^{A_I}$ and $P_v^{A_I A_I}|\Psi\rangle^{A_I} = 0$. Thus, we have

$$|X\rangle^{B'_I} = \sum_{m=0}^{2}\langle m|U|\Psi\rangle\;|m\rangle^{B'_I} = U|\Psi\rangle^{B'_I} \equiv |U\Psi\rangle^{B'_I}\,. \quad (57)$$

The computation of $|Y\rangle^{B'_I}$ proceeds in an analogous way to (55), and the result is

$$|Y\rangle^{B'_I} = \sum_{m=0}^{2} \left[\langle m|^{A_O} \tilde{U}^{A_O A_I} |v\rangle^{A_I} \right] |m\rangle^{B'_I} \,. \tag{58}$$

Again, using (37), the coefficient in the brackets can be evaluated as

$$\langle m|^{A_O} \tilde{U}^{A_O A_I} |v\rangle^{A_I} = \langle m|^{A_O} \left(U^{A_O A_I} P_{01}^{A_I A_I} + I^{A_O A_I} P_v^{A_I A_I} \right) |v\rangle^{A_I} = \langle m|v\rangle = \delta_{mv} \,, \tag{59}$$

since $P_{01}^{A_I A_I}|v\rangle^{A_I} = 0$ and $P_v^{A_I A_I}|v\rangle^{A_I} = |v\rangle^{A_I}$. Thus, we have

$$|Y\rangle^{B'_I} = \sum_{m=0}^{2} \delta_{mv} \, |m\rangle^{B'_I} = |v\rangle^{B'_I} \,. \tag{60}$$

Finally, substituting (57) and (60) back into (52), we obtain:

$$\langle\!\langle \tilde{U}^* |^{A_I A_O} | W_{QS_4} \rangle\!\rangle = \frac{1}{\sqrt{2}} \left(|U\Psi\rangle^{B'_I} |v\rangle^{B_I} + |v\rangle^{B'_I} |\Psi\rangle^{B_I} \right) |\mathbb{1}\rangle\!\rangle^{B_O A'_I} |\mathbb{1}\rangle\!\rangle^{(A'_O B'_O) S_{(AB)_I}} |\mathbb{1}\rangle\!\rangle^{S_{(AB)_O} T_{(AB)_I}} \,. \tag{61}$$

One should note, comparing (61) with (49), that the action of the gate A operation onto the process vector effectively performs the following transformation,

$$|\Psi\rangle^{A_I} \to |U\Psi\rangle^{A_O} \to |U\Psi\rangle^{B'_I} \,, \qquad |v\rangle^{A_I} \to |v\rangle^{A_O} \to |v\rangle^{B'_I} \,, \tag{62}$$

where the transport vector $|\mathbb{1}\rangle\!\rangle^{A_O B'_I}$ has been utilised for "transporting" the state from the output A_O of gate A to the input B'_I of the gate B', in line with the spacetime diagram. This scheme repeats itself with the action of all remaining gate operations on (61). In particular, the subsequent action of the gate B operation gives:

$$\begin{aligned} &\left(\langle\!\langle \tilde{V}^* |^{B_I B_O} \otimes \langle\!\langle \tilde{U}^* |^{A_I A_O} \right) | W_{QS_4} \rangle\!\rangle = \\ &\qquad \frac{1}{\sqrt{2}} \left(|U\Psi\rangle^{B'_I} |v\rangle^{A'_I} + |v\rangle^{B'_I} |V\Psi\rangle^{A'_I} \right) |\mathbb{1}\rangle\!\rangle^{(A'_O B'_O) S_{(AB)_I}} |\mathbb{1}\rangle\!\rangle^{S_{(AB)_O} T_{(AB)_I}} \,, \end{aligned} \tag{63}$$

which can also be verified with an explicit calculation similar to the above. Continuing on, the operations at the gates A' and B' give:

$$\begin{aligned} &\left(\langle\!\langle \tilde{V}^* |^{B'_I B'_O} \otimes \langle\!\langle \tilde{U}^* |^{A'_I A'_O} \otimes \langle\!\langle \tilde{V}^* |^{B_I B_O} \otimes \langle\!\langle \tilde{U}^* |^{A_I A_O} \right) | W_{QS_4} \rangle\!\rangle = \\ &\qquad \frac{1}{\sqrt{2}} \left(|VU\Psi\rangle^{S_{B_I}} |v\rangle^{S_{A_I}} + |v\rangle^{S_{B_I}} |UV\Psi\rangle^{S_{A_I}} \right) |\mathbb{1}\rangle\!\rangle^{S_{(AB)_O} T_{(AB)_I}} \,. \end{aligned} \tag{64}$$

Next, the action of the beam splitter at the gate S_f gives

$$\begin{aligned} &\left(\langle\!\langle \tilde{H}^* |^{S_I S_O} \otimes \langle\!\langle \tilde{V}^* |^{B'_I B'_O} \otimes \langle\!\langle \tilde{U}^* |^{A'_I A'_O} \otimes \langle\!\langle \tilde{V}^* |^{B_I B_O} \otimes \langle\!\langle \tilde{U}^* |^{A_I A_O} \right) | W_{QS_4} \rangle\!\rangle = \\ &\qquad \frac{1}{2} \sum_{i=0}^{1} \left(\langle i | \{ U \,, V \} | \Psi \rangle \, |i\rangle^{T_{A_I}} |v\rangle^{T_{B_I}} + \langle i | [U \,, V] | \Psi \rangle \, |v\rangle^{T_{A_I}} |i\rangle^{T_{B_I}} \right) \,. \end{aligned} \tag{65}$$

Finally, the action of the operations of the target gates T_A and T_B gives us the probability amplitude as a function of the measurement outcomes α and β,

$$\begin{aligned} &\mathcal{M}(\alpha, \beta) \equiv \\ &\left(\langle\!\langle \tilde{U}^* |^{A_I A_O} \otimes \langle\!\langle \tilde{U}^* |^{A'_I A'_O} \otimes \langle\!\langle \tilde{V}^* |^{B_I B_O} \otimes \langle\!\langle \tilde{V}^* |^{B'_I B'_O} \otimes \langle\!\langle H^* |^{S_I S_O} \otimes \langle\!\langle T^*_\alpha |^{T_{A_I} T_{A_O}} \otimes \langle\!\langle T^*_\beta |^{T_{B_I} T_{B_O}} \right) | W_{QS_4} \rangle\!\rangle \end{aligned}$$

$$= \frac{1}{2}\Big[\delta_{\beta v}\langle\alpha|\,\{\,U\,,\,V\,\}\,|\Psi\rangle + \delta_{\alpha v}\langle\beta|\,[\,U\,,\,V\,]\,|\Psi\rangle\Big]\,. \tag{66}$$

At this point we can employ (45) and calculate the probability distribution,

$$p(\alpha,\beta) = \frac{1}{4}\Big[\delta_{\beta v}\left|\langle\alpha|\,\{\,U\,,\,V\,\}\,|\Psi\rangle\right|^2 + \delta_{\alpha v}\left|\langle\beta|\,[\,U\,,\,V\,]\,|\Psi\rangle\right|^2\Big]\,, \tag{67}$$

where we have used the fact that the vacuum state $|v\rangle$ is orthogonal to both $\{\,U\,,\,V\,\}\,|\Psi\rangle$ and $[\,U\,,\,V\,]\,|\Psi\rangle$. In particular, we see that for $i \in \{0,1\}$ we have

$$p(i,v) = \frac{1}{4}\left|\langle i|\,\{\,U\,,\,V\,\}\,|\Psi\rangle\right|^2, \qquad p(v,i) = \frac{1}{4}\left|\langle i|\,[\,U\,,\,V\,]\,|\Psi\rangle\right|^2, \tag{68}$$

while all other choices of α and β give $p(\alpha,\beta) = 0$. The total probability that Alice will detect a particle is given by the marginal

$$p_A = \sum_{i=1}^{2} p(i,v) = \frac{1}{2}\left(1 + \mathrm{Re}\,\langle\Psi|U^\dagger V^\dagger U V|\Psi\rangle\right), \tag{69}$$

while the corresponding total probability that Bob will detect a particle is

$$p_B = \sum_{i=1}^{2} p(v,i) = \frac{1}{2}\left(1 - \mathrm{Re}\,\langle\Psi|U^\dagger V^\dagger U V|\Psi\rangle\right). \tag{70}$$

As a final point, we can verify that the probability distribution is correctly normalised. Using the fact that the only nonzero values for the probability are given in (68), we have

$$p_{\text{total}} = \sum_{\alpha=0}^{2}\sum_{\beta=0}^{2} p(\alpha,\beta) = \underbrace{p(0,v)+p(1,v)}_{p_A} + \underbrace{p(v,0)+p(v,1)}_{p_B} = 1\,, \tag{71}$$

as expected.

Instead of recombining the particle on the second beam splitter, one can consider the case in which the final gate $\mathcal{F}$ consists only of local measurements performed onto a particle in the Alice's and Bob's paths. In this case, the final gate is equivalent to two target gates T_A and T_B. Given that all the processes considered are pure, the corresponding process vector for the 4-event quantum switch implementation is given as (in order to compare the current with the previous works, we present the process that starts after $\mathcal{I}$, as was done in, say, [9]):

$$|W_{QS_4}\rangle\!\rangle = \frac{1}{\sqrt{2}}\left(|\Psi\rangle^{A_I}|v\rangle^{B_I} + |v\rangle^{A_I}|\Psi\rangle^{B_I}\right)|\mathbb{1}\rangle\!\rangle^{A_O B'_I}|\mathbb{1}\rangle\!\rangle^{B_O A'_I}|\mathbb{1}\rangle\!\rangle^{A'_O T_{A_I}}|\mathbb{1}\rangle\!\rangle^{B'_O T_{B_I}}. \tag{72}$$

D 3-event process vector

The detailed spacetime diagram for the 3-event quantum switch is given below (see Figure 15).

The process vector for this case is obtained from (44) by identifying the spacetime positions of the gates B and B', yet keeping the corresponding Hilbert spaces in the mathematical description (i.e., keeping the dimensionality of the problem). Thus, the corresponding circuit is *identical* to the 4-event circuit, and the process vector has the *identical* mathematical form as in the case of four gates. In order to emphasise the physical difference between the two cases, instead of $B_{I/O}$ and $B'_{I/O}$, we write B_{I_1/O_1} and B_{I_2/O_2}, respectively:

$$\begin{aligned} |W_{\text{3-event}}\rangle\!\rangle \;=\; & \underbrace{|\mathbb{1}\rangle\!\rangle^{P_{A_O} S^i_{A_I}}|\mathbb{1}\rangle\!\rangle^{P_{B_O} S^i_{B_I}}}_{\text{initial}}\underbrace{|\mathbb{1}\rangle\!\rangle^{S^i_{A_O} A_I}|\mathbb{1}\rangle\!\rangle^{A_O B_{I_2}}|\mathbb{1}\rangle\!\rangle^{B_{O_2} S^f_{B_I}}}_{\text{blue}} \\ & \underbrace{|\mathbb{1}\rangle\!\rangle^{S^i_{B_O} B_{I_1}}|\mathbb{1}\rangle\!\rangle^{B_{O_1} A'_I}|\mathbb{1}\rangle\!\rangle^{A'_O S^f_{A_I}}}_{\text{red}}\underbrace{|\mathbb{1}\rangle\!\rangle^{S^f_{A_O} T_{A_I}}|\mathbb{1}\rangle\!\rangle^{S^f_{B_O} T_{B_I}}}_{\text{final}}\,. \end{aligned} \tag{73}$$

The final probability distribution is identical to the one for the 4-event process, given by (67).

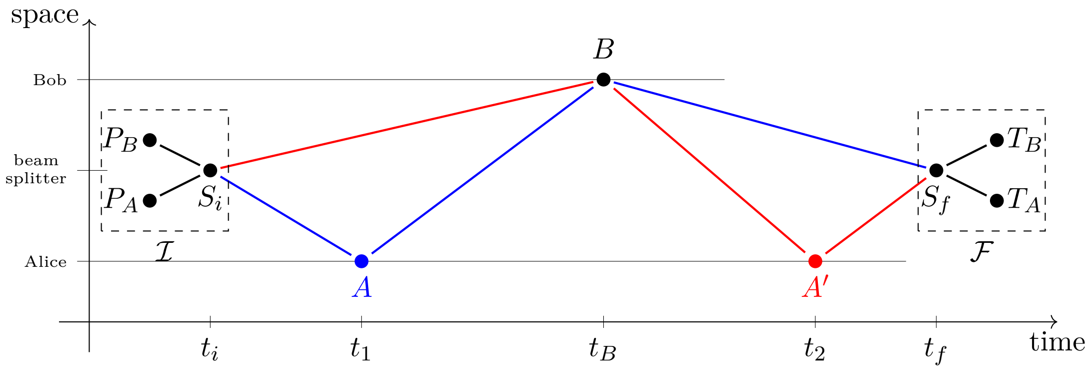


Figure 15: Spacetime diagram of the 3-event implementation of the quantum switch. The internal structures of the composite gates $\mathcal{I}$ and $\mathcal{F}$ are explicitly depicted.

E 2-event

In this Appendix we present process vectors for the two gravitational switches discussed in the main text. First, the process vector of the gravitational switch without recombination [15], is given by (since the "control" is now played by gravity, it is thus denoted as G, instead of C):

$$|W_{QS_2}\rangle\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle^G|\Psi\rangle^{A_I}|\mathbb{1}\rangle\rangle^{A_OB_I}|\mathbb{1}\rangle\rangle^{B_OT_{B_I}} + |1\rangle^G|\Psi\rangle^{B_I}|\mathbb{1}\rangle\rangle^{B_OA_I}|\mathbb{1}\rangle\rangle^{A_OT_{A_I}}\right)|\mathbb{1}\rangle\rangle^{GT_{G_I}}. \quad (74)$$

It is then straightforward to obtain the process vector for the case of recombining only the gravity on the final beam splitter S_f (a part of a bigger final gate $\mathcal{F}$), obtaining the analogue of (49), while the particle is not being recombined. Note that in this case the introduction of the vacuum state is not necessary, as in each branch of superposition all gates are acting upon a particle.

In contrast to the above case, the process vector describing the gravitational 2-event quantum switch with the recombination of both gravity and the particle is given as follows:

$$\begin{aligned}|W^{(r)}_{QS_2}\rangle\rangle = \frac{1}{\sqrt{2}}&\left(|0\rangle^G|\Psi\rangle^{A_I}|\mathbb{1}\rangle\rangle^{A_OB_I}|\mathbb{1}\rangle\rangle^{B_OS_{P_I}} + |1\rangle^G|\Psi\rangle^{B_I}|\mathbb{1}\rangle\rangle^{B_OA_I}|\mathbb{1}\rangle\rangle^{A_OS_{P_I}}\right)\\ &\otimes|\mathbb{1}\rangle\rangle^{GS_{G_I}}|\mathbb{1}\rangle\rangle^{(S_{G_O}S_{P_O})(T_{G_I}T_{P_I})}.\end{aligned} \quad (75)$$

Here, P stands for "the particle" (whose corresponding input space S_{P_I} is isomorphic to the tensor product of Alice's and Bob's output spaces, $S_{P_I} \simeq A_O \otimes B_O$), and S stands for a "beam splitter" (whose corresponding input space is $S_I = S_{G_I} \otimes S_{P_I}$, and analogously for the output space).

While defining the spaces $S_{G_{I/O}}$, $S_{P_{I/O}}$, T_{G_I}, T_{P_I}, and the vector $|\mathbb{1}\rangle\rangle^{(S_{G_O}S_{P_O})(T_{G_I}T_{P_O})}$ is straightforward, it is not so for the "final" recombination vector $|U^*_{BS}\rangle\rangle^{(S_{G_I}S_{P_I})(S_{G_O}S_{P_O})}$. Namely, note that in our gravitational switch *all* degrees of freedom, both gravitational and matter, are recombined by U_{BS} such that, by acting on the beam splitter input entangled state,

$$|\Psi_i\rangle^{S_{G_I}S_{P_I}} = \frac{1}{\sqrt{2}}\left(|0\rangle^{S_{G_I}} \otimes \left[UV|\Psi\rangle^{S_{P_I}}\right] + |1\rangle^{S_{G_I}} \otimes \left[VU|\Psi\rangle^{S_{P_I}}\right]\right), \quad (76)$$

the overall output state is a product one, of the form

$$|\Psi_o\rangle^{S_{G_O}S_{P_O}} = |\Gamma\rangle^{S_{G_O}} \otimes (\alpha UV + \beta VU)\,|\Psi\rangle^{S_{P_O}}, \quad (77)$$

where $|\Gamma\rangle^{S_{G_O}}$ is some (not necessarily classical) state of gravity. The above evolution is, at least in principle, allowed by the quantum laws, which is all that we need to know regarding the action of U_{BS} at this point. Its action on the rest of the overall Hilbert space is, for the purpose of our argument, irrelevant, and can thus be chosen arbitrarily.

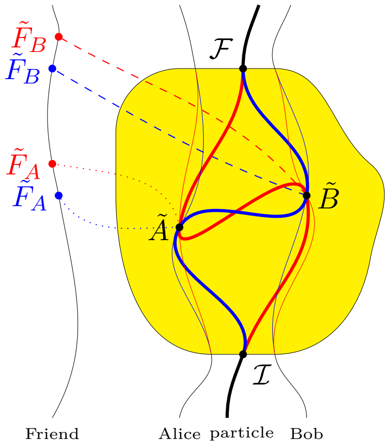
Finally, we would like to note that the same type of the 4-, or 3-event quantum switches in classical spacetimes can also be defined, resulting in the same type of the output state as (77), with the gravity degree of freedom being replaced by any additional matter degree of freedom that plays the role of the control.

F Various implementations of the gravitational switch

In this Appendix we present a few representative additional constructions of the gravitational quantum switch. First, we start with a 2-event switch for which the requirement (i) from Subsection 4.3 is not satisfied. It is obvious from the diagram on the left that each of the photon's superposed trajectories fail to meet at the boundary region, violating requirement (i), see the left diagram of Figure 16. Next, we proceed with the 2-event implementation for which requirement (i) is satisfied, but the requirement (ii) is not, since the superposed trajectories fail to recombine. This is depicted on the right diagram of Figure 16.

Finally, we present a 4-event implementation for which *both* requirements (i) and (ii) are satisfied (see Figure 17).

Of course, other variations are possible as well.



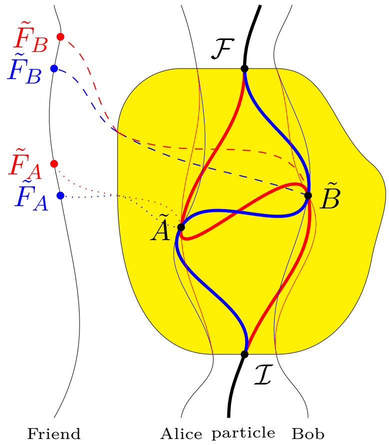


Figure 16: The spacetime diagrams of a 2-event gravitational switch implementations, with Friend's measurements, which fail to distinguish them from the optical implementation of the quantum switch.

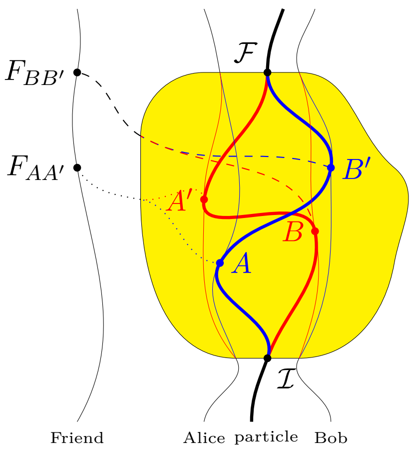


Figure 17: The spacetime diagram of a 4-event gravitational switch implementation, with Friend's measurement, which fails to distinguish it from the 2-event implementation of the gravitational switch.

Operational interpretation of the vacuum and process matrices for identical particles

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This work overviews the single-particle two-way communication protocol recently introduced by del Santo and Dakić (dSD), and analyses it using the process matrix formalism. We give a detailed account of the importance and the operational meaning of the interaction of an agent with the vacuum — in particular its role in the process matrix description. Our analysis shows that the interaction with the vacuum should be treated as an operation, on equal footing with all other interactions. This raises the issue of counting such operations in an operational manner. Motivated by this analysis, we apply the process matrix formalism to capped Fock spaces using the framework of second quantisation, in order to characterise protocols with an indefinite number of identical particles.

1 Introduction

In recent years there have been advances in quantum information theory related to new techniques for discussing quantum circuits and quantum computation. One of those techniques is the recently developed process matrix formalism [1]. This formalism is general enough to describe all known quantum processes, in particular the superposed orders of operations in a quantum circuit. Moreover, its most prominent feature is that it allows for a description of more general situations of indefinite causal orders of spacetime points. A formal example of such a process has been introduced and discussed in [1], leading to the violation of the so-called *causal inequalities*. The latter represent device-independent conditions that need to be satisfied in order for a given process to have a well-defined causal order. It is still an open question whether such a process is physical and can be realised in nature. Also, a lot of attention in the literature has been devoted to the *quantum switch* operation, which has been discussed through both theoretical descriptions [2, 3, 4, 5] and experimental implementations [6, 7, 8].

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One of the interesting aspects of the quantum switch is that it gives rise to a superposition of orders of quantum operations. In a recent work [9], the difference between the superposition of orders of quantum operations and the superposition of causal orders in spacetime was discussed in detail, and it was demonstrated that the latter can in principle be realised only in the context of quantum gravity (see also [10, 11, 12]). The detailed analysis of the causal structure of the quantum switch has revealed one important qualitative aspect of the process matrix description — in order to properly account for the causal structure of an arbitrary process, it is *necessary* to introduce the notion of the quantum vacuum as a possible physical state. Otherwise, the naive application of the process matrix formalism may suggest a misleading conclusion that quantum switch implementations in flat spacetime feature genuine superpositions of spacetime causal orders. This demonstrates the importance of the concept of vacuum in quantum information processing. Regarding the general role of the vacuum in quantum circuits and optical experiments, see [13] and [14, 15], respectively, and the references therein.

Simultaneously with these developments, another interesting quantum process has been recently proposed [16] by del Santo and Dakić — dSD protocol (see also subsequent theoretical [17, 18] and experimental work [19]). As it turns out, while this process enables Alice and Bob to guess each other's input bits with certainty by exchanging a single particle only once, it cannot be correctly described within the process matrix formalism without the introduction of the interaction between the vacuum and the apparatus as an *operation*. Thus, it represents an additional motivation to introduce the vacuum state into the process matrix formalism, independent of the reasons related to the description of the quantum switch process.

Moreover, while the dSD protocol employs only one photon, it is also relevant for multiphoton processes, which opens the question of the treatment of identical particles within the process matrix formalism. Also, taking into account the presence of the vacuum state, one is steered towards the application of the abstract process matrix formalism to systems with variable number of identical particles, to the second quantisation and ultimately generalisation to quantum field theory (QFT). See also a related work on the causal boxes framework [20].

In this work we give a detailed description and treatment of dSD protocol within the process matrix formalism. We analyse in detail the role of the vacuum in the protocol and the formalism, and its operational interpretation. Specifically, our aim is to discuss the following question:

Is the interaction with the vacuum an operation, or not?

Our analysis of dSD protocol leads to a conclusion that the interaction with the vacuum should be considered an operation. The alternative would mean that one could extract information from the system at the final moment of the protocol without performing an operation at all. Since the same physical situation should always be described in the same way, we conclude that the interaction with the vacuum should be treated as an operation, and thus as a resource, in all quantum information protocols. This includes the optical implementation of the quantum switch protocol, leading one to infer that it features *four, rather than just two* operations, as was claimed in a number of papers [3, 4, 5, 6, 7, 8]. In addition, we make use of the dSD protocol as an illuminative example to apply the process matrix formalism to multipartite systems of identical particles.

The paper is organised as follows. In Section 2 we give a short overview of the process matrix formalism and the dSD protocol. Section 3 is devoted to the process matrix formalism description of dSD protocol, and to the discussion of the *operational* role and importance of the vacuum state for its description. In particular, in Subsection 3.4 we present the argument for our main conclusion, namely that the interaction with the vacuum should be considered an operation. In Section 4 we provide the basic rules for the application of the process matrix formalism to identical multiparticle systems. Section 5 is devoted to the summary of our results, discussion and prospects for future research. The Appendix contains various technical details of the calculations.

2 State of the art

In this section, we present an overview of the relevant background results. First, we give a short introduction to the process matrix formalism, and then we present the dSD protocol. This overview is not intended to be complete or self-contained, but merely of informative type. The reader should consult the literature for more details.

2.1 The process matrix formalism

The process matrix formalism is based on an idea of a set of laboratories, interacting with the outside world by exchanging quantum systems. Each laboratory is assumed to be spatially local in the sense that one can consider its size negligible for the problem under discussion. Inside the laboratory, it is assumed that the ordinary laws of quantum theory hold. The laboratory interacts with the outside world by receiving an *input* quantum system and by sending an *output* quantum system. Inside the laboratory, the input and output quantum systems are being manipulated using the notion of an *instrument*, denoting the most general operation one can perform over quantum systems. Each interaction is also assumed to be localised in time, such that each operation of a given laboratory has a separate spacetime point assigned to it (see Subsection 3.4 for a discussion of time delocalised laboratories and operations [21]). Thus, we introduce the notion of a *gate*, which represents the action of an instrument at a given spacetime point (see Section 2 of [9]); for simplicity, both the gate and its corresponding spacetime point will be denoted by the same symbol, G. By G_I and G_O we denote the Hilbert spaces of the input and the output quantum systems, respectively. These Hilbert spaces are assumed to be finite-dimensional or trivial. The action of the instrument is described by an operator, $\mathcal{M}^G_{x,a} : G_I \otimes G_I^* \to G_O \otimes G_O^*$, which may depend on some classical input information a available to the gate G, and some readouts x of eventual measurement results that may take place in G. Thus, the instrument maps a generic mixed input state ρ_I into the output state $\rho_O = \mathcal{M}^G_{x,a}(\rho_I)$.

Given such a setup, one defines a *process*, denoted $\mathcal{W}$, as a functional over the instruments of all gates, as

$$p(x, y, \dots |a, b, \dots) = \mathcal{W}(\mathcal{M}^{G^{(1)}}_{x,a} \otimes \mathcal{M}^{G^{(2)}}_{y,b} \otimes \dots) ,$$

where $p(x, y, \dots |a, b, \dots)$ represents the probability of obtaining measurement results $x, y, \dots$, given the inputs $a, b, \dots$. In order for the right-hand side to be interpreted as a probability distribution, the process $\mathcal{W}$ must satisfy three basic axioms,

$$\begin{aligned} \mathcal{W} &\geq 0 , \\ \operatorname{Tr} \mathcal{W} &= \prod\nolimits_i \dim G_O^{(i)} , \\ \mathcal{W} &= \mathcal{P}_G(\mathcal{W}) , \end{aligned} \tag{1}$$

where $\mathcal{P}_G$ is a certain projector onto a subspace of $\bigotimes_i \left(G_I^{(i)} \otimes G_O^{(i)} \right)$ which, together with the second requirement, ensures the normalisation of the probability distribution (see [3] for details).

In order to have a computationally manageable formalism, one often employs the Choi-Jamiołkowski (CJ) map over the instrument operations, such that a given operation $\mathcal{M}^G_{x,a}$ is being represented by a matrix,

$$\begin{aligned} M^G_{x,a} = \Big[\left(\mathcal{I} \otimes \mathcal{M}^G_{x,a} \right) (|\mathbb{1}\rangle\!\rangle\langle\!\langle \mathbb{1}|) \Big]^T \\ \in (G_I \otimes G_O) \otimes (G_I \otimes G_O)^* , \end{aligned} \tag{2}$$

where

$$|\mathbb{1}\rangle\!\rangle \equiv \sum_i |i\rangle \otimes |i\rangle \in G_I \otimes G_I \tag{3}$$

is the so-called *transport vector*, representing the non-normalised maximally entangled state, and $\mathcal{I}$ is the identity operator. Then, one can describe the process $\mathcal{W}$ using the *process matrix* W to write

$$\begin{aligned} p(x, y, \dots |a, b, \dots) = \\ \operatorname{Tr} \left[(M^{G_1}_{x,a} \otimes M^{G_2}_{y,b} \otimes \dots) W \right] . \end{aligned} \tag{4}$$

Finally, if an instrument $\mathcal{M}^G_{x,a}$ is linear, one can also use a corresponding "vector" notation (see Appendix A.1 in [3]),

$$|(\mathcal{M}^G_{x,a})^*\rangle\!\rangle \equiv \left[\mathcal{I} \otimes (\mathcal{M}^G_{x,a})^* \right] |\mathbb{1}\rangle\!\rangle \in G_I \otimes G_O , \tag{5}$$

so that

$$M^G_{x,a} = |(\mathcal{M}^G_{x,a})^*\rangle\!\rangle\langle\!\langle(\mathcal{M}^G_{x,a})^*| . \tag{6}$$

In cases where all instruments are linear, and in addition the process matrix W is a one-dimensional projector, one can introduce the the corresponding *process vector* $|W\rangle\!\rangle$, such that $W = |W\rangle\!\rangle\langle\!\langle W|$, and rewrite (4) in the form:

$$\begin{aligned} p(x, y, \dots |a, b, \dots) = \\ \left\| \left(\langle\!\langle \mathcal{M}^{G^{(1)}*}_{x,a} | \otimes \langle\!\langle \mathcal{M}^{G^{(2)}*}_{y,b} | \otimes \dots \right) |W\rangle\!\rangle \right\|^2 . \end{aligned} \tag{7}$$

2.2 The dSD protocol

In a recent paper [16], del Santo and Dakić have introduced a protocol which allows two agents to guess each other's input bits with certainty by exchanging a single particle only once. The protocol goes as follows. Initially, a single particle is prepared in a superposition state of being sent to Alice and being sent to Bob. Upon receiving the particle, both Alice and Bob perform unitary operations on it, encoding their bits of information, a and b, respectively, about the outcomes of their coin tosses. They do this by changing the local phase of the particle by $(-1)^a$ and $(-1)^b$. The particle is subsequently forwarded to a beam splitter, and after that again to Alice and Bob, who now measure the presence or absence of the particle.

This way, the state of the particle stays in *coherent* superposition of different paths in a Mach-Zehnder interferometer. The interference of its paths gives rise to *deterministic* outcome that depends on the relative phase $e^{i\phi} = (-1)^{a \oplus b}$ between the two branches: in case $\phi = 0$, the particle will end up in Alice's laboratory, while otherwise it will end in Bob's. Thus, knowing their own inputs and the outcomes of their local measurements, both agents can determine each other's inputs, allowing for two-way communication using only one particle. This is clearly impossible in classical physics, demonstrating yet another example of the advantage of quantum over classical strategies.

The crucial aspect of the protocol lies in the fact that the *absence* of the particle represents a useful piece of information for an agent. This gives rise to the notion of the *vacuum state* as a carrier of information, playing the central role in the protocol. Thus, in order to describe the protocol using the process matrix formalism, one has to incorporate the notion of the vacuum in the formalism itself. We show this in detail in the next section.

It is interesting to note that the crucial role of the vacuum plays an important part not only in the dSD protocol, but also in a completely different setup that has been discussed a lot in recent literature, namely the *quantum switch* [2]. As analysed in detail in [9], if one takes care to distinguish the two temporal positions of a given laboratory and introduces the notion of a vacuum explicitly, one can demonstrate that the optical implementations of the quantum switch in flat spacetime do not feature any superposition of causal orders induced by the spacetime metric. Instead, it was argued that superpositions of spacetime causal orders can be present only within the context of a theory of quantum gravity. As we shall see below, the notion of the interaction with the vacuum will prove essential to the process matrix description of the dSD protocol as well.

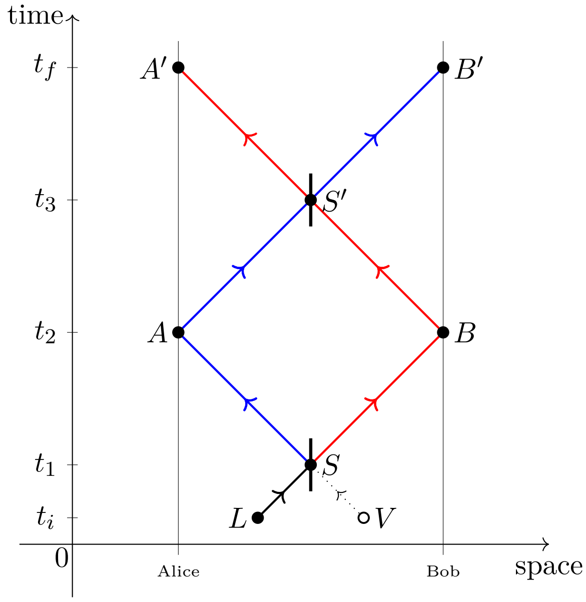

Figure 1: The complete spacetime diagram of the process corresponding to the dSD protocol.

3 Process matrix description of the dSD protocol

3.1 The spacetime diagram

We begin by drawing the spacetime diagram of the process corresponding to the dSD protocol (see Figure 1).

At the initial time t_i the laser L creates a photon and shoots it towards the beam splitter S, which at time t_1 performs the Hadamard operation and entangles it with the incoming vacuum state (described by the dotted arrow from the grey gate V). The entangled state of the photon and the vacuum continues on towards Alice's and Bob's gates A and B, respectively. At time t_2, Alice and Bob generate their random bits a and b, and encode them into the phase of the incoming photon-vacuum system. The system then proceeds to the beam splitter S' which again performs the Hadamard operation at time t_3. The photon-vacuum system then proceeds to the gates A' and B', where it is measured at time t_f by Alice and Bob, respectively. Note that the spatial distance Δl between Alice and Bob is precisely equal to the time distance between the generation of the random bits and the final measurements,

$$\Delta l = c(t_f - t_2)\,,$$

so that a single photon has time to traverse the space between Alice and Bob *only once*. Also, note that the gate V, which generates the vacuum state, corresponds to a "trivial instrument", since the vacuum does not require any physical device to be generated. Nevertheless, the vacuum is still a legitimate physical state of the EM field, so the appropriate gate V has to be formally introduced and accounted for in the process matrix formalism calculations.

3.2 Formulation of the process matrix

Based on the spacetime diagram, we formulate the process matrix description as follows. All spacetime points, where interaction between the EM field and some apparatus may happen, are assigned a gate and an operation which describes the interaction. Each gate has an input and output Hilbert space, as follows:

$$
\begin{array}{llllllll}
L: & \mathbb{C} & \to & L_O\,, & A: & A_I & \to & A_O\,,\\
V: & \mathbb{C} & \to & V_O\,, & B: & B_I & \to & B_O\,,
\end{array}
$$

$$
\begin{array}{llllllll}
S: & S_I & \to & S_O\,, & A': & A'_I & \to & \mathbb{C}\,,\\
S': & S'_I & \to & S'_O\,, & B': & B'_I & \to & \mathbb{C}\,.
\end{array}
$$

The initial gates, L and V, have trivial input spaces and nontrivial output spaces. The final gates, A' and B', have trivial output spaces and nontrivial input spaces. The gates A and B have nontrivial input and output spaces. Each nontrivial space is isomorphic to $\mathcal{H}_1 \oplus \mathcal{H}_0 \subset \mathcal{F}$, where $\mathcal{H}_0$ and $\mathcal{H}_1$ are the vacuum and single-excitation subspaces of the Fock space $\mathcal{F}$ in perturbative QED. Namely, by design of the dSD protocol, Alice and Bob may exchange at most one photon, which means that multiparticle Hilbert subspaces of the Fock space can be omitted. Moreover, the resulting probability distribution of the experiment outcomes does not in principle depend on the frequency or the polarisation of the photon in use, so we can approximate the single-excitation space as a one-dimensional Hilbert space. Given that the vacuum Hilbert space $\mathcal{H}_0$ is by definition one-dimensional, we can write

$$
\mathcal{H}_0 = \mathrm{span}\{|0\rangle\} \equiv \mathbb{C}\,, \qquad \mathcal{H}_1 \approx \mathrm{span}\{|1\rangle\} \equiv \mathbb{C}\,,
$$

so that $\mathcal{H}_0 \oplus \mathcal{H}_1 \equiv \mathbb{C} \oplus \mathbb{C}$. Here, $|0\rangle$ and $|1\rangle$ denote the states of the vacuum and the photon in the occupation number basis of the Fock space. Therefore, we have

$$
\begin{aligned}
L_O \cong V_O \cong A_I \cong A_O \cong \\
B_I \cong B_O \cong A'_I \cong B'_I \cong \mathbb{C} \oplus \mathbb{C}\,.
\end{aligned}
$$

Finally, the input and output spaces of beam splitters S and S' are “doubled”, since a beam splitter operates over two inputs to produce two outputs. In particular,

$$
\begin{array}{lllllll}
S_I & = & S_I^L \otimes S_I^V\,, & \qquad & S'_I & = & S_I'^A \otimes S_I'^B\,,\\
S_O & = & S_O^A \otimes S_O^B\,, & \qquad & S'_O & = & S_O'^A \otimes S_O'^B\,,
\end{array}
$$

where again

$$
\begin{aligned}
S_I^L \cong S_I^V \cong S_O^A \cong S_O^B \cong \\
S_I'^A \cong S_I'^B \cong S_O'^A \cong S_O'^B \cong \mathbb{C} \oplus \mathbb{C}\,.
\end{aligned}
$$

With all relevant Hilbert spaces defined, we formulate the action of each gate, using the CJ map in the form (5). The gates L and V simply generate the photon and the vacuum,

$$
|L^*\rangle\!\rangle^{L_O} = |1\rangle^{L_O}\,, \qquad |V^*\rangle\!\rangle^{V_O} = |0\rangle^{V_O}\,, \tag{8}
$$

where $*$ is the complex conjugation. The action of the beam splitters is

$$
|S^*\rangle\!\rangle^{S_I S_O} = \left[I^{S_I S_I} \otimes (H^*)^{S_O S_I} \right] |\mathbb{1}\rangle\!\rangle^{S_I S_I}\,, \tag{9}
$$

and

$$
|S'^*\rangle\!\rangle^{S'_I S'_O} = \left[I^{S'_I S'_I} \otimes (H^*)^{S'_O S'_I} \right] |\mathbb{1}\rangle\!\rangle^{S'_I S'_I}\,, \tag{10}
$$

where the Hadamard operator for S is defined as

$$
\begin{aligned}
H^{S_O S_I} = \\
\frac{1}{\sqrt{2}} \left(|1\rangle^{S_O^A} |0\rangle^{S_O^B} + |0\rangle^{S_O^A} |1\rangle^{S_O^B} \right) \langle 1|^{S_I^L} \langle 0|^{S_I^V} \\
+ \frac{1}{\sqrt{2}} \left(|1\rangle^{S_O^A} |0\rangle^{S_O^B} - |0\rangle^{S_O^A} |1\rangle^{S_O^B} \right) \langle 0|^{S_I^L} \langle 1|^{S_I^V}\,,
\end{aligned}
$$

and analogously for $H^{S'_O S'_I}$. The unit operator is denoted as I. Next, in the gates A and B, Alice and Bob generate their random bits a and b, and encode them into the phase of the photon. The corresponding actions are defined as

$$
|A^*\rangle\!\rangle^{A_I A_O} = \left[I^{A_I A_I} \otimes (A^*)^{A_O A_I} \right] |\mathbb{1}\rangle\!\rangle^{A_I A_I}\,, \tag{11}
$$

and

$$
|B^*\rangle\!\rangle^{B_I B_O} = \left[I^{B_I B_I} \otimes (B^*)^{B_O B_I} \right] |\mathbb{1}\rangle\!\rangle^{B_I B_I}, \tag{12}
$$

where

$$
A^{A_O A_I} = (-1)^a |1\rangle^{A_O} \langle 1|^{A_I} \oplus |0\rangle^{A_O} \langle 0|^{A_I}\,,
$$

and

$$
B^{B_O B_I} = (-1)^b |1\rangle^{B_O} \langle 1|^{B_I} \oplus |0\rangle^{B_O} \langle 0|^{B_I}\,.
$$

Finally, the gates A' and B' describe Alice's and Bob's measurement of the incoming state in the occupation number basis,

$$
|A'^*\rangle\!\rangle^{A'_I} = |a'\rangle\,, \qquad |B'^*\rangle\!\rangle^{B'_I} = |b'\rangle\,, \tag{13}
$$

where their respective measurement outcomes a' and b' take values from the set $\{0, 1\}$, depending on whether the vacuum or the photon has been measured, respectively.

After specifying the actions of the gates, the last step is the construction of the process vector

$|W_{dSD}\rangle\rangle$ itself. The dSD protocol assumes that the state of the photon remains unchanged during its travel between the gates. Therefore, the process vector will be a tensor product of transport vectors (3), one for each line connecting two gates in the spacetime diagram. The input and output spaces of the gates connected by the line determine the spaces of the corresponding transport vector. Thus, the total process vector is:

$$\begin{aligned} &|W_{dSD}\rangle\rangle = \\ &\quad |\mathbb{1}\rangle\rangle^{L_O S_I^L} |\mathbb{1}\rangle\rangle^{V_O S_I^V} |\mathbb{1}\rangle\rangle^{S_O^A A_I} |\mathbb{1}\rangle\rangle^{S_O^B B_I} \\ &\quad |\mathbb{1}\rangle\rangle^{A_O S_I'^A} |\mathbb{1}\rangle\rangle^{B_O S_I'^B} |\mathbb{1}\rangle\rangle^{S_O'^A A_I'} |\mathbb{1}\rangle\rangle^{S_O'^B B_I'} . \end{aligned} \tag{14}$$

3.3 Evaluation of the probability distribution

Now that the process vector and the operations of all gates have been specified in detail, we can evaluate the probability distribution

$$p(a', b'|a, b) = \|\mathcal{M}\|^2 , \tag{15}$$

where the probability amplitude $\mathcal{M}$ is obtained by taking the scalar product of $|W_{dSD}\rangle\rangle$ with the tensor product of all gates, see (7). It is most instructive to perform the computation iteratively, taking the partial scalar product of $|W_{dSD}\rangle\rangle$ with each gate, one by one. The explicit calculation of each step is based on two lemmas from Appendix A.

We begin by taking the partial scalar product of (14) and the preparation gates (8). Using Lemma 1 from Appendix A, we obtain:

$$\begin{aligned} &\left(\langle\langle L^*|^{L_O} \otimes \langle\langle V^*|^{V_O}\right) |W_{dSD}\rangle\rangle = \\ &\qquad |1\rangle^{S_I^L} |0\rangle^{S_I^V} |\mathbb{1}\rangle\rangle^{S_O^A A_I} |\mathbb{1}\rangle\rangle^{S_O^B B_I} \\ &\qquad |\mathbb{1}\rangle\rangle^{A_O S_I'^A} |\mathbb{1}\rangle\rangle^{B_O S_I'^B} |\mathbb{1}\rangle\rangle^{S_O'^A A_I'} |\mathbb{1}\rangle\rangle^{S_O'^B B_I'} . \end{aligned}$$

Next we take the partial scalar product with the beam splitter S gate operation (9). Using Lemma 2 from Appendix A, we obtain:

$$\begin{aligned} &\left(\langle\langle S^*|^{S_I S_O} \otimes \langle\langle L^*|^{L_O} \otimes \langle\langle V^*|^{V_O}\right) |W_{dSD}\rangle\rangle = \\ &\qquad \frac{1}{\sqrt{2}} \left(|1\rangle^{A_I} |0\rangle^{B_I} + |0\rangle^{A_I} |1\rangle^{B_I} \right) \\ &\qquad |\mathbb{1}\rangle\rangle^{A_O S_I'^A} |\mathbb{1}\rangle\rangle^{B_O S_I'^B} |\mathbb{1}\rangle\rangle^{S_O'^A A_I'} |\mathbb{1}\rangle\rangle^{S_O'^B B_I'} . \end{aligned}$$

Now we apply the Alice's gate operation (11) to obtain:

$$\begin{aligned} &\Big(\langle\langle A^*|^{A_I A_O} \otimes \langle\langle S^*|^{S_I S_O} \otimes \\ &\quad \langle\langle L^*|^{L_O} \otimes \langle\langle V^*|^{V_O}\Big) |W_{dSD}\rangle\rangle = \\ &\qquad \frac{1}{\sqrt{2}} \left((-1)^a |1\rangle^{S_I'^A} |0\rangle^{B_I} + |0\rangle^{S_I'^A} |1\rangle^{B_I} \right) \\ &\qquad |\mathbb{1}\rangle\rangle^{B_O S_I'^B} |\mathbb{1}\rangle\rangle^{S_O'^A A_I'} |\mathbb{1}\rangle\rangle^{S_O'^B B_I'} . \end{aligned}$$

Similarly, applying Bob's gate (12) we get:

$$\begin{aligned} &\Big(\langle\langle B^*|^{B_I B_O} \otimes \langle\langle A^*|^{A_I A_O} \otimes \langle\langle S^*|^{S_I S_O} \otimes \\ &\quad \langle\langle L^*|^{L_O} \otimes \langle\langle V^*|^{V_O}\Big) |W_{dSD}\rangle\rangle = \\ &\frac{1}{\sqrt{2}} \left((-1)^a |1\rangle^{S_I'^A} |0\rangle^{S_I'^B} + (-1)^b |0\rangle^{S_I'^A} |1\rangle^{S_I'^B} \right) \\ &|\mathbb{1}\rangle\rangle^{S_O'^A A_I'} |\mathbb{1}\rangle\rangle^{S_O'^B B_I'} . \end{aligned}$$

The next step is the application of the second beam splitter gate (10). After a little bit of algebra, the result is:

$$\begin{aligned} &\left(\langle\langle S'^*|^{S_I' S_O'} \otimes \langle\langle B^*|^{B_I B_O} \otimes \langle\langle A^*|^{A_I A_O} \otimes \langle\langle S^*|^{S_I S_O} \otimes \langle\langle L^*|^{L_O} \otimes \langle\langle V^*|^{V_O}\right) |W_{dSD}\rangle\rangle = \\ &\qquad \frac{(-1)^a + (-1)^b}{2} |1\rangle^{A_I'} |0\rangle^{B_I'} + \frac{(-1)^a - (-1)^b}{2} |0\rangle^{A_I'} |1\rangle^{B_I'} . \end{aligned}$$

Finally, applying the measurement gates (13), we obtain the complete probability amplitude,

$$\begin{aligned} \mathcal{M} \;=\; & \frac{(-1)^a + (-1)^b}{2} \delta_{a'1} \delta_{b'0} \\ & + \frac{(-1)^a - (-1)^b}{2} \delta_{a'0} \delta_{b'1} , \end{aligned}$$

and substituting this into (15), we obtain the desired probability distribution of the dSD process:

$$\begin{aligned} p(a', b'|a, b) \;=\; & \frac{1 + (-1)^{a+b}}{2} \delta_{a'1} \delta_{b'0} \\ & + \frac{1 - (-1)^{a+b}}{2} \delta_{a'0} \delta_{b'1} . \end{aligned}$$

From the probability distribution we can now conclude that there are two distinct possibilities:

either Alice detects the photon and Bob does not, $a' = 1, b' = 0$, or vice versa, $a' = 0, b' = 1$. In the first case, because total probability must be equal to one, we have

$$\frac{1+(-1)^{a+b}}{2} = 1\,, \qquad \frac{1-(-1)^{a+b}}{2} = 0\,.$$

The only solution to these equations is $a = b$, which means that Alice and Bob have initially generated equal bits. Since both know the probability distribution and their own bit, they both know each other's bit as well, with certainty. In the second case, when Bob detects the photon, we instead have

$$\frac{1+(-1)^{a+b}}{2} = 0\,, \qquad \frac{1-(-1)^{a+b}}{2} = 1\,,$$

and the only solution is $a \neq b$, meaning that Alice and Bob have initially generated opposite bits. Again, both parties know the probability distribution and their own bit, and therefore each other's bit as well, with certainty.

In order to formalise this result, one can also introduce the parity $\pi \equiv a \oplus b$ and rewrite the probability distribution in the form

$$\begin{aligned} p(a',b'|\pi) \;\; = \;\; & \frac{1+(-1)^{\pi}}{2}\delta_{a'1}\delta_{b'0} \\ & + \frac{1-(-1)^{\pi}}{2}\delta_{a'0}\delta_{b'1}\,. \end{aligned} \tag{16}$$

Thus, if Alice detects the photon, then π is even, while if Bob detects the photon, π must be odd. In both cases, they can "guess" each other's bits with certainty by calculating

$$x = \pi \oplus a\,, \qquad y = \pi \oplus b\,,$$

where x is Alice's prediction of the value of Bob's bit, and y is Bob's prediction of the value of Alice's bit. Therefore, the probability of guessing each other's input bit is

$$p_{\text{success}} \equiv p(x = b \wedge y = a) = 1\,. \tag{17}$$

3.4 Analysis of the process matrix description — operational interpretation of the vacuum

After we have given the detailed process matrix description of the dSD protocol and derived the result (17), we analyse in more detail the role of the vacuum in the formalism, giving its operational interpretation.

In order to clarify the exposition, let us give an overview of the argument, as follows:

- In the next paragraph below, we analyse the role of the vacuum in the dSD protocol, and conclude that the interaction with the vacuum should be regarded as an operation, on the same footing with all other interactions.
- In the following four paragraphs, we discuss the optical implementation of the quantum switch protocol, which also features interactions between the agents and the vacuum. Since the same physical situation should always be described in the same way, we conclude that the interaction with the vacuum should be treated as an operation in this protocol as well. Thus, the protocol features a total of four, rather than two, operations.
- Finally, in the remaining three paragraphs, we discuss the alternative point of view, namely that the interaction with the vacuum is not regarded as an operation. This is the case in the method for counting operations proposed in [22]. We conclude that it would then mean that in the dDS protocol an agent could extract information from the system at t_f without performing an operation at all.

In the dSD protocol four operations (gates), A, A', B and B' are performed (see Figure 1). Note that for each choice of input bits a and b one of the two operations performed, A' and B', is of a special form: it represents the absence of the particle. This gives rise to an *operational interpretation* of the vacuum state as a carrier of information, playing the central role in the protocol — the very interaction between the apparatus and the vacuum (the absence of a particle) plays *exactly* the same role in this protocol as any other operation, i.e., not detecting a particle ("seeing the vacuum") is an operation on its own. From the mathematical point of view, supported by the structure of the process vector (14) that explicitly features the vacuum state, it is perfectly natural to consider the interaction between the apparatus and the vacuum state on equal footing with the interaction between the apparatus and the field excitation (i.e., the particle). Both interactions equally represent operations. Therefore, one should regard the interaction with the vacuum as a resource, in the same way as the interaction with the particle.

Let us now consider the optical quantum switch, a similar protocol in which the notion of

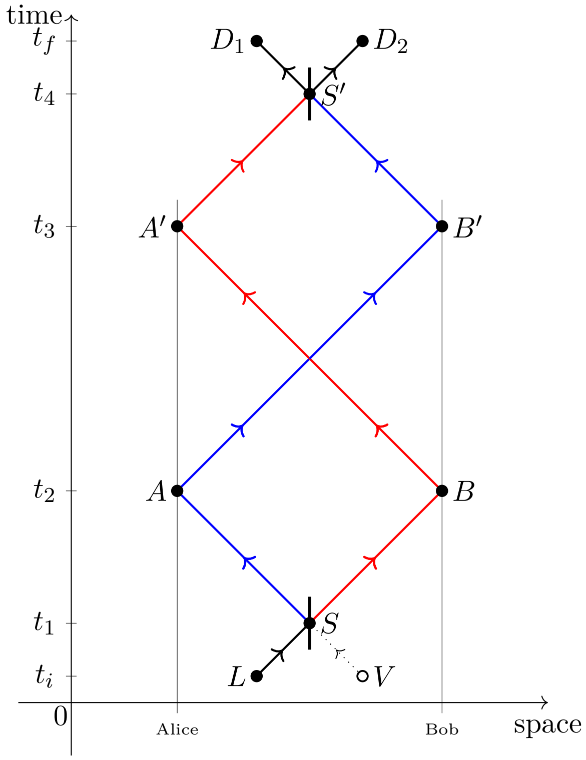

Figure 2: The complete spacetime diagram of the process corresponding to the optical quantum switch. Upon receiving the photon, Alice rotates its polarisation by the unitary U. Analogously, Bob performs rotation V on the photon entering his lab.

the vacuum also plays a role. Current optical implementations of the quantum switch feature four spacetime points, the same as the dSD protocol [9, 10, 11, 12], thus having the similar type of the spacetime schematic description, see Figure 2. However, by introducing the notion of time delocalised operations it was argued that the optical switch implements only two operations, U in spacetime points A or A', and V in spacetime points B or B' [21]. Nevertheless, the optical switch features the same apparatus-vacuum interaction as the one from the dSD protocol: whenever the particle is in, say, the blue branch, and the operations U and V are applied at spacetime points A and B', respectively, Alice's and Bob's labs experience the interaction with the vacuum at spacetime points B and A' (and analogously for the red branch). Therefore, the treatment of the vacuum in the optical quantum switch is mutually incoherent with the treatment of the vacuum in the dSD protocol.

Our analysis can thus serve as motivation for a search towards a more coherent treatment of the vacuum within the operational approach, since the same physical situation — interaction between the apparatus and the vacuum — is currently treated differently in the descriptions of the two protocols.

One might consider the following possible chain of inference. From the examples of both the quantum switch and the dSD protocol, we have that unitary operations (be it "genuine rotations" U and V, as well as phase flips $\pm I$) are considered to be operations. From the example of the dSD protocol, we see that the interaction with the vacuum is an operation as well. Further, in reference [21] it was argued that the optical switch features two "time-delocalised operations", U and V. Thus, by the same token, it follows that within this operational approach the optical switch should feature two additional "time-delocalised operations": interactions with the vacuum, one performed by Alice, and the other by Bob (see Appendix B). Therefore, the protocol features a total of four, rather than two, operations. Note that this is a possible treatment of the vacuum, which still features superposition of orders of operations U and V in the optical switch.

It is obvious that the interaction with the vacuum plays a prominent role in achieving the goal of the dSD protocol — communication between Alice and Bob. But interactions with the vacuum are also crucial in the optical switch. Indeed, without those operations, it would be *impossible* to achieve superposition of orders of operations U and V in flat spacetime with fixed causal order of spacetime points [9].

In [22] the so-called "flag" systems were introduced to count the number of operations performed in a lab without destroying the superposition, which count only one operation per each lab of the optical switch. Note though that using this method, which effectively counts the number of times a particle enters the lab, one would count three rather than four operations in the dSD protocol. This means that either the method is not appropriate, or in fact the dSD protocol features three, instead of four operations. In the case of the former, it would be useful to introduce a formal operational definition of a general method of counting operations, given that the above "flag" method cannot count interactions with the vacuum. In the case of the latter, it would mean that one could extract the information from the system at t_f without performing an operation at all.

Indeed, if the interaction between the vacuum and the apparatus would not be considered an operation, an issue with formulating the process vector for the dSD protocol would arise. The one we formulated in (14) contains input and output Hilbert spaces associated with the interaction between the vacuum and the detectors. It is not possible to formulate a process matrix for the dSD protocol that would feature three operations, without the mentioned interaction with the vacuum. Namely, depending on the choice of input bits a and b, the photon will end up either in Alice's or Bob's lab, rendering it impossible to know in advance which of the two agents is supposed to perform the final operation. Thus, it is not possible to formulate a process matrix which features only one operation at the final moment t_f. Note that the process matrices themselves were introduced as the main tool for describing quantum processes in the operational approach. In other words, the impossibility of formulating the main operational tool for the dSD protocol without introducing the interaction with the vacuum as an operation, suggests that the latter should be considered as an operation in that protocol.

Note that, if the dSD and the optical switch protocols featured incoherent mixtures of the two possible paths instead of coherent superpositions, then one could formulate the corresponding process matrices without treating the interaction with the vacuum as an operation, indeed without even mentioning the vacuum at all. These would be purely classical processes, which would not feature any interference effects. In general, ommiting the vacuum is a natural point of view in classical physics. However, if one wants to describe quantum physics, the notions of the vacuum and its interaction with the apparatus are unavoidable.

4 Identical particles

The above analysis shows that the vacuum state plays a physically relevant role in transmitting information, and cannot be ignored. From the point of view of QFT this is a perfectly natural state of affairs, but from the point of view of quantum mechanics (QM) it is not, since the notion of vacuum as a physical state does not exist in QM a priori, and needs to be explicitly introduced by hand. Moreover, in QFT one can naturally study systems of indefinite number of identical particles. Therefore, as a first step towards the generalization of the process matrix formalism to QFT, we apply the existing abstract process matrix formalism to the representation of the second quantization.

In this section, we give basic elements of the process matrix formalism, when applied to systems of identical particles. In order to avoid working with (anti-)symmetrised vectors of multi-particle states that contain non-physical entanglement whenever two or more identical particles are fully distinguishable (say, one photon is in Alice's, and another in Bob's lab), we will use the representation of the second quantisation in which the effects of particle statistics are governed by the creation and annihilation (anti-)commutation rules. First, we need to move from the single-particle Hilbert spaces associated to the gates and the process matrix to the corresponding capped Fock spaces.

To each gate G, we assign the input/output Fock spaces, $\mathcal{G}_{I/O}$, given in terms of the vacuum state $|0\rangle$ and the single-particle Hilbert spaces $G_{I/O}$. The single-particle input Hilbert space is given as

$$G_I = \text{span}\{|i\rangle = a_i^\dagger |0\rangle \mid i = 1, 2, \dots d_I\},$$

such that its creation and annihilation operators satisfy the standard (anti-)commutation relations,

$$[a_i^\dagger, a_j^\dagger]_\pm = [a_i, a_j]_\pm = 0\,, \quad [a_i, a_j^\dagger]_\pm = \delta_{ij}\,, \quad (18)$$

where $[\_\,,\_]_+$ stands for anti-commutator, and $[\_\,,\_]_-$ for commutator. The overall bosonic input Fock space is then

$$\mathcal{G}_I = \bigoplus_{\ell=0}^{\infty} G_I(\ell), \quad (19)$$

where $G_I(0) = \text{span}\{|0\rangle\}$ is the zero-particle, $G_I(1) = G_I$ the single-particle, and

$$G_I(\ell) = \{[(a_1^\dagger)^{s_1} \dots (a_{d_I}^\dagger)^{s_{d_I}}]|0\rangle \mid s_1 + \dots + s_{d_I} = \ell\}$$

are the ℓ-particle orthogonal subspaces of the input Fock space. For fermions, each $s_i \in \{0, 1\}$, and the orthogonal sum in Equation (19) goes until d_I, instead of ∞. For a given gate, the output Fock space $\mathcal{G}_O$ is defined analogously, and we denote its creation and annihilation operators as $\tilde{a}_i^\dagger$

and $\tilde{a}_i$, respectively, in order to distinguish them from the corresponding operators in $\mathcal{G}_I$.

Our formalism is constructed for quantum circuits which consist of finite number of gates. This means that we work in the approximation of a finite number of spacetime points, as opposed to the standard QFT where one works with an uncountably infinitely many spacetime points. Thus, given the algebra (18) for the creation and annihilation operators at a single gate, the full algebra across all gates is normalised to a Kronecker delta, instead of the standard Dirac delta function. Moreover, the operators in (18) are operators in coordinate space, as opposed to the momentum space operators which are standard in QFT, since they create and annihilate modes at a given gate (i.e., a given spacetime point), instead of modes with a given momentum. Taking into account our assumption of finite number of gates, the single-particle Hilbert spaces $G_{I/O}$ are finite-dimensional, i.e., $d_{I/O} \in \mathbb{N}$. Since the gates are distinguishable, the modes assigned to different gates *always* (anti-)commute.

We restrict ourselves to the Minkowski spacetime, so that the global Poincaré symmetry implies that the vacuum state $|0\rangle$ is identical across different gates, as well as between input and output Fock spaces for a given gate. In this sense, each gate is assumed to be stationary in some inertial reference frame, since the Fock spaces of non-inertial gates would be subject to the Unruh effect. We leave the discussion of non-inertial gates and spacetimes with more general geometries for future work.

Once the Fock spaces have been defined, we pass on to the process matrix description of gate operations. Since a process matrix has to satisfy the normalisation rule (1), the corresponding input and output spaces have to be finite-dimensional. To that end, we restrict ourselves to capped Fock spaces, which contain only a finite number of elements in the sum (19), denoted $N \in \mathbb{N}$. Together with the fact that $d_{I/O}$ is finite, it follows that the capped Fock spaces are finite-dimensional. A gate operation is represented via a CJ isomorphism of the corresponding operator between the input and the output capped Fock spaces, defined in equation (2),

$$M = \Big[(\mathcal{I} \otimes \mathcal{M}) \left(|\mathbb{1}\rangle\!\rangle \langle\!\langle \mathbb{1}| \right) \Big]^T , \qquad (20)$$

where the transport vector

$$|\mathbb{1}\rangle\!\rangle = \sum_{k=0}^{N} |\mathbb{1}_k\rangle\!\rangle \,, \qquad (21)$$

is given in terms of k-transport vectors defined as

$$|\mathbb{1}_k\rangle\!\rangle = \sum \Big[\prod_{i=1}^{d} \frac{(a_i^\dagger)^{s_i}}{\sqrt{s_i!}} \Big] \otimes \Big[\prod_{i=1}^{d} \frac{(a_i^\dagger)^{s_i}}{\sqrt{s_i!}} \Big] |0\rangle \,, \quad (22)$$

where the sum is taken over all s_i satisfying the constraint $s_1 + ... + s_d = k$.

One special case of the general formula (20) is the case where gates destroy all coherence between k-particle sectors, for example by measuring the number of particles,

$$M = \sum_{k=0}^{N} \Big[(\mathcal{I} \otimes \mathcal{M}_k) \left(|\mathbb{1}_k\rangle\!\rangle \langle\!\langle \mathbb{1}_k| \right) \Big]^T , \qquad (23)$$

where $\mathcal{M}_k$ represents the k-particle operator for the gate. The above gate represents a classical mixture of operations on each k-particle sector, as opposed to coherent superpositions of them.

Another special case of (20), which does preserve the coherence between k-particle sectors, is represented by linear operations. For a linear gate operation, one can analogously use the "vector" formalism, and the generalisation of the CJ vector (5). With a slight abuse of notation, using $\mathcal{M}$ to denote the operator instead of its superoperator, we can now write

$$\begin{aligned} |\mathcal{M}^*\rangle\!\rangle &= \Big[\mathcal{I} \otimes \mathcal{M}^* \Big] |\mathbb{1}\rangle\!\rangle \\ &= \sum_{k,k',k''=0}^{N} \Big[\mathcal{I}_k \otimes \mathcal{M}^*_{k'} \Big] |\mathbb{1}_{k''}\rangle\!\rangle \\ &= \sum_{k=0}^{N} \Big[\mathcal{I}_k \otimes \mathcal{M}^*_k \Big] |\mathbb{1}_k\rangle\!\rangle \,, \end{aligned}$$

since it is assumed that by definition

$$\Big[\mathcal{I}_k \otimes \mathcal{M}^*_{k'} \Big] |\mathbb{1}_{k''}\rangle\!\rangle \equiv 0 \,, \qquad k'' \notin \{k, k'\} \,.$$

Now, using (6) one can rewrite (20) into the form

$$\begin{aligned} M &= |\mathcal{M}^*\rangle\!\rangle \langle\!\langle \mathcal{M}^*| \\ &= \sum_{k,k'=0}^{N} \Big[\mathcal{I}_k \otimes \mathcal{M}^*_k \Big] |\mathbb{1}_k\rangle\!\rangle \langle\!\langle \mathbb{1}_{k'}| \Big[\mathcal{I}_{k'} \otimes \mathcal{M}^*_{k'} \Big]^\dagger , \end{aligned}$$

which is clearly different from the case (23), since it contains off-diagonal elements which preserve coherence between k-particle sectors. One concrete example of this special case is the dSD protocol, discussed in the previous Section. Another example is a single-particle unitary operator

$$U = \sum_{i,j} u_{ij} \tilde{a}_i^\dagger a_j \,.$$

Then, its capped Fock-space generalisation is given as

$$\mathcal{M} = \sum_{k=0}^{N} \mathcal{M}_k = |0\rangle\langle 0| + \sum_{k=1}^{N} \frac{1}{k!} : U^{\otimes k} : ,$$

where $: U^{\otimes k} :$ is the normal ordering of $U^{\otimes k}$.

Given the capped Fock spaces and actions of instruments in all gates, a process matrix is defined in the same way as in Section 2, according to Eq. (4). A process matrix maps the tensor product of output spaces for all gates into the tensor product of input spaces for all gates. For example, if the process under consideration is a quantum circuit (see Section 2 of [9]), the corresponding process matrix can be represented as a tensor product of transport vectors, each corresponding to a wire connecting two gates. Transport vectors are defined in the same way as (21), where in (22) the first set of creation operators corresponds to the input space of the wire, while the second set corresponds to its output space. Given that a wire is connecting two gates, its input and output spaces correspond to the output and input subspaces of the two gates, respectively. A gate can in general have multiple incoming or outgoing wires attached to it. Therefore, its input (output) space is a tensor product of all output (input) spaces of the corresponding wires.

5 Conclusions

5.1 Summary of the results

In this work we have presented a detailed account of the dSD protocol, formulating it within the process matrix formalism. Analysing the role of the vacuum state in the dSD protocol and its process matrix description, we gave the operational interpretation of the vacuum. Our analysis shows that the interaction with the vacuum should be treated as an operation, on equal footing with all other interactions, thus representing a resource in quantum information protocols (including, for example, [23, 24]). As a consequence, the optical implementation of the quantum switch protocol features four rather than just two operations, in contrast to what was claimed in the literature [3, 4, 5, 6, 7, 8]. Furthermore, we have applied the process matrix formalism to the second quantisation framework restricted to capped Fock spaces, providing the description of systems of identical particles.

5.2 Discussion

The first important point of this work is the necessity of explicitly introducing the interaction with the vacuum as a legitimate operation in the dSD protocol, on equal footing with any other operation. Indeed, the very lack of detection of the particle in the protocol provides an equal amount of information as its detection (*explicit* interaction). As a consequence, instead of interpreting the absence of particle as noninteraction, one should interpret it as the interaction between the vacuum and the apparatus, and thus as an operation. Including the interaction with the vacuum as an operation poses a question of the method of counting operations in a given protocol, since the operations corresponding to the interaction with the vacuum cannot be counted.

The introduction of the vacuum into the process matrix formalism gives a natural motivation to extend the latter to the case of identical particles, both bosons and fermions, which is the second important point of this work. However, note that while employing the formalism of second quantisation, our construction still features only a discrete number of gates. This discreteness means that we still work in *particle ontology* (i.e., mechanics). Nevertheless, our construction is an important first step towards defining the process matrix formalism in *field ontology*, i.e., fully fledged QFT.

5.3 Future lines of investigation

As mentioned in the discussion, a natural next line of investigation would be a generalisation of the process matrix formalism to full, or at least perturbative, QFT. This would include an analysis of non-inertial gates and the corresponding Unruh effect. In addition, a mathematically rigorous formulation of the axioms for the process matrix description in Fock spaces is also an important topic to be addressed. While the primary interest in process matrices lies in their application to higher order processes [25, 26], their generalisation to QFT would also be of great interest. Finally, addressing in more detail the interaction between the agent and the vacuum within the operational approach is an interesting topic of future research.

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A Two lemmas for the process matrix evaluation

Lemma 1. Let $|\Psi^*\rangle\!\rangle^{X_O} = |\Psi^*\rangle^{X_O}$ represent a gate which has no input, while it prepares the state $|\Psi\rangle \in X_O$ as its output. Then, the scalar product of that vector and the transport vector $|\mathbb{1}\rangle\!\rangle^{X_O Y_I}$ is given as:

$$^{X_O}\langle\!\langle \Psi^* | \mathbb{1} \rangle\!\rangle^{X_O Y_I} = |\Psi\rangle^{Y_I} .$$

Proof. Using the fact that the transport vector is an unnormalized maximally entangled state, the explicit calculation goes as follows:

$$\begin{aligned} ^{X_O}\langle\!\langle \Psi^* | \mathbb{1} \rangle\!\rangle^{X_O Y_I} &= \langle \Psi^* |^{X_O} \sum_k |k\rangle^{X_O} |k\rangle^{Y_I} \\ &= \sum_k \langle \Psi^* | k\rangle \; |k\rangle^{Y_I} \\ &= \sum_k \langle k | \Psi\rangle \; |k\rangle^{Y_I} \\ &= |\Psi\rangle^{Y_I} , \end{aligned}$$

where we have used the unit decomposition $I = \sum_k |k\rangle\langle k|$ and the fact that $\langle \Psi^* | k\rangle = \langle \Psi | k\rangle^* = \langle k | \Psi\rangle$.

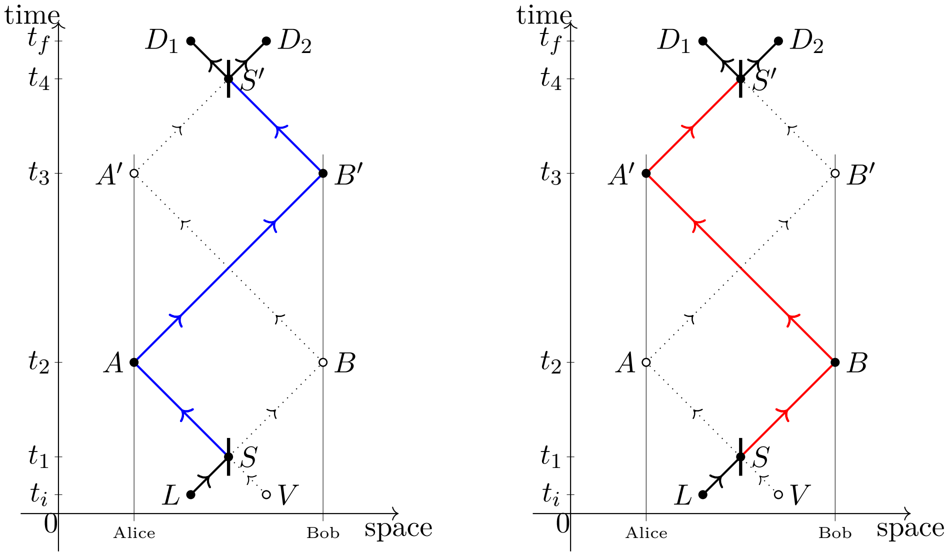

Figure 3: Two branches of the coherent superposition of the optical switch protocol.

Lemma 2. Let

$$|U^*\rangle\rangle^{X_I X_O} = \left[I^{X_I X_I} \otimes (U^*)^{X_O X_I} \right] |\mathbb{1}\rangle\rangle^{X_I X_I}$$

represent a gate which performs the operation $U : X_I \to X_O$, and let $|W\rangle\rangle = |\Psi\rangle^{X_I} |\mathbb{1}\rangle\rangle^{X_O Y_I}$. Then the scalar product of the two is

$${}^{X_I X_O}\langle\langle U^* | W \rangle\rangle = \Big(U |\Psi\rangle \Big)^{Y_I} .$$

Proof. Again using the expansion of the transport vectors as unnormalized maximally entangled states, the explicit calculation goes as follows:

$$\begin{aligned}
{}^{X_I X_O}\langle\langle U^* | W \rangle\rangle &= \langle\langle \mathbb{1} |^{X_I X_I} \left[I^{X_I X_I} \otimes (U^T)^{X_I X_O} \right] |\Psi\rangle^{X_I} |\mathbb{1}\rangle\rangle^{X_O Y_I} \\
&= \sum_k \langle k|^{X_I} \langle k|^{X_I} \left[I^{X_I X_I} \otimes (U^T)^{X_I X_O} \right] |\Psi\rangle^{X_I} \sum_m |m\rangle^{X_O} |m\rangle^{Y_I} \\
&= \sum_{k,m} \Big(\langle k|^{X_I} I^{X_I X_I} |\Psi\rangle^{X_I} \Big) \Big(\langle k|^{X_I} (U^T)^{X_I X_O} |m\rangle^{X_O} \Big) |m\rangle^{Y_I} \\
&= \sum_{k,m} \Big(\langle k|\Psi\rangle \Big) \Big(\langle m|U|k\rangle \Big) |m\rangle^{Y_I} \\
&= \sum_m \langle m|U \left(\sum_k |k\rangle\langle k| \right) |\Psi\rangle \; |m\rangle^{Y_I} \\
&= \sum_m \langle m|U|\Psi\rangle \; |m\rangle^{Y_I} \\
&= \Big(U|\Psi\rangle \Big)^{Y_I} ,
\end{aligned}$$

where we have again used the unit decomposition and the fact that $\langle k|U^T|m\rangle = \langle m|U|k\rangle$.

B Time-delocalised operations in the optical switch

Figure 3 depicts two branches coherently superposed in the optical switch. The left diagram represents the branch in which the photon first enters Alice's lab, and then Bob's. On the right, the photon first visits Bob's lab, and then Alice's. Whenever the photon enters Alice's lab, she applies unitary U (in A, left diagram, or A', right diagram), while Bob interacts with the vacuum (in B, left diagram, or B', right diagram). Analogously, whenever the photon enters Bob's lab, he applies unitary V (in B, right diagram, or B', left diagram), while Alice interacts with the vacuum (in A, right diagram, or A', left diagram).

Since applying the unitaries in a quantum protocol are operations, and since in the optical switch they are applied by Alice (U) and Bob (V) at two different times, we say that the optical switch features two time-delocalised operations U (at A and A') and V (at B and B').

Since the interaction with the vacuum in the dSD protocol is an operation, and since in the optical switch it is applied by Alice and Bob at two different times, one can say that the optical switch features two time-delocalised operations of the interaction with the vacuum (at A and A', as well as at B and B').

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Topological invariant of 4-manifolds based on a 3-group

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Abstract: We study a generalization of 4-dimensional BF-theory in the context of higher gauge theory. We construct a triangulation independent topological state sum Z, based on the classical $3BF$ action for a general 3-group and a 4-dimensional spacetime manifold $\mathcal{M}_4$. This state sum coincides with Porter's TQFT for $d = 4$ and $n = 3$. In order to verify that the constructed state sum is a topological invariant of the underlying 4-dimensional manifold, its behavior under Pachner moves is analyzed, and it is obtained that the state sum Z remains the same. This paper is a generalization of the work done by Girelli, Pfeiffer, and Popescu for the case of state sum based on the classical $2BF$ action with the underlying 2-group structure.

Keywords: Differential and Algebraic Geometry, Models of Quantum Gravity, Topological Field Theories, Gauge Symmetry

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1 Introduction

Within the Loop Quantum Gravity framework, one studies the nonperturbative quantization of gravity, both canonically and covariantly, see [1–4] for an overview and a comprehensive introduction. The covariant approach focuses on defining the path integral for the gravitational field by considering a triangulation of a spacetime manifold and specifying the path integral as a discrete state sum of the gravitational field configurations living on the simplices in the triangulation. This quantization technique is usually referred to as the *spinfoam quantization method*, and it can be divided into three major steps:

1. first, one writes the classical action $S[g]$ as a topological BF-like action plus simplicity constraints,

2. then one uses the algebraic structure underlying the topological sector of the action to define a topological state sum Z,

3. and finally, one deforms the topological state sum by imposing simplicity constraints, thus promoting it into a path integral for a physical theory.

Spinfoam models for gravity are usually constructed by constraining the topological gauge theory known as BF theory, obtaining the Plebanski formulation of general relativity [5]. For example, in 3 dimensions, the prototype spinfoam model is known as the Ponzano-Regge model [6]. In 4 dimensions there are multiple models, such as the Barrett-Crane model [7, 8], the Ooguri model [9], and the most sophisticated EPRL/FK model [10, 11] (see also [12–14]). All these models aim to define a viable theory of a quantum gravitational field alone, without matter fields. The attempts to include matter fields have had limited success [15], mainly because the mass terms cannot be expressed in the theory due to the absence of the tetrad fields from the topological BF sector of the theory.

In order to overcome this problem, a new approach has been developed within the framework of *higher gauge theory* (for a review of higher gauge theory, see [16, 17], and for its applications in physics see [18–29]). Within higher gauge theory formalism, one generalizes the BF action, based on some Lie group, to an $2BF$ action based on the 2-group structure. Within this approach [30], one rewrites the action for general relativity as a constrained $2BF$ action, such that the tetrad fields are present in the topological sector. This result opened up the possibility to couple all matter fields to gravity in a straightforward way. Nevertheless, the matter fields could not be naturally expressed using the underlying algebraic structure of a 2-group, rendering the spinfoam quantization method only half-implementable, since the matter sector of the classical action could not be expressed as a topological term plus a simplicity constraint, which means that the steps 2 and 3 above could not be performed for the matter sector of the action.

This final issue has recently been resolved in [31], where one more step in the categorical ladder is performed in order to generalize the underlying algebraic structure from a 2-group to a 3-group (see also [32] for the 4-group formulation). This generalization then naturally gives rise to the so-called $3BF$ action, which proves to be suitable for a unified description of both gravity and matter fields. The first step of the spinfoam quantization program is carried out in [31] where the suitable gauge 3-groups have been specified, and the corresponding constrained $3BF$ actions constructed so that the desired classical dynamics of the gravitational and matter fields are obtained. A reader interested in the construction of the constrained $2BF$ actions describing the Yang-Mills field and Einstein-Cartan gravity, and $3BF$ actions describing the Klein-Gordon, Dirac, Weyl, and Majorana fields, each coupled to gravity in the standard way, is referred to [30, 31].

In this paper, we focus our attention on the second step of the spinfoam quantization program: we will construct a triangulation independent topological state sum Z, based on the classical $3BF$ action for a general 3-group and a 4-dimensional spacetime manifold $\mathcal{M}_4$. This state sum coincides with Porter's TQFT [33, 34] for $d = 4$ and $n = 3$. In order to verify that the constructed state sum is topological, we analyze its behavior under Pachner moves [35]. Pachner moves are local changes of a triangulation that preserve topology, such that any two triangulations of the same manifold are connected by a finite number of Pachner moves. In 4 dimensions, there are five different Pachner moves: the $3-3$ move,

$4-2$ move, and $5-1$ move, and their inverses. After defining the state sum, we calculate its behavior under these Pachner moves. We obtain that the state sum Z remains the same, proving that it is a topological invariant of the underlying 4-dimensional manifold. This construction thus completes the second step of the quantization procedure. Our result paves the way for the third step of the covariant quantization procedure and a formulation of a quantum theory of gravity and matter by imposing the simplicity constraints on the state sum. We leave the third step for future work.

The layout of the paper is as follows. In section 2 we review the pure and the constrained nBF theories describing some of the physically relevant models — the constrained $2BF$ actions describing the Yang-Mills field and Einstein-Cartan gravity, and constrained $3BF$ actions describing the Klein-Gordon and Dirac fields coupled to Yang-Mills fields and gravity in the standard way. In section 3, we review the relevant algebraic tools involved in the description of higher gauge theory, 2-crossed modules, and 3-gauge theory. Starting from the notion of Lie 3-groups, we generalize the integral picture of gauge theory to a 3-gauge theory that involves curves, surfaces, and volumes labeled with elements of non-Abelian groups. In section 4, we define the discrete state sum model of topological higher gauge theory in dimension $d = 4$. The model is defined for any closed and oriented combinatorial 4-dimensional manifold $\mathcal{M}_4$. The proof that the state sum is invariant under the Pachner moves and thus independent of the chosen triangulation is presented in appendix B.

Notations and conventions throughout the paper are as follows. The local Lorentz indices are denoted by the Latin letters $a, b, c, \dots$, that take values $0, 1, 2, 3$, and are raised and lowered using the Minkowski metric η_{ab} with signature $(-,+,+,+)$. The spacetime indices are denoted by the Greek letters $\mu, \nu, \dots$, and are raised and lowered by the spacetime metric $g_{\mu\nu} = \eta_{ab} e^a{}_\mu e^b{}_\nu$, where $e^a{}_\mu$ denotes the tetrad fields. If G is a finite group, $\int_G dg = 1/|G| \sum_{g\in G}$ denotes the normalized sum over all group elements, while δ_G denotes the corresponding δ-distribution on G. The δ-distribution is defined for every element $g \in G$ such that $\delta_G(g) = |G|$ if g is the unit element of the group, i.e., $g = e$, and $\delta_G(g) = 0$ if it is not, i.e., $g \neq e$. If G is a Lie group, $\int_G dg$ and δ_G denote the Haar measure and the δ-distribution on G, respectively. The set of all k-simplices, $0 \le k \le d$, is denoted by Λ_k. The set of vertices Λ_0 is finite and ordered, and every k-simplex is labeled by $(k+1)$-tuples of vertices $(i_0 \dots i_k)$, where $i_0, \dots, i_k \in \Lambda_0$ such that $i_0 < \dots < i_k$.

2 Review of the classical theory

2.1 Topological nBF theories

For a given Lie group G whose Lie algebra $\mathfrak{g}$ is equipped with the G-invariant symmetric nondegenerate bilinear form $\langle \_\,,\_ \rangle_{\mathfrak{g}}$, and for a given 4-dimensional spacetime manifold $\mathcal{M}_4$, one can introduce the BF action as

$$S_{BF} = \int_{\mathcal{M}_4} \langle B \wedge F \rangle_{\mathfrak{g}}\,, \tag{2.1}$$

where 2-form $F \equiv \mathrm{d}\alpha + \alpha \wedge \alpha$ is the curvature for the $\mathfrak{g}$-valued connection 1-form $\alpha \in \mathcal{A}^1(\mathcal{M}_4\,, \mathfrak{g})$ and 2-form $B \in \mathcal{A}^2(\mathcal{M}_4\,, \mathfrak{g})$ is an $\mathfrak{g}$-valued Lagrange multiplier. Varying the

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action (2.1) with respect to the Lagrange multiplier B and the connection α, one obtains the equations of motion of the theory,

$$F = 0\,, \qquad \nabla B \equiv \mathrm{d}B + \alpha \wedge B = 0\,. \tag{2.2}$$

From the first equation of motion, one sees that α is a flat connection, which then, together with the second equation of motion, implies that B is constant. Therefore, the theory given by the BF action has no local propagating degrees of freedom, i.e., the theory is topological. For more details about the BF theory see [5, 36, 37].

Within the framework of Higher Gauge Theory, by passing from the notion of a gauge group to the notion of a gauge 2-group, one defines the categorical generalization of the BF action, called the $2BF$ action. A 2-group has a naturally associated notion of a 2-connection $(\alpha\,,\beta)$, described by the usual $\mathfrak{g}$-valued 1-form $\alpha \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{g})$ and an $\mathfrak{h}$-valued 2-form $\beta \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{h})$, where $\mathfrak{h}$ is a Lie algebra of the Lie group H. The 2-connection gives rise to the so-called fake 2-curvature $(\mathcal{F},\mathcal{G})$, where $\mathcal{F}$ is a $\mathfrak{g}$-valued fake curvature 2-form $\mathcal{F} \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{g})$ and $\mathcal{G}$ is an $\mathfrak{h}$-valued curvature 3-form $\mathcal{G} \in \mathcal{A}^3(\mathcal{M}_4\,,\mathfrak{h})$, defined as

$$\mathcal{F} = \mathrm{d}\alpha + \alpha \wedge \alpha - \partial\beta\,, \qquad \mathcal{G} = \mathrm{d}\beta + \alpha \wedge^{\triangleright} \beta\,. \tag{2.3}$$

Representing the 2-group as a crossed-module $(H \stackrel{\partial}{\to} G\,,\triangleright)$, and seeing the next section for the definition and notation, one introduces a $2BF$ action using the fake 2-curvature (2.3) as

$$S_{2BF} = \int_{\mathcal{M}_4} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} + \langle C \wedge \mathcal{G} \rangle_{\mathfrak{h}}\,, \tag{2.4}$$

where the 2-form $B \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{g})$ and the 1-form $C \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{h})$ are Lagrange multipliers, and $\langle\_\,,\_\rangle_{\mathfrak{g}}$ and $\langle\_\,,\_\rangle_{\mathfrak{h}}$ denote the G-invariant symmetric nondegenerate bilinear forms for the algebras $\mathfrak{g}$ and $\mathfrak{h}$, respectively. Similarly as in the case of the BF theory, varying the $2BF$ action (2.4) with respect to the Lagrange multipliers B and C one obtains the equations of motion,

$$\mathcal{F} = 0\,, \qquad \mathcal{G} = 0\,, \tag{2.5}$$

i.e., the conditions that the curvature 2-form $\mathcal{F}$ and the curvature 3-form $\mathcal{G}$ vanish, while varying with respect to the connections α and β one obtains

$$\nabla B + C \wedge^{\mathcal{T}} \beta = 0\,, \qquad \nabla C - \partial(B) = 0\,. \tag{2.6}$$

Similar to the case of the BF action, the $2BF$ action defines a topological theory, i.e., a theory with no propagating degrees of freedom, see [38–41] for review and references.

Continuing the categorical ladder one step further, one can generalize the $2BF$ action to the $3BF$ action, by passing from the notion of a 2-group to the notion of a 3-group. Representing the 3-group with a 2-crossed module $(L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G\,,\triangleright\,,\{\_\,,\_\}_{\mathrm{p}})$, and seeing next section for definition and notation, one can define a 3-connection as an ordered triple (α, β, γ), where α, β, and γ are appropriate algebra-valued differential forms, $\alpha \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{g})$, $\beta \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{h})$, and $\gamma \in \mathcal{A}^3(\mathcal{M}_4, \mathfrak{l})$. The corresponding fake 3-curvature

$(\mathcal{F},\mathcal{G},\mathcal{H})$ is defined as:

$$\begin{aligned}&\mathcal{F}=\mathrm{d}\alpha+\alpha\wedge\alpha-\partial\beta\,, \qquad\qquad \mathcal{G}=\mathrm{d}\beta+\alpha\wedge^{\rhd}\beta-\delta\gamma\,,\\ &\mathcal{H}=\mathrm{d}\gamma+\alpha\wedge^{\rhd}\gamma+\{\beta\wedge\beta\}_{\mathrm{p}}\,.\end{aligned}\tag{2.7}$$

Then, similar to the construction of BF and $2BF$ actions, one defines the $3BF$ action as

$$S_{3BF}=\int_{\mathcal{M}_4}\langle B\wedge\mathcal{F}\rangle_{\mathfrak{g}}+\langle C\wedge\mathcal{G}\rangle_{\mathfrak{h}}+\langle D\wedge\mathcal{H}\rangle_{\mathfrak{l}}\,,\tag{2.8}$$

where $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$ denote the Lie algebras corresponding to the Lie groups G, H, and L and the forms $\langle\_,\_\rangle_{\mathfrak{g}}$, $\langle\_,\_\rangle_{\mathfrak{h}}$, and $\langle\_,\_\rangle_{\mathfrak{l}}$ are G-invariant symmetric nondegenerate bilinear forms on $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$, respectively. The variables $B\in\mathcal{A}^2(\mathcal{M}_4,\mathfrak{g})$, $C\in\mathcal{A}^1(\mathcal{M}_4,\mathfrak{h})$, and $D\in\mathcal{A}^0(\mathcal{M}_4,\mathfrak{l})$ are Lagrange multipliers, and their associated equations of motion are the conditions that the 3-curvature $(\mathcal{F},\mathcal{G},\mathcal{H})$ vanishes,

$$\mathcal{F}=0\,,\qquad \mathcal{G}=0\,,\qquad \mathcal{H}=0\,.\tag{2.9}$$

Additionally, varying with respect to the 3-connection variables α, β, and γ one gets:

$$\nabla B+C\wedge^{\mathcal{T}}\beta-D\wedge^{\mathcal{S}}\gamma=0\,,\tag{2.10}$$

$$\nabla C-\partial(B)-D\wedge^{(\chi_1+\chi_2)}\beta=0\,,\tag{2.11}$$

$$\nabla D+\delta(C)=0\,.\tag{2.12}$$

For further details see [22, 42, 43] for the definition of the 3-group, and [31] for the definition of the pure $3BF$ action.

All the above actions are topological, in the sense that they do not contain any local propagating degrees of freedom [44, 45]. In this sense, they are not very interesting for the description of realistic physics, which should feature nontrivial dynamics. Nevertheless, by choosing the convenient underlying 2-crossed module structure and imposing the appropriate simplicity constraints onto the degrees of freedom present in the $3BF$ action, one can obtain the nontrivial classical dynamics of the gravitational and matter fields, as we will see in the following subsection.

2.2 Models with relevant dynamics

Let us review how one can employ the n-group structure to introduce the topological nBF actions corresponding to gravity and matter fields, as well as the form of the appropriate simplicity constraints to be imposed on these fields to obtain the classical dynamics.

First we review the most important constrained $2BF$ actions. We begin by rewriting general relativity as a constrained $2BF$ action based on the underlying Poincaré 2-group. The Poincaré 2-group is equivalent to a crossed module $(H\xrightarrow{\partial}G,\rhd)$, where the groups are choosen as $G=\mathrm{SO}(3,1)$ and $H=\mathbb{R}^4$, and the map ∂ is trivial. The action $\rhd$ is a natural action of $\mathrm{SO}(3,1)$ on $\mathbb{R}^4$, defined as

$$M_{ab}\rhd P_c=\eta_{[bc}P_{a]}\,,\tag{2.13}$$

where M_{ab} and P_a are the generators of groups $\mathrm{SO}(3,1)$ and $\mathbb{R}^4$, respectively. The action $\triangleright$ of $\mathrm{SO}(3,1)$ on itself is given via conjugation, by definition of a crossed module. Then, Poincaré 2-group gives rise to the 2-connection (α, β), given by the algebra-valued differential forms

$$\alpha = \omega^{ab} M_{ab} \,, \qquad \beta = \beta^a P_a \,, \tag{2.14}$$

where we have interpreted the connection 1-form α^{ab} as the ordinary spin connection ω^{ab}. Also, the corresponding 2-curvature $(\mathcal{F}, \mathcal{G})$ is given as

$$\begin{aligned} \mathcal{F} &= (\mathrm{d}\omega^{ab} + \omega^a{}_c \wedge \omega^{cb}) M_{ab} \equiv R^{ab} M_{ab} \,, \\ \mathcal{G} &= (\mathrm{d}\beta^a + \omega^a{}_b \wedge \beta^b) P_a \qquad \equiv \nabla \beta^a P_a \equiv G^a P_a \,, \end{aligned} \tag{2.15}$$

where we can recognize the standard Riemann curvature 2-form R^{ab} in $\mathcal{F}$. Having these variables in hand, one defines $2BF$ action (2.4) for the Poincaré 2-group as

$$S_{2BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a \,. \tag{2.16}$$

Here, the crucial insight is that the Lagrange multiplier fields C^a can be identified with the tetrads [30], since one can show that 1-forms C^a transform in the same way as the tetrad 1-forms e^a under the Lorentz transformations and diffeomorphisms. One can now construct the action for general relativity by simply adding the additional simplicity constraint term to the action (2.16):

$$S = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right) . \tag{2.17}$$

Here λ_{ab} is a Lagrange multiplier 2-form associated to the simplicity constraint term, and l_p is the Planck length. It is straightforward to show that the corresponding equations of motion reduce to vacuum Einstein field equations. Thus the action (2.17) is classically equivalent to general relativity. The construction of the action (2.17) is analogous to the Plebanski model, where general relativity is constructed by adding a simplicity constraint to the BF theory based on the Lorentz group. However, one clear advantage of this model over the Plebanski model is that the tetrads are explicitly present in the topological sector of the action. Upon the covariant quantization, tetrads are therefore fundamental, off-shell quantities, in contrast to the Plebanski model where they appear only on-shell, as solutions of the classical equations of motion. The off-shell presence of the tetrads facilitates the straightforward coupling of the matter fields to gravity, and thus overcomes the problems present in the spinfoam models [15].

The Poincaré 2-group can be easily extended to include the coupling of the $\mathrm{SU}(N)$ Yang-Mills fields to gravity [31]. To achieve this, one constructs the crossed module $(H \xrightarrow{\partial} G, \triangleright)$, where the groups are chosen as $G = \mathrm{SO}(3,1) \times \mathrm{SU}(N)$ and $H = \mathbb{R}^4$, while the map ∂ remains trivial, as before. The action $\triangleright$ of the group G on H is such that the $\mathrm{SO}(3,1)$ subgroup acts on $\mathbb{R}^4$ via the vector representation (2.13), while the action of the $\mathrm{SU}(N)$ subgroup is trivial,

$$\tau_I \triangleright P_a = 0 \,, \tag{2.18}$$

where τ_I are the SU(N) generators. This crossed module yields the 2-connection (α, β), where algebra-valued 1-form α and algebra valued 2-form β are defined as follows,

$$\alpha = \omega^{ab} M_{ab} + A^I \tau_I \,, \qquad \beta = \beta^a P_a \,, \tag{2.19}$$

where we can identify the gauge connection 1-form A^I. This connection gives rise to the 2-curvature $(\mathcal{F}, \mathcal{G})$, where $\mathcal{F}$ as defined as

$$\mathcal{F} = R^{ab} M_{ab} + F^I \tau_I \,, \qquad F^I \equiv \mathrm{d}A^I + f_{JK}{}^I A^J \wedge A^K \,, \tag{2.20}$$

while the curvature $\mathcal{G}$ for β remains the same as before. Given these variables, the Lagrange multiplier B in the first term of the topological action (2.4) also splits into two pieces corresponding to the direct product of the group G, giving

$$S_{2BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + B^I \wedge F_I + e_a \wedge \nabla \beta^a \,, \tag{2.21}$$

where 2-form $B^I \in \mathcal{A}^2(\mathcal{M}_4\,, \mathfrak{su}(N))$ is the second piece of the Lagrange multiplier. To obtain the non-trivial classical dynamics for gravity and the Yang-Mills field, we add the appropriate simplicity constraint terms to the action (2.21), and construct the constrained $2BF$ action:

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + B^I \wedge F_I + e_a \wedge \nabla \beta^a - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right) \\ & + \lambda^I \wedge \left(B_I - \frac{12}{g} M_{abI} e^a \wedge e^b \right) + \zeta^{abI} \left(M_{abI} \varepsilon_{cdef} e^c \wedge e^d \wedge e^e \wedge e^f - g_{IJ} F^J \wedge e_a \wedge e_b \right) . \end{aligned} \tag{2.22}$$

Here, the first row is the topological sector and the familiar simplicity constraint for gravity from (2.17), while the second row contains the appropriate simplicity constraints for Yang Mills field, featuring the Lagrange multipliers λ^I and ζ^{abI}. The action (2.22) provides two dynamical equations — the equation for A^I,

$$\nabla_\rho F^{I\rho\mu} \equiv \partial_\rho F^{I\rho\mu} + \Gamma^\rho{}_{\lambda\rho} F^{I\lambda\mu} + f_{JK}{}^I A^J{}_\rho F^{K\rho\mu} = 0 \,, \tag{2.23}$$

where $\Gamma^\lambda{}_{\mu\nu}$ is the standard Levi-Civita connection, and an equation for e^a which is the Einstein field equation with the SU(N) gauge field source term,

$$R^{\mu\nu} - \frac{1}{2} g^{\mu\nu} R = 8\pi l_p^2 \, T^{\mu\nu} \,, \quad T^{\mu\nu} \equiv -\frac{1}{4g} \left(F_{\rho\sigma}{}^I F^{\rho\sigma}{}_I g^{\mu\nu} + 4 F^{\mu\rho}{}_I F_\rho{}^{\nu I} \right) . \tag{2.24}$$

In this way, we see that both gravity and gauge fields can be successfully represented within a unified framework of higher gauge theory, based on a 2-group structure. A generalization from SU(N) Yang-Mills case to the more complicated cases, such as SU(3) × SU(2) × U(1), is straightforward.

Let us now review how one can use the 3-group structure and the corresponding constrained $3BF$ theory to describe general relativity coupled to Klein-Gordon and Dirac fields. To describe a single real Klein-Gordon field coupled to gravity, one begins by specifying a 2-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \triangleright\,, \{\_\,,\_\}_{\mathrm{p}})$, as follows. The groups are given as

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$G = \mathrm{SO}(3,1)$, $H = \mathbb{R}^4$, and $L = \mathbb{R}$. The group G acts on H via the vector representation, and on L via the trivial representation. The maps ∂ and δ are chosen to be trivial, as well as the Peiffer lifting. Given this choice of a 2-crossed module, the 3-connection $(\alpha\,, \beta\,, \gamma)$ takes the form

$$\alpha = \omega^{ab} M_{ab}\,, \qquad \beta = \beta^a P_a\,, \qquad \gamma = \gamma \mathbb{I}\,, \tag{2.25}$$

where $\mathbb{I}$ is the sole generator of the Lie group L. This 3-connection gives rise to the fake 3-curvature $(\mathcal{F}, \mathcal{G}, \mathcal{H})$,

$$\mathcal{F} = R^{ab} M_{ab}\,, \qquad \mathcal{G} = \nabla \beta^a P_a\,, \qquad \mathcal{H} = \mathrm{d}\gamma\,. \tag{2.26}$$

The importance of the $3BF$ theory for this choice of the 2-crossed module lies in the fact that the Lagrange multiplier D can transform as a scalar with respect to Lorentz symmetry, $M_{ab} \triangleright \mathbb{I} = 0$, and it transforms as a scalar with respect to diffeomorphisms since D is also a 0-form. In other words, one can interpret the Lagrange multiplier D to be a real scalar field, $D \equiv \phi$, and write the topological $3BF$ action (2.8) as:

$$S_{3BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a + \phi \, \mathrm{d}\gamma\,. \tag{2.27}$$

In order to obtain the Klein-Gordon field ϕ of mass m coupled to gravity in the standard way, the appropriate simplicity constraints are imposed, and the constrained $3BF$ action takes the form:

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a + \phi \, \mathrm{d}\gamma - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right) \\ & + \lambda \wedge \left(\gamma - \frac{1}{2} H_{abc} e^a \wedge e^b \wedge e^c \right) + \Lambda^{ab} \wedge \left(H_{abc} \varepsilon^{cdef} e_d \wedge e_e \wedge e_f - \mathrm{d}\phi \wedge e_a \wedge e_b \right) \\ & - \frac{1}{2 \cdot 4!} m^2 \phi^2 \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d\,. \end{aligned} \tag{2.28}$$

The first row is the topological sector (2.27) and the simplicity constraint for gravity from the action (2.17), the second row contains two new simplicity constraints featuring the Lagrange multiplier 1-forms λ and Λ^{ab} and the 0-form H_{abc}, and the third row features the mass term for the scalar field. The action (2.28) has two dynamical equations of motion — the equation for the scalar field ϕ is the covariant Klein-Gordon equation,

$$\left(\nabla_\mu \nabla^\mu - m^2 \right) \phi = 0\,, \tag{2.29}$$

while the equation for the tetrads e^a is the Einstein field equation with the scalar field source term,

$$R^{\mu\nu} - \frac{1}{2} g^{\mu\nu} R = 8\pi l_p^2 \, T^{\mu\nu}\,, \quad T^{\mu\nu} \equiv \partial^\mu \phi \partial^\nu \phi - \frac{1}{2} g^{\mu\nu} \left(\partial_\rho \phi \partial^\rho \phi + m^2 \phi^2 \right)\,. \tag{2.30}$$

We see that the obtained theory is classically equivalent to general relativity coupled to a scalar field. Most importantly, one sees that the choice of the group L dictates the matter

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content of the theory, while the action $\triangleright$ of G on L specifies the transformation properties of the matter fields.

Finally, in order to describe the Dirac field coupled to Einstein-Cartan gravity, the 2-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \triangleright\,, \{\_\,,\_\}_{\rm p})$ has to be chosen as follows. The groups are $G = {\rm SO}(3,1)$. $H = \mathbb{R}^4$, and $L = \mathbb{R}^8(\mathbb{G})$, where $\mathbb{G}$ is the algebra of complex Grassmann numbers. The maps ∂, δ, and the Peiffer lifting are trivial, as before. The action of the group G on H is via vector representation, and on L via spinor representation, in the following way. Denoting the eight generators of the Lie group $\mathbb{R}^8(\mathbb{G})$ as P_α and P^α, where the bispinor index α takes the values $1,\dots,4$, the action $\triangleright$ of G on L is given explicitly as

$$M_{ab} \triangleright P_\alpha = \frac{1}{2}(\sigma_{ab})^\beta{}_\alpha P_\beta\,, \qquad M_{ab} \triangleright P^\alpha = -\frac{1}{2}(\sigma_{ab})^\alpha{}_\beta P^\beta\,, \tag{2.31}$$

where $\sigma_{ab} = \frac{1}{4}[\gamma_a, \gamma_b]$, and γ_a are the usual Dirac matrices. This choice of the 2-crossed module gives rise to the 3-connection $(\alpha\,, \beta\,, \gamma)$, defined as

$$\alpha = \omega^{ab} M_{ab}\,, \qquad \beta = \beta^a P_a\,, \qquad \gamma = \gamma^\alpha P_\alpha + \bar{\gamma}_\alpha P^\alpha\,, \tag{2.32}$$

where the 3-connection 3-forms γ^α and $\bar{\gamma}_\alpha$ should not be confused with the Dirac matrices γ_a due to different types of indices. The 3-curvature $(\mathcal{F}\,, \mathcal{G}\,, \mathcal{H})$ is given as:

$$\begin{aligned}
&\mathcal{F} = R^{ab} M_{ab}\,, \qquad\qquad \mathcal{G} = \nabla \beta^a P_a\,, \\
&\mathcal{H} = \Big({\rm d}\gamma^\alpha + \frac{1}{2}\omega^{ab}(\sigma_{ab})^\alpha{}_\beta \gamma^\beta\Big)P_\alpha + \Big({\rm d}\bar{\gamma}_\alpha - \frac{1}{2}\omega^{ab}\bar{\gamma}_\beta(\sigma_{ab})^\beta{}_\alpha\Big)P^\alpha \equiv (\overset{\rightarrow}{\nabla}\gamma)^\alpha P_\alpha + (\bar{\gamma}\overset{\leftarrow}{\nabla})_\alpha P^\alpha\,.
\end{aligned} \tag{2.33}$$

As in the case of the scalar field, the choice of the group L and action $\triangleright$ of G on L dictates the matter content of the theory and its transformation properties. The group L prescribes that D contains eight independent real anticommuting matter fields as its components. Then, since D is a 0-form and it transforms according to the spinorial representation of ${\rm SO}(3,1)$, these eight real Grassmann-valued fields can be identified with the four complex Dirac bispinor fields, and one can write the corresponding topological $3BF$ action as:

$$S_{3BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla\beta^a + (\bar{\gamma}\overset{\leftarrow}{\nabla})_\alpha \psi^\alpha + \bar{\psi}_\alpha(\overset{\rightarrow}{\nabla}\gamma)^\alpha\,. \tag{2.34}$$

In order to obtain the action that gives us the dynamics of Einstein-Cartan theory of gravity coupled to a Dirac field, we add the following simplicity constraints:

$$\begin{aligned}
S = \int_{\mathcal{M}_4} &B^{ab} \wedge R_{ab} + e_a \wedge \nabla\beta^a + (\bar{\gamma}\overset{\leftarrow}{\nabla})_\alpha \psi^\alpha + \bar{\psi}_\alpha(\overset{\rightarrow}{\nabla}\gamma)^\alpha - \lambda_{ab} \wedge \Big(B^{ab} - \frac{1}{16\pi l_p^2}\varepsilon^{abcd} e_c \wedge e_d\Big) \\
&- \lambda^\alpha \wedge \Big(\bar{\gamma}_\alpha - \frac{i}{6}\varepsilon_{abcd} e^a \wedge e^b \wedge e^c (\bar{\psi}\gamma^d)_\alpha\Big) + \bar{\lambda}_\alpha \wedge \Big(\gamma^\alpha + \frac{i}{6}\varepsilon_{abcd} e^a \wedge e^b \wedge e^c (\gamma^d \psi)^\alpha\Big) \\
&- \frac{1}{12} m\, \bar{\psi}\psi\, \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d + 2\pi i l_p^2\, \bar{\psi}\gamma_5\gamma^a\psi\, \varepsilon_{abcd} e^b \wedge e^c \wedge \beta^d.
\end{aligned} \tag{2.35}$$

The topological sector is in the first row, as well as the gravitational simplicity constraint, the second row contains the new simplicity constraints for the Dirac field, while the third row contains the mass term for the Dirac field and a term that ensures the correct coupling between the torsion and the spin of the Dirac field. Varying the action (2.35), one obtains the following dynamical equations of motion — the equations for ψ and $\bar{\psi}$ which are the standard covariant Dirac equation and its conjugate,

$$(i\gamma^a e^\mu{}_a \overrightarrow{\nabla}_\mu - m)\psi = 0\,, \quad \bar{\psi}(i\overleftarrow{\nabla}_\mu e^\mu{}_a \gamma^a + m) = 0\,, \tag{2.36}$$

and the differential equation of motion for e^a which is the Einstein field equation with a Dirac field source term,

$$R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R = 8\pi l_p^2\, T^{\mu\nu}\,, \quad T^{\mu\nu} \equiv \frac{i}{2}\bar{\psi}\gamma^a \overleftrightarrow{\nabla}^\nu e^\mu{}_a \psi - \frac{1}{2}g^{\mu\nu}\bar{\psi}\Big(i\gamma^a\overleftrightarrow{\nabla}_\rho e^\rho{}_a - 2m\Big)\psi\,, \tag{2.37}$$

where $\overleftrightarrow{\nabla} = \overrightarrow{\nabla} - \overleftarrow{\nabla}$. Moreover, one obtains the desired equation of motion for the torsion,

$$T_a \equiv \nabla e_a = 2\pi l_p^2 s_a\,, \quad s_a = i\varepsilon_{abcd} e^b \wedge e^c \bar{\psi}\gamma_5\gamma^d\psi\,, \tag{2.38}$$

where s_a is the Dirac spin 2-form. The equations of motion (2.36), (2.37), and (2.38) are precisely the equations of motion of the Einstein-Cartan-Dirac theory.

The natural presence of a scalar and Dirac field in the $3BF$ action is an essential property of the specific choices of the 3-group structures in a 4-dimensional spacetime, just like the existence of the tetrad field e^a in the topological $2BF$ action is an essential property of the $2BF$ action and the Poincaré 2-group. In this way, both the scalar field and the Dirac field appear in the topological sector of the action, making the quantization procedure feasible. Similarly, one can introduce Weyl and Majorana fields as well, see [31].

3 A review of 2-groups and 3-groups

As we have seen in the previous section, the gauge symmetry of 3-gauge theory is described by an algebraic structure known as a 3-*group*. In this section, we present the relevant definition of the 3-group, and we briefly explain how this structure is used to equip curves, surfaces, and volumes with holonomies. The results obtained in this section are necessary for the construction of the topological invariant, which will be studied in section IV.

3.1 3-Groups

In the category theory, a 2-group is defined as a 2-category consisting of only one object, where all the morphisms and 2-morphisms are invertible. It has been shown that every strict 2-group is equivalent to a crossed module $(H \xrightarrow{\partial} G\,, \triangleright)$.

A *pre-crossed module* $(H \xrightarrow{\partial} G\,, \triangleright)$ of groups G and H, is given by a group map $\partial : H \to G$, together with a left action $\triangleright$ of G on both groups, by automorphisms, such that the group G acts on itself via conjugation, i.e. , for each $g_1, g_2 \in G$,

$$g_1 \triangleright g_2 = g_1 g_2 g_1^{-1}\,,$$

and for each $h_1\,, h_2 \in H$ and $g \in G$ the following identity holds:

$$g\partial h g^{-1} = \partial(g \triangleright h)\,.$$

In a pre-crossed module the *Peiffer commutator* is defined as:

$$\langle h_1\,, h_2\rangle_{\mathrm{p}} = h_1 h_2 h_1^{-1} \partial(h_1) \rhd h_2^{-1}\,. \tag{3.1}$$

A pre-crossed module is said to be a *crossed module* if all of its Peiffer commutators are trivial, which is to say that the *Peiffer identity* is satisfied:

$$(\partial h_1) \rhd h_2 = h_1 h_2 h_1^{-1}\,. \tag{3.2}$$

Continuing the categorical generalization one step further, one can generalize the notion of a 2-group to the notion of a 3-group. Similar to the definition of a group and a 2-group within the category theory formalism, a 3-group is defined as a 3-category with only one object, where all morphisms, 2-morphisms, and 3-morphisms are invertible. Moreover, in analogy with how a crossed module encodes a strict 2-group, it has been proved that a semistrict 3-group — Gray group is equivalent to a 2-crossed module [42, 46].

A 2-*crossed module* $(L \xrightarrow{\delta} H \xrightarrow{\partial} G,\, \rhd,\, \{\_\,,\,\_\}_{\mathrm{p}})$ is a chain complex of groups, given by three groups G, H, and L, together with maps ∂ and δ,

$$L \xrightarrow{\delta} H \xrightarrow{\partial} G\,,$$

such that $\partial\delta = 1_G$, an action $\rhd$ of the group G on all three groups, and a map $\{\_\,,\_\}_{\mathrm{p}}$ called the *Peiffer lifting*:

$$\{\_\,,\_\}_{\mathrm{p}} : H \times H \to L\,.$$

The maps ∂ and δ, and the Peiffer lifting are G-equivariant, i.e., for each $g \in G$ and $h \in H$

$$g \rhd \partial(h) = \partial(g \rhd h)\,, \qquad g \rhd \delta(l) = \delta(g \rhd l)\,,$$

and for each h_1, $h_2 \in H$ and $g \in G$:

$$g \rhd \{h_1\,, h_2\}_{\mathrm{p}} = \{g \rhd h_1,\, g \rhd h_2\}_{\mathrm{p}}\,.$$

The action of the group G on the groups H and L is a smooth left action by automorphisms, i.e., for each $g, g_1, g_2 \in G,\;\; h_1, h_2 \in H,\;\; l_1, l_2 \in L$ and $k \in H, L$,

$$g_1 \rhd (g_2 \rhd k) = (g_1 g_2) \rhd k\,, \qquad g \rhd (h_1 h_2) = (g \rhd h_1)(g \rhd h_2)\,, \qquad g \rhd (l_1 l_2) = (g \rhd l_1)(g \rhd l_2)\,.$$

The action of the group G on itself is again via conjugation. Further, the following identities are satisfied:

$$\delta(\{h_1, h_2\}_{\mathrm{p}}) = \langle h_1\,, h_2\rangle_{\mathrm{p}}\,, \qquad \forall h_1, h_2 \in H\,; \tag{3.3a}$$

$$[l_1, l_2] = \{\delta(l_1)\,, \delta(l_2)\}_{\mathrm{p}}\,, \qquad \forall l_1\,, l_2 \in L\,, \quad \text{where } [l,k] = lkl^{-1}k^{-1}; \tag{3.3b}$$

$$\{h_1 h_2, h_3\}_{\mathrm{p}} = \{h_1, h_2 h_3 h_2^{-1}\}_{\mathrm{p}} \partial(h_1) \rhd \{h_2, h_3\}_{\mathrm{p}}\,, \qquad \forall h_1, h_2, h_3 \in H\,; \tag{3.3c}$$

$$\{h_1, h_2 h_3\}_{\mathrm{p}} = \{h_1, h_2\}_{\mathrm{p}} \{h_1, h_3\}_{\mathrm{p}} \{\langle h_1, h_3\rangle_{\mathrm{p}}^{-1}\,, \partial(h_1) \rhd h_2\}_{\mathrm{p}}\,, \qquad \forall h_1, h_2, h_3 \in H\,; \tag{3.3d}$$

$$\{\delta(l), h\}_{\mathrm{p}} \{h, \delta(l)\}_{\mathrm{p}} = l(\partial(h) \rhd l^{-1})\,, \qquad \forall h \in H\,, \qquad \forall l \in L\,. \tag{3.3e}$$

In a 2-crossed module the structure $(L \xrightarrow{\delta} H, \triangleright')$ is a crossed module, with action of the group H on the group L defined for each $h \in H$ and $l \in L$ as:

$$h \triangleright' l = l\,\{\delta(l)^{-1},\, h\}_{\mathrm{p}}\,,$$

and it follows that the Peiffer identity is satisfied for each $l_1, l_2 \in L$:

$$\delta(l_1) \triangleright' l_2 = l_1\, l_2\, l_1^{-1}\,.$$

However, the structure $(H \xrightarrow{\partial} G\,, \triangleright)$ in the general case does not form a crossed module, but a pre-crossed module, and for each $h, h' \in H$ the Peiffer commutator does not necessarily vanish.

The following identities hold, for each $h_1, h_2, h_3 \in H$ [42]:

$$\{h_1h_2, h_3\}_{\mathrm{p}} = (h_1 \triangleright' \{h_2, h_3\}_{\mathrm{p}})\{h_1, \partial(h_2) \triangleright h_3\}_{\mathrm{p}}\,, \tag{3.4}$$

$$\{h_1, h_2h_3\}_{\mathrm{p}} = \{h_1, h_2\}_{\mathrm{p}}(\partial(h_1) \triangleright h_2) \triangleright' \{h_1, h_3\}_{\mathrm{p}}\,, \tag{3.5}$$

and are of prime importance for the proof of the Pachner moves invariance. By using the condition (3.3e) of the definition of a 2-crossed module, it follows that for each $h \in H$ and $l \in L$ the following identity holds:

$$\{h, \delta(l)^{-1}\}_{\mathrm{p}} = (h \triangleright' l^{-1})(\partial(h) \triangleright l)\,. \tag{3.6}$$

Moreover, for each $h_1, h_2 \in H$,

$$\{h_1, h_2\}_{\mathrm{p}}^{-1} = h_1 \triangleright' \{h_1^{-1}, \partial(h_1) \triangleright h_2\}_{\mathrm{p}}\,, \tag{3.7}$$

$$\{h_1, h_2\}_{\mathrm{p}}^{-1} = \partial(h_1) \triangleright \{h_1^{-1}, h_1h_2h_1^{-1}\}_{\mathrm{p}}\,, \tag{3.8}$$

$$\{h_1, h_2\}_{\mathrm{p}}^{-1} = (h_1h_2h_1^{-1}) \triangleright' \{h_1, h_2^{-1}\}_{\mathrm{p}}\,, \tag{3.9}$$

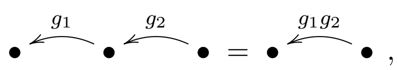
$$\{h_1, h_2\}_{\mathrm{p}}^{-1} = (\partial(h_1) \triangleright h_2) \triangleright' \{h_1, h_2^{-1}\}_{\mathrm{p}}\,. \tag{3.10}$$

A reader interested in more details about 3-groups is referred to [43].

3.2 3-gauge theory

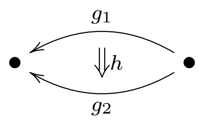
In this subsection, we will describe how the language of 3-gauge theory can be used in order to define compositions of labeled paths, surfaces, and volumes. In a 3-gauge theory, one labels geometric objects at three levels. Curves are labeled by elements of G. Their composition and orientation reversal is defined as in conventional gauge theory. In addition, surfaces are labeled with elements of H, and volumes are labeled with the elements of L. The reader interested in the formulation of a 2-gauge theory is referred to [47].

Curves are labeled with the elements of G, and the elements are composed as in the ordinary gauge theory, i.e. , for each $g_1, g_2 \in G$,



the composition of the elements results in the element $g_1 g_2 \in G$. The orientation of a curve can be reversed if it is labeled by the inverse element g^{-1} instead.

Surfaces are labeled with the elements $h \in H$. For each surface, we choose two reference points on the boundary, and split the boundary into two curves, the source curve labeled with $g_1 \in G$, and the target curve labeled with $g_2 \in G$, as demonstrated in the diagram



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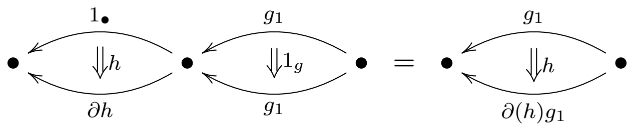
The 2-arrow $h \in H$ maps the curve $g_1 \in G$ to the curve $\partial(h) g_1 \in G$,



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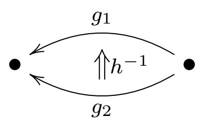
so that the label $h \in H$ of the surface is required to satisfy the following condition:

$$\partial(h) = g_2 g_1^{-1} . \tag{3.11}$$

The orientation of the surface can be reversed and labeled with the inverse element instead,



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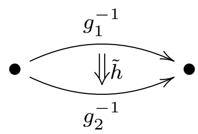
while the orientation reversal of the curves leads to the surface element labeled with $\tilde{h} = g_1^{-1} \triangleright h^{-1}$:



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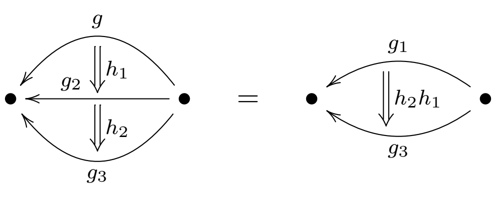
One can now compose 2-morphisms vertically. Let us denote the source and the target of the k-arrow ($k = 1, 2$) of the 2-morphism h as $\partial_k^-(h)$ and $\partial_k^+(h)$, respectively. Then, the vertical composition of 2-morphisms (g_1, h_1) and (g_2, h_2), when they are compatible, i.e., when $\partial_2^+(h_1) = \partial_2^-(h_2)$,

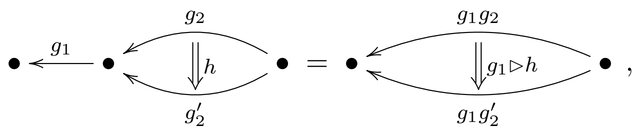


,

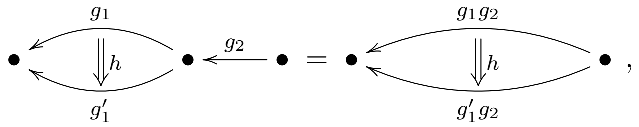
results in a 2-morphism $(g_1, h_2 h_1)$,

$$(g_2, h_2) \#_2 (g_1, h_1) = (g_1, h_2 h_1) . \tag{3.12}$$

An important operation is known as whiskering. One can whisker a 2-morphism h with a morphism g_1 by attaching the whisker g_1 to the surface h from the left, i.e., such that $\partial_1^-(g_1) = \partial_1^+(h)$,

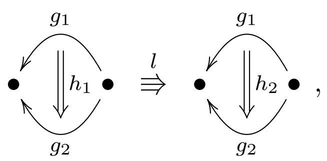


which results in the 2-morphism with the source curve $g_1 g_2$ and target curve $g_1 g_2'$, carrying the label $g_1 \triangleright h$. Similarly, by attaching whisker g_2 to a surface h from the right, i.e. , such that $\partial_1^-(h) = \partial_1^+(g_2)$,



one obtains the 2-morphism with the source curve $g_1 g_2$ and target curve $g_1' g_2$, carrying the label h.

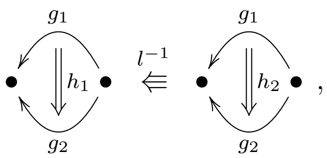
The volumes are labeled with the elements $l \in L$. Let us denote the source and the target of the k-arrow ($k = 1, 2, 3$) of the 3-morphism l as $\partial_k^-(l)$ and $\partial_k^+(l)$, respectively. For each volume, we split the boundary into two surfaces, the source surface labeled with $\partial_3^-(l) = h_1$ and the target surface labeled with $\partial_3^+(l) = h_2$. On the common boundary of the source and target surface, we choose two reference points, and split the boundary into two curves, the source curve labeled with $\partial_2^-(l) = g_1$ and the target curve labeled with $\partial_2^+(l) = g_2$, as demonstrated in the diagram below



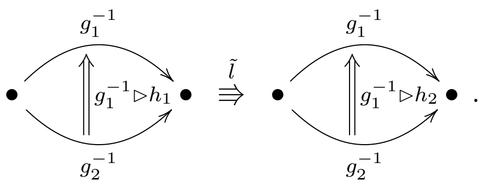
so that the volume label $l \in L$ is required to satisfy the following condition:

$$\delta(l) = h_2 h_1^{-1} . \tag{3.13}$$

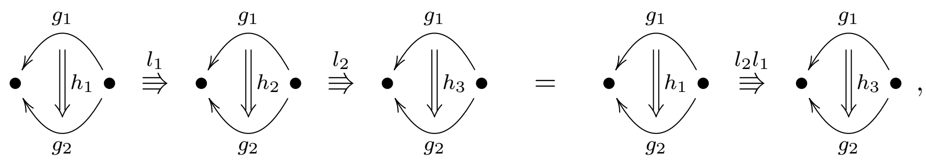
The orientation of the volume can be reversed if one labels it with the inverse element l^{-1}:



while the orientation reversal of the curves and surfaces leads to the surface element labeled with $\tilde{l} = g_1^{-1} \triangleright l$,



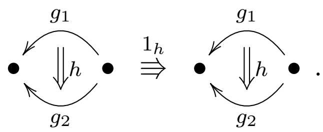
One can compose two 3-morphisms via the *upward composition* (visualizing a third axis, orthogonal to the plane of the paper, as the direction up). The upward composition of 3-morphisms (g_1, h_1, l_1) and (g_1, h_2, l_2), when they are compatible, i.e., when $\partial_3^+(l_1) = \partial_3^-(l_2)$,



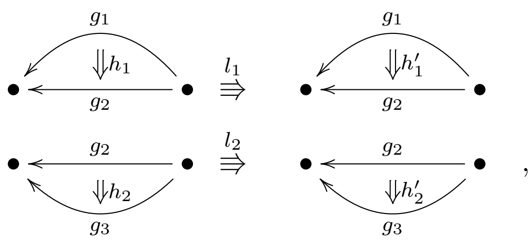
results in a 3-morphism $(g_1, h_1, l_2 l_1)$:

$$(g_1, h_2, l_2) \#_3 (g_1, h_1, l_1) = (g_1, h_1, l_2 l_1) \,. \tag{3.14}$$

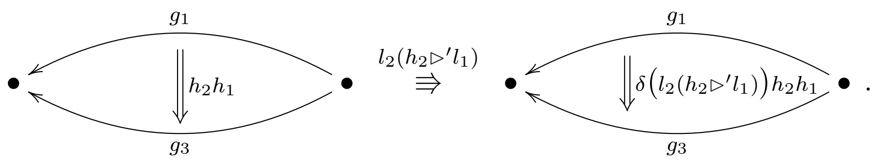
The upward composition of 3-morphisms is associative, and for every $h \in H$ there is a 3-morphism that is an identity for the upward composition of 3-morphisms



The vertical composition of two 3-morphisms (g_1, h_1, l_1) and (g_2, h_2, l_2), when they are compatible, i.e., when $\partial_2^+(l_1) = \partial_2^-(l_2)$,



results in a 3-morphism $(g_1, h_2 h_1, l_2(h_2 \rhd' l_1))$,



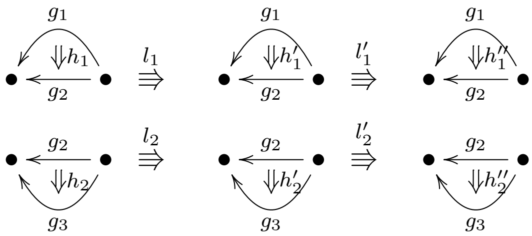
One can write, for (g_1, h_1, l_1) and (g_2, h_2, l_2),

$$(g_2, h_2, l_2) \#_2 (g_1, h_1, l_1) = (g_1, h_2 h_1, l_2(h_2 \rhd' l_1)) \,. \tag{3.15}$$

The vertical composition of 3-morphisms is an associative operation. Composition of 3-morphisms is invariant under the change of order of upward composition and vertical composition of 3-morphisms, i.e.,

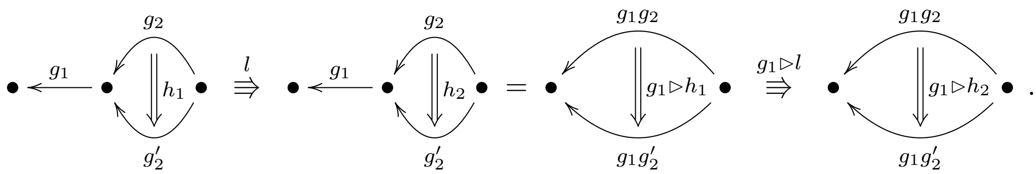
$$\begin{aligned} &((g_2, h_2', l_2') \#_3 (g_2, h_2, l_2)) \#_2 ((g_1, h_1', l_1') \#_3 (g_1, h_1, l_1)) \\ =&((g_2, h_2', l_2') \#_2 (g_1, h_1', l_1')) \#_3 ((g_2, h_2, l_2) \#_2 (g_1, h_1, l_1)) \,, \end{aligned} \tag{3.16}$$

which is demonstrated in the diagram notation, where the diagram



uniquely determines the 3-morphism. The proof of the equation (3.16) is given in the appendix A.

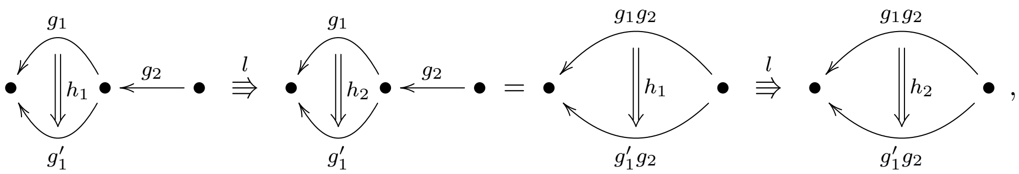
One can whisker the 3-morphisms with morphisms and 2-morphisms. Whiskering of a 3-morphism by a morphism from the left is the composition of a volume $l \in L$ and curve $g_1 \in G$ from the left, when they are compatible, i.e. , when $\partial_1^+(l) = \partial_1^-(g_1)$,



The composition results in a 3-morphism:

$$g_1 \#_1 (g_2, h_1, l) = (g_1g_2, g_1 \triangleright h_1, g_1 \triangleright l)\,. \tag{3.17}$$

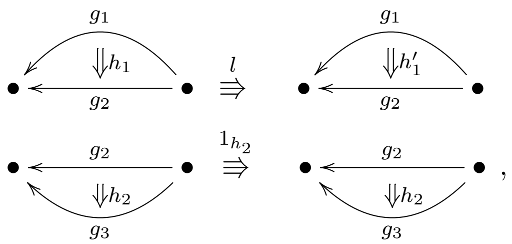
Similarly, one can whisker a 3-morphism by a morphism from the right, when they are compatible, i.e. , $\partial_1^-(l) = \partial_1^+(g_2)$,



which results in the 3-morphism:

$$(g_1, h_1, l) \#_1 g_2 = (g_1g_2, h_1, l)\,. \tag{3.18}$$

Whiskering of a 3-morphism with a 2-morphisms from below, when they are compatible, i.e. , $\partial_2^+(l) = \partial_2^-(h_2)$, is formed as a vertical composition of 3-morphisms (g_1, h_1, l) and $(g_2, h_2, 1_{h_2})$,



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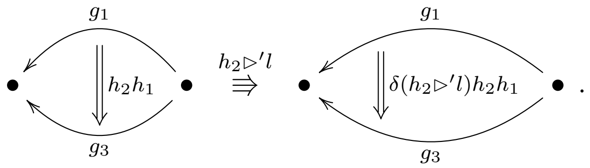
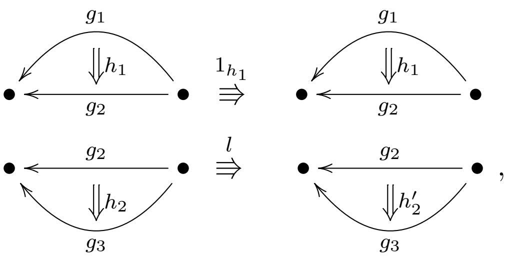
which results in a 3-morphism



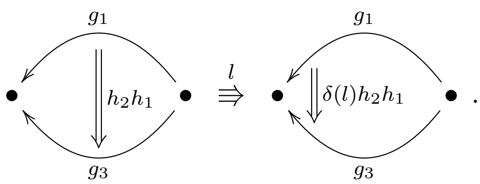
One writes,

$$(g_2, h_2)\#_2(g_1, h_1, l) = (g_1, h_2h_1, h_2 \triangleright' l)\,. \tag{3.19}$$

Whiskering a 3-morphism by 2-morphism from above, when they are compatible, i.e., when $\partial_2^-(l) = \partial_2^+(h_1)$, is formed as a vertical composition of 3-morphisms $(g_1, h_1, 1_{h_1})$ and (g_2, h_2, l),



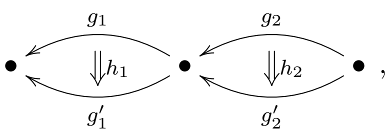
which results in a 3-morphism,



One obtains

$$(g_2, h_2, l)\#_2(g_1, h_1) = (g_1, h_2h_1, l)\,. \tag{3.20}$$

The interchanging 3-arrow is the horizontal composition of two 2-morphisms h_1 and h_2, when they are compatible, i.e., when $\partial_1^-(h_1) = \partial_1^+(h_2)$,

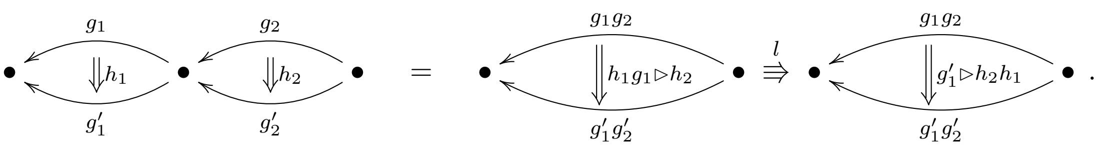


that results in a 3-morphism l, with source surface

$$\partial_3^-(l) = ((g_1, h_1)\#_1 g_2')\#_2(g_1\#_1(g_2, h_2))\,,$$

and target surface

$$\partial_3^+(l) = (g_1'\#_1(g_2, h_2))\#_2((g_1, h_1)\#_1 g_2)\,,$$



One obtains,

$$(g_1, h_1)\#_1(g_2, h_2) = (g_1 g_2, h_1 g_1 \rhd h_2, l)\,, \tag{3.21}$$

where the 3-morphism l is Peiffer lifting $\{h_1, g_1 \rhd h_2\}_{\mathrm{p}}^{-1}$. Using the condition (3.13), one obtains

$$((\partial(h_1)g_1) \rhd h_2)h_1 = \delta(l)h_1(g_1 \rhd h_2)\,, \tag{3.22}$$

and from the definition of the Peiffer commutator, the identity (3.1), and the property (3.3a) of the 2-crossed module, i.e. , $\delta(\{h_1, h_2\}_{\mathrm{p}}) = \langle h_1\,, h_2\rangle_{\mathrm{p}}$, one obtains

$$\delta(l)^{-1} = h_1 g_1 \rhd h_2 h_1^{-1}(\partial(h_1)g_1) \rhd h_2{}^{-1} = \langle h_1, g_1 \rhd h_2\rangle_{\mathrm{p}} = \delta(\{h_1, g_1 \rhd h_2\}_{\mathrm{p}})\,. \tag{3.23}$$

Given any collection of curves, surfaces, and volumes, a configuration of 3-gauge theory is an assignment of elements of G to the curves, elements of H to the surfaces, and elements of L to volumes so that the following conditions hold:

1. For each surface labeled by $h \in H$, one has that $\partial(h) = g_2 g_1^{-1}$ where g_1 and g_2 are the source and target curve, respectively;

2. For each volume labeled by $l \in L$, one has that $\delta(l) = h_2 h_1^{-1}$, where h_1 and h_2 are the source and target surface, respectively;

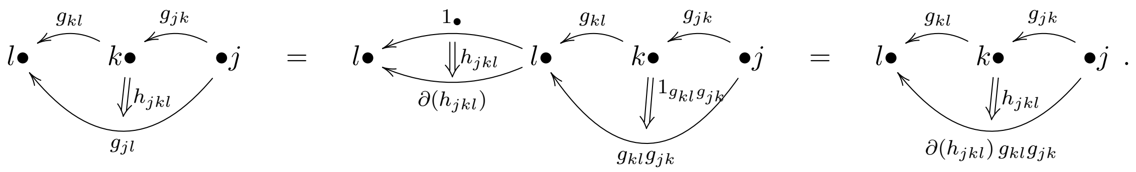
3. For each 4-simplex labeled by $(jk\ell mn) \in \Lambda_4$, the volume holonomy around it is trivial.

The defined configurations can be viewed as the classical configurations of 3-gauge theory or, in a path integral quantum theory, these are the configurations over which one integrates in the path integral.

3.3 Gauge invariant quantities

In subsection 3.2, we have introduced a number of operations by which we can combine labeled paths, surfaces, and volumes, in order to calculate the composition of elementary paths, surfaces, and volumes, to arbitrarily large ones. In this subsection, we will make use of these compositions in order to construct gauge invariant quantities that are associated with closed paths, surfaces, and volumes. In Lemmas 3.1, 3.2, and 3.3, this procedure is used for the boundary path of a triangle, the boundary surface of a tetrahedron, and the boundary volume of the 4-simplex. The result of Lemma 3.1 is already derived for the case of 2-groups and remains unchanged in the 3-gauge theory, see [38]. The higher flatness condition for the boundary surface of a tetrahedron derived in [38], is generalized for the case of 3-groups is Lemma 3.2. One of the main results of the paper is Lemma 3.3 where we derived the higher flatness condition for the boundary volume of the 4-simplex.

Lemma 3.1. Let us consider a triangle, $(jk\ell)$. The edges $(jk)\,, j < k$, are labeled by group elements $g_{jk} \in G$ and the triangle $(jk\ell)\,, j < k < \ell$, by element $h_{jk\ell} \in H$. Consider the diagram (3.24).



(3.24)

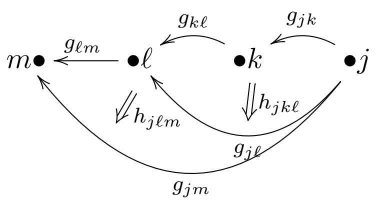
The curve $\gamma_1 = g_{k\ell}g_{jk}$ is the source and the curve $\gamma_2 = g_{j\ell}$ is the target of the surface morphism $\Sigma : \gamma_1 \to \gamma_2$, labeled by the group element $h_{jk\ell}$, i.e.,

$$g_{j\ell} = \partial(h_{jk\ell})g_{k\ell}g_{jk} \,. \tag{3.25}$$

Lemma 3.2. Let us consider a tetrahedron, $(jk\ell m)$. The edges $(jk)\,, j < k$, are labeled by group elements $g_{jk} \in G$ and the triangles $(jk\ell)\,, j < k < \ell$, by elements $h_{jk\ell} \in H$, and the tetrahedron $(jk\ell m)\,, j < k < \ell < m$ by the group element $l_{jk\ell m} \in L$. We have oriented the triangles $(jk\ell)$ so that they have the source is $g_{k\ell}g_{jk}$ and the target is $g_{j\ell}$, i.e. $g_{j\ell} = \partial(h_{jk\ell})g_{k\ell}g_{jk}$.

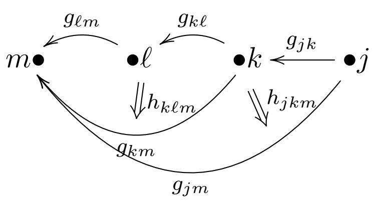
Let us first cut the tetrahedron surface along the edge (jm). This determines the ordering of the vertical composition of the constituent surfaces. One just has to make sure that all surfaces are composable, i.e., they have the suitable reference points and the correct orientation in order to compose them vertically.

Consider the diagram (3.26). We first move the curve from $g_{k\ell}g_{jk}$ to the curve $g_{j\ell}$. At this stage, one cannot compose the result with the triangle $(j\ell m)$, and one first has to whisker it from the left by $g_{\ell m}$. Now the two morphisms are vertically composable, and this moves the curve to g_{jm}. The following 2-morphism is obtained



$$\begin{aligned} &= (g_{\ell m}g_{j\ell}, h_{j\ell m})\#_2(g_{\ell m}\#_1(g_{k\ell}g_{jk}, h_{jk\ell})) \\ &= (g_{\ell m}g_{k\ell}g_{jk}, h_{j\ell m}(g_{\ell m} \triangleright h_{jk\ell}))\,. \end{aligned} \tag{3.26}$$

Let us then consider the diagram (3.27). We first move the curve from $g_{\ell m}g_{k\ell}$ to the curve g_{km}. At this stage, one cannot compose the result with the triangle (jkm), and one first has to whisker it from the right by g_{jk}. Now the two morphisms are vertically composable, and this moves the curve to g_{jm}. The following 2-morphism is obtained



$$\begin{aligned} &= (g_{km}g_{jk}, h_{jkm})\#_2((g_{\ell m}g_{k\ell}, h_{k\ell m})\#_1 g_{jk}) \\ &= (g_{\ell m}g_{k\ell}g_{jk}, h_{jkm}h_{k\ell m})\,. \end{aligned} \tag{3.27}$$

The two surfaces have the same source and target, $\Sigma_1 : g_{\ell m}g_{k\ell}g_{jk} \to g_{jm}$ and $\Sigma_2 : g_{\ell m}g_{k\ell}g_{jk} \to g_{jm}$. Now, transition from the surface shown on the diagram (3.26) to the surface shown on the diagram (3.27) is given by the volume morphism $\mathcal{V} : \Sigma_1 \to \Sigma_2$

determined by the group element $l_{jk\ell m}$, i.e.,

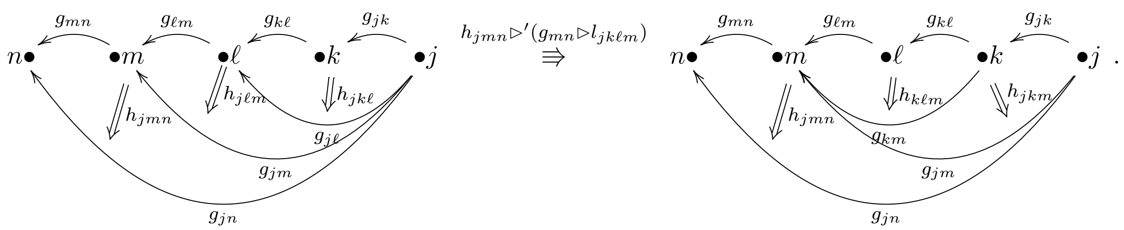
$$(g_{\ell m}g_{k\ell}g_{jk}, h_{jkm}h_{k\ell m}) = (g_{\ell m}g_{k\ell}g_{jk}, \delta(l_{jk\ell m})h_{j\ell m}(g_{\ell m} \rhd h_{jk\ell}))\,, \tag{3.28}$$

that gives the relation,

$$h_{jkm}h_{k\ell m} = \delta(l_{jk\ell m})h_{j\ell m}(g_{\ell m} \rhd h_{jk\ell})\,. \tag{3.29}$$

Lemma 3.3. Let us consider a 4-simplex, $(jk\ell mn)$. The edges $(jk)\,, j < k$, are labeled by group elements $g_{jk} \in G$, the triangles $(jk\ell)\,, j < k < \ell$, by elements $h_{jk\ell} \in H$, and the tetrahedrons $(jk\ell m)\,, j < k < \ell < m$, by the group element $l_{jk\ell m} \in L$. We have oriented the triangles $(jk\ell)$ so that the source curve is $g_{k\ell}g_{jk}$ and the target curve is $g_{j\ell}$, i.e., $g_{j\ell} = \partial(h_{jk\ell})g_{k\ell}g_{jk}$, and the tetrahedrons $(jk\ell m)$ so that the source surface is $h_{j\ell m}(g_{\ell m} \rhd h_{jk\ell})$ and the target surface is $h_{jkm}h_{k\ell m}$, i.e., $h_{jkm}h_{k\ell m} = \delta(l_{jk\ell m})h_{j\ell m}(g_{\ell m} \rhd h_{jk\ell})$.

Let us first cut the 4-simplex volume along the surface $h_{jmn}g_{mn} \rhd (h_{j\ell m}g_{\ell m} \rhd h_{jk\ell})$. This surface determines the ordering of the vertical composition of the constituent volumes. We have to make sure that all volumes are composable, i.e., they have the suitable reference points and the correct orientation in order to compose them vertically. First, let us consider the diagram (3.30). We first move the surface from $h_{j\ell m}g_{\ell m} \rhd h_{jk\ell}$ to surface $h_{jkm}h_{k\ell m}$ with the 3-arrow $l_{jk\ell m}$. To compose the resulting 3-morphism with the surface h_{jmn} one must first whisker it from the left with g_{mn}. The obtained 3-morphism $(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, g_{mn} \rhd (h_{j\ell m}g_{\ell m} \rhd h_{jk\ell}), g_{mn} \rhd l_{jk\ell m})$ can be whiskered from below with the 2-morphism $(g_{mn}g_{jm}, h_{jmn})$, and the resulting 3-morphism is $(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{jmn}g_{mn} \rhd (h_{j\ell m}g_{\ell m} \rhd h_{jk\ell}), h_{jmn} \rhd' (g_{mn} \rhd l_{jk\ell m}))$, with the source surface $h_{jmn}g_{mn} \rhd (h_{j\ell m}g_{\ell m} \rhd h_{jk\ell})$ and the target surface $h_{jmn}g_{mn} \rhd (h_{jkm}h_{k\ell m})$,



(3.30)

Let us move the surface to $h_{jkn}h_{kmn}g_{m\ell} \rhd h_{k\ell m}$, see diagram (3.31). To do that, we consider the 3-morphism $(g_{mn}g_{km}g_{jk}, h_{jmn}g_{mn} \rhd h_{jkm}, l_{jkmn})$ with the source surface $h_{jmn}g_{mn} \rhd h_{jkm}$ and target surface $h_{jkn}h_{kmn}$. This 3-morphism can be whiskered from above with the 2-morphism $(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, g_{mn} \rhd h_{k\ell m})$, and the obtained 3-morphism is $(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{jmn}\, g_{mn} \rhd (h_{jkm}h_{k\ell m}), l_{jkmn})$, with the source surface $h_{jmn}g_{mn} \rhd (h_{jkm}h_{k\ell m})$ and target surface

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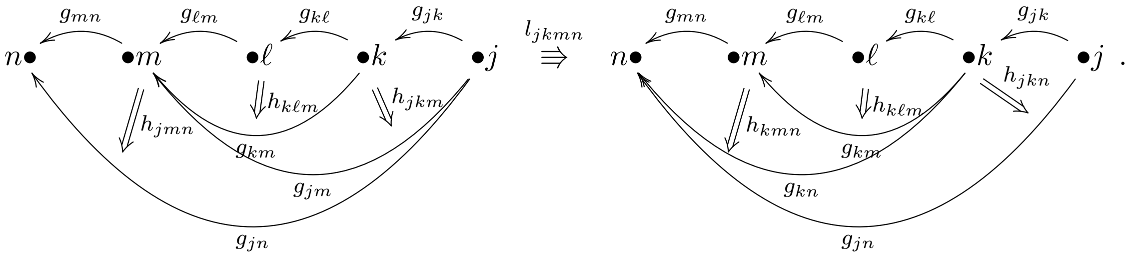
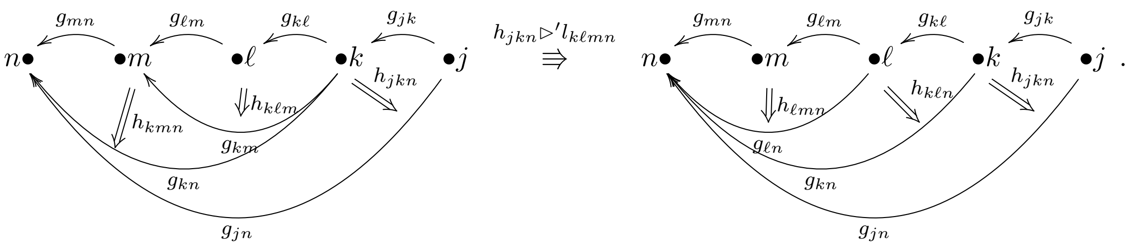
$h_{jkn} h_{kmn} g_{mn} \rhd h_{k\ell m}$,



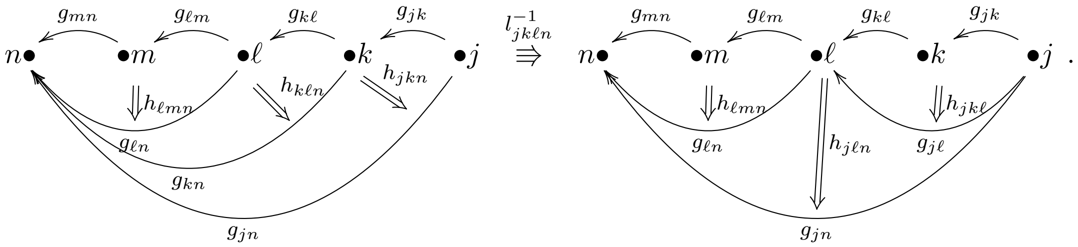
(3.31)

Next, we want to move the surface $h_{jkn} h_{kmn} g_{mn} \rhd h_{k\ell m}$ to surface $h_{jkn} h_{k\ell n} h_{\ell mn}$, as shown on the diagram (3.32). We whisker the 3-morphism $(g_{mn} g_{\ell m} g_{k\ell}, h_{kmn} g_{mn} \rhd h_{k\ell m}, l_{k\ell mn})$, with the source surface $h_{kmn} g_{mn} \rhd h_{k\ell m}$ and target surface $h_{k\ell n} h_{\ell mn}$, with the morphism g_{jk} from the right, obtaining the 3-morphism $(g_{mn} g_{\ell m} g_{k\ell} g_{jk}, h_{kmn} g_{mn} \rhd h_{k\ell m}, l_{k\ell mn})$. Now, we whisker this 3-morphism with the 2-morphism $(g_{kn} g_{jk}, h_{jkn})$ from below, and we obtain the 3-morphism $(g_{mn} g_{\ell m} g_{k\ell} g_{jk}, h_{jkn} h_{kmn} g_{mn} \rhd h_{k\ell m}, h_{jkn} \rhd' l_{k\ell mn})$,



(3.32)

The mapping of the surface $h_{jkn} h_{k\ell n} h_{\ell mn}$ to the surface $h_{j\ell n} g_{\ell n} \rhd h_{jk\ell} h_{\ell mn}$ in shown on the diagram (3.33). The 3-morphism with the appropriate source and target is constructed by whiskering the 3-morphism $(g_{\ell n} g_{k\ell} g_{jk}, h_{jkn} h_{k\ell n}, l^{-1}_{jk\ell n})$ with 2-morphism $(g_{mn} g_{\ell m} g_{k\ell} g_{jk}, h_{\ell mn})$ from above. The obtained 3-morphism is $(g_{mn} g_{\ell m} g_{k\ell} g_{jk}, h_{jkn} h_{k\ell n} h_{\ell mn}, l^{-1}_{jk\ell n})$,



(3.33)

Next we map the surface $h_{j\ell n} g_{\ell n} \rhd h_{jk\ell} h_{\ell mn}$ to the surface $h_{j\ell n} h_{\ell mn} (g_{mn} g_{\ell m}) \rhd h_{jk\ell}$, see the diagram (3.34). We use the inverse interchanging 2-arrow composition to map the surface $g_{\ell n} \rhd h_{jk\ell} h_{\ell mn}$ to the surface $h_{\ell mn} (g_{mn} g_{\ell m}) \rhd h_{jk\ell}$, resulting in the 3-morphism $(g_{mn} g_{\ell m} g_{k\ell} g_{jk}, g_{\ell n} \rhd h_{jk\ell} h_{\ell mn}, \{h_{\ell mn}, (g_{mn} g_{\ell m}) \rhd h_{jk\ell}\}_{\mathrm{p}})$. Next, we whisker the obtained 3-morphism with the 2-morphism $(g_{\ell n} g_{j\ell}, h_{j\ell n})$ from below. The obtained 3-morphism with the appropriate source and target surfaces is $(g_{mn} g_{\ell m} g_{k\ell} g_{jk}, h_{j\ell n} g_{\ell n} \rhd h_{jk\ell} h_{\ell mn}, h_{j\ell n} \rhd'$

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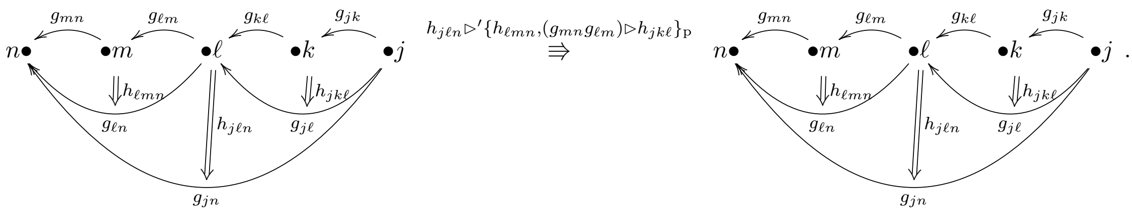
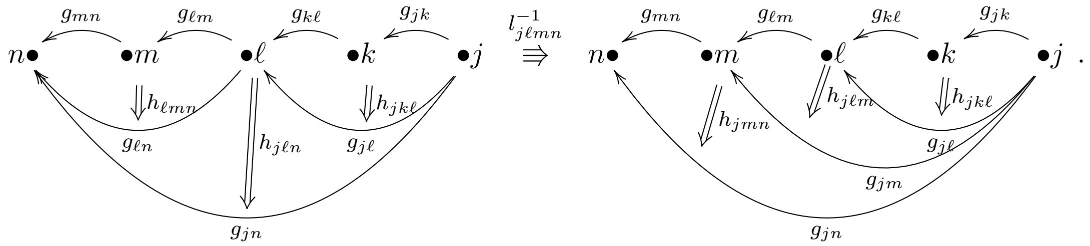
$\{h_{\ell mn}, (g_{mn}g_{\ell m}) \triangleright h_{jk\ell}\}_{\mathrm{p}}),$



(3.34)

Finally, we construct the 3-morphism that maps the surface $h_{j\ell n}h_{\ell mn}(g_{mn}g_{\ell m}) \triangleright h_{jk\ell}$ to the starting surface $h_{jmn}g_{mn} \triangleright (h_{j\ell m}g_{\ell m} \triangleright h_{jk\ell})$. To obtain the 3-morphism with the appropriate source and target surfaces we first move the surface $h_{j\ell n}h_{\ell mn}$ to the surface $h_{jmn}g_{mn} \triangleright h_{j\ell m}$ with the 3-arrow $(g_{mn}g_{\ell m}g_{j\ell}, h_{j\ell n}h_{\ell mn}, l^{-1}_{j\ell mn})$. Next, we whisker the 3-morphism $(g_{mn}g_{\ell m}g_{j\ell}, h_{j\ell n}h_{\ell mn}, l^{-1}_{j\ell mn})$ with the 2-morphism $(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, (g_{mn}g_{\ell m}) \triangleright h_{jk\ell})$ from above. The obtained 3-morphism $(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{j\ell n}h_{\ell mn}(g_{mn}g_{\ell m}) \triangleright h_{jk\ell}, l^{-1}_{j\ell mn})$ moves the surface to the starting surface, as shown on the diagram (3.35),



(3.35)

After the upward composition of the 3-morphisms given by the diagrams (3.30)–(3.35), the obtained 3-morphism is:

$$
\begin{aligned}
&(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{j\ell n}h_{\ell mn}(g_{mn}g_{\ell m}) \triangleright h_{jk\ell}, l^{-1}_{j\ell mn})\#_3 \\
&(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, g_{\ell n} \triangleright h_{jk\ell}h_{\ell mn}, h_{j\ell n} \triangleright' \{h_{\ell mn}, (g_{mn}g_{\ell m}) \triangleright h_{jk\ell}\}_{\mathrm{p}})\#_3 \\
&(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{jkn}h_{k\ell n}h_{\ell mn}, l^{-1}_{jk\ell n})\#_3 \\
&(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{jkn}h_{kmn}g_{m\ell} \triangleright h_{k\ell m}, h_{jkn} \triangleright' l_{jkmn})\#_3 \\
&(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{jmn}g_{mn} \triangleright (h_{jkm}h_{k\ell m}), l_{jkmn})\#_3 \\
&(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{jmn}g_{mn} \triangleright (h_{j\ell m}g_{\ell m} \triangleright h_{jk\ell}), h_{jmn} \triangleright' (g_{mn} \triangleright l_{jk\ell m})) \\
= &(g_{mn}g_{\ell m}g_{k\ell}g_{jk}, h_{jmn}g_{mn} \triangleright (h_{j\ell m}g_{\ell m} \triangleright h_{jk\ell}), l^{-1}_{j\ell mn}\, h_{j\ell n} \triangleright' \{h_{\ell mn}, (g_{mn}g_{\ell m}) \triangleright h_{jk\ell}\}_{\mathrm{p}} \\
&l^{-1}_{jk\ell n}(h_{jkn} \triangleright' l_{k\ell mn})l_{jkmn}h_{jmn} \triangleright' (g_{mn} \triangleright l_{jk\ell m}))\,.
\end{aligned}
\tag{3.36}
$$

The obtained 3-morphism is the identity morphism with source and target surface $\mathcal{V}_1 = \mathcal{V}_2 = h_{jmn}g_{mn} \triangleright (h_{j\ell m}g_{\ell m} \triangleright h_{jk\ell})$, i.e.,

$$
l^{-1}_{j\ell mn}\, h_{j\ell n} \triangleright' \{h_{\ell mn}, (g_{mn}g_{\ell m}) \triangleright h_{jk\ell}\}_{\mathrm{p}}\, l^{-1}_{jk\ell n}(h_{jkn} \triangleright' l_{k\ell mn})l_{jkmn}h_{jmn} \triangleright' (g_{mn} \triangleright l_{jk\ell m}) = e\,. \tag{3.37}
$$

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4 Quantization of the topological 3BF theory

In conventional BF theory, one chooses the action in such a way that the theory does not depend on any background field, but only the spacetime manifold. The classical field equations of the theory require the gauge connection to be flat, i.e., in terms of the holonomy variables, that any null-homotopic closed curve corresponds to the identity of the gauge group. In the framework of higher gauge theory, specifically 2-gauge theory, one generalizes this idea by imposing the *higher flatness condition* requiring that the surface holonomy around the boundary 2-sphere of any 3-ball be trivial instead. One can continue further categorical generalization by choosing a 3-group structure to describe the gauge symmetry of the theory, and formulate a 3BF theory whose equations of motion impose a higher flatness condition for a 3-curvature $(\mathcal{F},\mathcal{G},\mathcal{H})$. In this section, a combinatorial description of such model for any triangulation of any smooth manifold of dimension $d=4$ is presented. This model coincides with Porter's abstract definition of a TQFT [33] for $d=4$ and $n=3$, which is itself a generalization of Yetter's work [48, 49].

Let us show how to construct a state sum model from the classical action (2.8) by the usual heuristic spinfoam quantization procedure. We consider the path integral for the action S_{3BF},

$$Z=\int \mathcal{D}\alpha\,\mathcal{D}\beta\,\mathcal{D}\gamma\,\mathcal{D}B\,\mathcal{D}C\,\mathcal{D}D\,\exp\left(i\int_{M_4}\langle B\wedge\mathcal{F}\rangle_{\mathfrak{g}}+\langle C\wedge\mathcal{G}\rangle_{\mathfrak{h}}+\langle D\wedge\mathcal{H}\rangle_{\mathfrak{l}}\right). \tag{4.1}$$

The formal integration over the Lagrange multipliers B, C, and D leads to:

$$Z=\mathcal{N}\int \mathcal{D}\alpha\,\mathcal{D}\beta\,\mathcal{D}\gamma\;\delta(\mathcal{F})\delta(\mathcal{G})\delta(\mathcal{H})\,. \tag{4.2}$$

Similarly to conventional gauge theory, the connection 1-form $\alpha\in\mathcal{A}^1(\mathcal{M}_4,\mathfrak{g})$ is discretized by colouring the edges $\epsilon=(jk)\in\Lambda_1$ of the triangulation with group elements $g_\epsilon\in G$. The connection 2-form $\beta\in\mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{h})$ is represented by group elements $h_\Delta\in H$ coloring the triangles $\Delta=(jk\ell)\in\Lambda_2$. The connection 3-form $\gamma\in\mathcal{A}^3(\mathcal{M}_4\,,\mathfrak{l})$ is represented by group elements $l_\tau\in L$ coloring the tetrahedrons $\tau=(jk\ell m)\in\Lambda_3$.

The path integral measures of (4.1) are discretized by replacing

$$\int\mathcal{D}\alpha\quad\mapsto\quad\prod_{(jk)\in\Lambda_1}\int_G dg_{jk}\,, \tag{4.3}$$

$$\int\mathcal{D}\beta\quad\mapsto\quad\prod_{(jk\ell)\in\Lambda_2}\int_H dh_{jk\ell}, \tag{4.4}$$

$$\int\mathcal{D}\gamma\quad\mapsto\quad\prod_{(jk\ell m)\in\Lambda_3}\int_L dl_{jk\ell m}\,, \tag{4.5}$$

where dg_{jk}, $dh_{jk\ell}$, and $dl_{jk\ell m}$ denote integration with respect to the Haar measures of G, H, and L, respectively. The vanishing fake curvature condition is discretized on each triangle $(jkl)\in\Lambda_2$ by discretizing $\delta(\mathcal{F})$. When passing from a smooth manifold to its triangulation, the δ distribution is defined over the appropriate set of simplices as follows,

$$\delta(\mathcal{F})=\prod_{(jk\ell)\in\Lambda_2}\delta_G(g_{jk\ell})\,, \tag{4.6}$$

where for each $(jkl) \in \Lambda_2$ the δ-function $\delta_G(g_{jkl})$ is given by:

$$\delta_G(g_{jk\ell}) = \delta_G\big(\partial(h_{jk\ell})\, g_{k\ell}\, g_{jk}\, g_{j\ell}^{-1}\big)\,. \tag{4.7}$$

Similarly, on the triangulated manifold the condition $\delta(\mathcal{G})$ on the fake curvature 3-form reads

$$\delta(\mathcal{G}) = \prod_{(jk\ell m)\in\Lambda_3} \delta_H(h_{jk\ell m})\,, \tag{4.8}$$

where for every tetrahedron $(jk\ell m) \in \Lambda_3$ one has:

$$\delta_H(h_{jk\ell m}) = \delta_H\big(\delta(l_{jk\ell m}) h_{j\ell m}\,(g_{\ell m} \rhd h_{jk\ell})\, h_{k\ell m}^{-1}\, h_{jkm}^{-1}\big)\,. \tag{4.9}$$

Finally, the condition $\delta(\mathcal{H})$ is discretized as

$$\delta(\mathcal{H}) = \prod_{(jk\ell mn)\in\Lambda_4} \delta_L(l_{jk\ell mn})\,, \tag{4.10}$$

where for each 4-simplex $(jk\ell mn) \in \Lambda_4$ one has:

$$\delta_L(l_{jk\ell mn}) = \delta_L\big(l_{j\ell mn}^{-1}\, h_{j\ell n} \rhd' \{h_{\ell mn}, (g_{mn} g_{\ell m}) \rhd h_{jk\ell}\}_{\mathrm{p}}\, l_{jk\ell n}^{-1} (h_{jkn} \rhd' l_{k\ell mn}) l_{jkmn} h_{jmn} \rhd' (g_{mn} \rhd l_{jk\ell m})\big)\,. \tag{4.11}$$

The identities (4.7), (4.9), and (4.11) are the results of Lemmas 3.1, 3.2, and 3.3, respectively.

After substituting the expressions for discretized measures (4.3)–(4.5) and δ-functions (4.6), (4.8), and (4.10) into the equation (4.2) one obtains:

$$Z = \mathcal{N} \prod_{(jk)\in\Lambda_1} \int_G dg_{jk} \prod_{(jk\ell)\in\Lambda_2} \int_H dh_{jk\ell} \prod_{(jk\ell m)\in\Lambda_3} \int_L dl_{jk\ell m} \Big(\prod_{(jk\ell)\in\Lambda_2} \delta_G(g_{jk\ell})\Big)\Big(\prod_{(jk\ell m)\in\Lambda_3} \delta_H(h_{jk\ell m})\Big)\Big(\prod_{(jk\ell mn)\in\Lambda_4} \delta_L(l_{jk\ell mn})\Big). \tag{4.12}$$

By inserting (4.7), (4.9), and (4.11) into (4.12), we obtain an explicit expression for the state sum over a given triangulation of the manifold $\mathcal{M}_4$. This expression can be made independent of the triangulation if one appropriately chooses the constant factor $\mathcal{N}$, obtained after the integration over the Lagrange multipliers B, C, and D. This is done by requiring that the state sum is invariant under the Pachner moves, which leads us to the appropriate form of the constant factor $\mathcal{N}$, as given by the definition 4.1.

Definition 4.1. Let $\mathcal{M}_4$ be a compact and oriented combinatorial d-manifold, $d = 4$, and $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \rhd\,, \{\_\,,\_\}_{\mathrm{pf}})$ be a 2-crossed module. The state sum of *topological higher gauge theory* is defined by

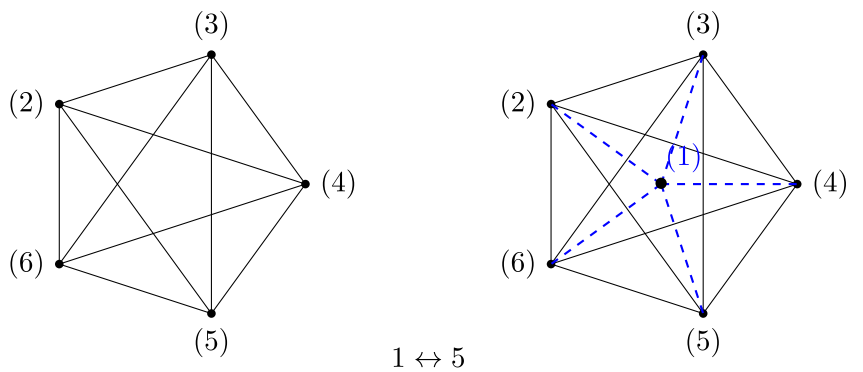
$$\begin{aligned} Z = {} & |G|^{-|\Lambda_0|+|\Lambda_1|-|\Lambda_2|} |H|^{|\Lambda_0|-|\Lambda_1|+|\Lambda_2|-|\Lambda_3|}\, |L|^{-|\Lambda_0|+|\Lambda_1|-|\Lambda_2|+|\Lambda_3|-|\Lambda_4|} \\ & \times \Big(\textstyle\prod_{(jk)\in\Lambda_1} \int_G dg_{jk}\Big) \Big(\prod_{(jk\ell)\in\Lambda_2} \int_H dh_{jk\ell}\Big) \Big(\prod_{(jk\ell m)\in\Lambda_3} \int_L dl_{jk\ell m}\Big) \\ & \times \Big(\textstyle\prod_{(jk\ell)\in\Lambda_2} \delta_G\big(\partial(h_{jk\ell})\, g_{k\ell}\, g_{jk}\, g_{j\ell}^{-1}\big)\Big) \Big(\prod_{(jk\ell m)\in\Lambda_3} \delta_H\big(\delta(l_{jk\ell m}) h_{j\ell m}\,(g_{\ell m} \rhd h_{jk\ell})\, h_{k\ell m}^{-1}\, h_{jkm}^{-1}\big)\Big) \\ & \times \Big(\textstyle\prod_{(jk\ell mn)\in\Lambda_4} \delta_L\big(l_{j\ell mn}^{-1}\, h_{j\ell n} \rhd' \{h_{\ell mn}, (g_{mn} g_{\ell m}) \rhd h_{jk\ell}\}_{\mathrm{p}}\, l_{jk\ell n}^{-1} (h_{jkn} \rhd' l_{k\ell mn}) l_{jkmn} h_{jmn} \rhd' (g_{mn} \rhd l_{jk\ell m})\big)\Big)\,. \end{aligned} \tag{4.13}$$

Here we integrate over $g_{jk} \in G$ for every edge $(jk) \in \Lambda_1$, over $h_{jk\ell} \in H$ for every triangle $(jk\ell) \in \Lambda_2$ and over l_{jklm} for every tetrahedron $(jk\ell m) \in \Lambda_3$. The δ-distributions under the integral impose the following conditions. First, the condition that $\partial(h_{jk\ell})\, g_{k\ell}\, g_{jk} = g_{j\ell}$ for each triangle $(jk\ell) \in \Lambda_2$, i.e., that each surface label $h_{jk\ell}$ has got the appropriate source and target, see Lemma 3.1. Second, the condition that $h_{jkm}\, h_{k\ell m} = \delta(l_{jk\ell m}) h_{j\ell m}\, (g_{\ell m} \triangleright h_{jk\ell})$ for each tetrahedron $(jk\ell m) \in \Lambda_3$, i.e., that each volume label $l_{jk\ell m}$ has got the appropriate source and target, see Lemma 3.2. Finally, the condition that the volume holonomy around every 4-simplex $(jk\ell mn) \in \Lambda_4$ is trivial, i.e., that $l^{-1}_{j\ell mn}\, h_{j\ell n} \triangleright' \{h_{\ell mn}, (g_{mn} g_{\ell m}) \triangleright h_{jk\ell}\}_{\mathrm{p}}\, l^{-1}_{jk\ell n} (h_{jkn} \triangleright' l_{k\ell mn}) l_{jkmn} h_{jmn} \triangleright' (g_{mn} \triangleright l_{jk\ell m})$ is equal to the neutral element of the group L for each 4-simplex $(jk\ell mn) \in \Lambda_4$, see Lemma 3.3.

Theorem 4.2. Let $\mathcal{M}_4$ be a closed and oriented combinatorial 4-manifold and $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \triangleright\,, \{\_\,,\_\}_{\mathrm{pf}})$ be a 2-crossed module. The state sum (4.13) is invariant under Pachner moves.

The statements of Pachner move invariance are formulated in the following subsections, while corresponding proofs are given in the appendix B.

4.1 Pachner move $1 \leftrightarrow 5$



$1 \leftrightarrow 5$

Let us verify that the state sum (4.13) is invariant under $1-5$ Pachner move. Since the partition function is independent of the total order of vertices, let us fix the ordering and verify the move in only one case. Let us denote the vertices of the 4-simplex on the left hand side of the $1-5$ Pachner move as (23456). Then, adding a vertex 1 on the right hand side of the Pachner move one obtains five 4-simplices $M_4 = \{(13456), (12456), (12356), (12346), (12345)\}$. On the r.h.s. there are tetrahedrons $M_3 = \{(1234), (1235), (1236), (1245), (1246), (1256), (1345), (1346), (1356), (1456)\}$, triangles $(jk\ell) \in M_2 = \{(123), (124), (125), (126), (134), (135), (136), (145), (146), (156)\}$, edges $(jk) \in M_1 = \{(12), (13), (14), (15), (16)\}$ and vertices $(j) \in M_0 = \{(1)\}$. All other simplices are present on both sides of the move.

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	$\vert\Lambda_0\vert$	$\vert\Lambda_1\vert$	$\vert\Lambda_2\vert$	$\vert\Lambda_3\vert$	$\vert\Lambda_4\vert$
l.h.s.	5	10	10	5	1
r.h.s.	6	15	20	15	5

Table 1. Number of vertices $|\Lambda_0|$, edges $|\Lambda_1|$, triangles $|\Lambda_2|$, tetrahedrons $|\Lambda_3|$, and 4-simplices $|\Lambda_4|$ on both sides of the $1 \leftrightarrow 5$ move.

If the $1-5$ Pachner move does not change the state sum (4.13), then the state sum of the right hand side,

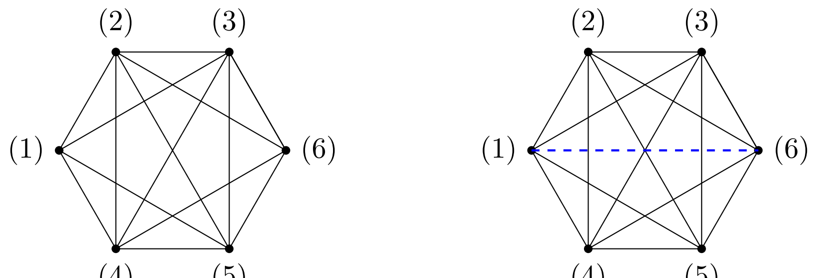
$$Z^{1\leftrightarrow 5}_{\text{right}} = |G|^{-11}|H|^{-4}|L|^{-1}\int_{G^5}\prod_{(jk)\in M_1} dg_{jk}\int_{H^{10}}\prod_{(jk\ell)\in M_2} dh_{jk\ell}\int_{L^{10}}\prod_{(jklm)\in M_3} dl_{jklm} \cdot\left(\prod_{(jk\ell)\in M_2}\delta_G(g_{jk\ell})\right)\left(\prod_{(jk\ell m)\in M_3}\delta_H(h_{jk\ell m})\right)\left(\prod_{(jk\ell mn)\in M_4}\delta_L(l_{jk\ell mn})\right)Z_{\text{remainder}}\,, \tag{4.14}$$

should be equal to the state sum of the left hand side,

$$Z^{1\leftrightarrow 5}_{\text{left}} = |G|^{-5}|H|^{0}|L|^{-1}\delta_L(l_{23456})Z_{\text{remainder}}\,. \tag{4.15}$$

Here, the prefactors $|G|^{-|\Lambda_0|+|\Lambda_1|-|\Lambda_2|}$, $|H|^{|\Lambda_0|-|\Lambda_1|+|\Lambda_2|-|\Lambda_3|}$, and $|L|^{-|\Lambda_0|+|\Lambda_1|-|\Lambda_2|+|\Lambda_3|-|\Lambda_4|}$ are $|G|^{-11}|H|^{-4}|L|^{-1}$ on the r.h.s. and $|G|^{-5}|H|^{0}|L|^{-1}$ on the l.h.s., as obtained by counting the numbers of the k-simplices on both sides of the $1-5$ move, shown in the table 1. The $Z_{\text{remainder}}$ denotes the part of the state sum that is the same on both sides of the move, and thus irrelevant for the proof of invariance. The proof that $Z_{\text{left}} = Z_{\text{right}}$ is given in the appendix B.

4.2 Pachner move $2 \leftrightarrow 4$



$2 \leftrightarrow 4$

In order to verify the state sum (4.13) invariance under $2-4$ Pachner move, we order the vertices in such a way that on the l.h.s. of the move we have two 4-simplices $M_4^{\text{left}} = \{(23456),(12345)\}$, while on the r.h.s. we have four 4-simplices $M_4^{\text{right}} = \{(12346),(12356),(12456),(13456)\}$. On the l.h.s. we have one tetrahedron $M_3^{\text{left}} = \{(2345)\}$, whereas on the r.h.s. there are six tetrahedrons $M_3^{\text{right}} = \{(1236),(1246),(1256),(1346),(1356),(1456)\}$. All other tetrahedrons appear on both sides of the move. On the r.h.s. there are triangles $M_2^{\text{right}} = \{(126),(136),(146),(156)\}$, and one edge $M_1^{\text{right}} = \{(16)\}$, while the rest of the triangles and edges appear on both sides of the move.

	$\lvert\Lambda_0\rvert$	$\lvert\Lambda_1\rvert$	$\lvert\Lambda_2\rvert$	$\lvert\Lambda_3\rvert$	$\lvert\Lambda_4\rvert$
l.h.s.	6	14	16	9	2
r.h.s.	6	15	20	14	4

Table 2. Number of vertices $|\Lambda_0|$, edges $|\Lambda_1|$, triangles $|\Lambda_2|$, tetrahedrons $|\Lambda_3|$, and 4-simplices $|\Lambda_4|$ on both sides of the $2 \leftrightarrow 4$ move.

On the l.h.s. there is the state sum,

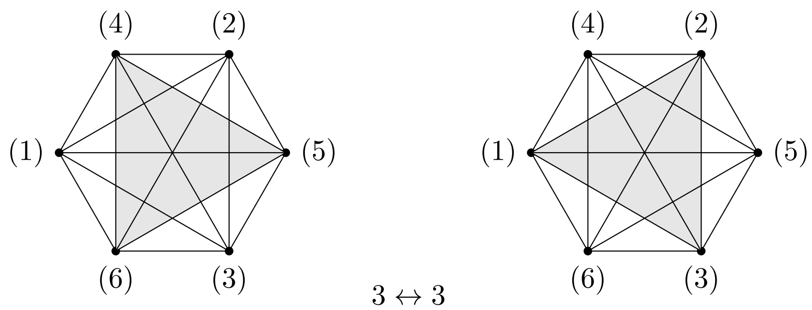
$$Z^{2\leftrightarrow 4}_{\text{left}} = |G|^{-8}|H|^{-1}|L|^{-1} \int_L dl_{2345}\delta_H(h_{2345})\left(\prod_{(jk\ell mn)\in M_4^{\text{left}}} \delta_L(l_{jk\ell mn})\right) Z_{\text{remainder}}\,, \quad (4.16)$$

whereas on the r.h.s. the state sum reads:

$$Z^{2\leftrightarrow 4}_{\text{right}} = |G|^{-11}|H|^{-3}|L|^{-1} \int_G dg_{16} \int_{H^4} dh_{126}dh_{136}dh_{146}dh_{156} \int_L dl_{1236}dl_{1246}dl_{1256}dl_{1346}dl_{1356}dl_{1456}$$
$$\left(\prod_{(jk\ell)\in M_2^{\text{right}}} \delta_G(g_{jk\ell})\right)\left(\prod_{(jk\ell m)\in M_3^{\text{right}}} \delta_H(h_{jk\ell m})\right)\left(\prod_{(jk\ell mn)\in M_4^{\text{right}}} \delta_L(l_{jk\ell mn})\right) Z_{\text{remainder}}. \quad (4.17)$$

Here the prefactors $|G|^{-8}|H|^{-1}|L|^{-1}$ on the l.h.s. and $|G|^{-11}|H|^{-3}|L|^{-1}$ on the r.h.s. are obtained by counting the numbers of k-simplices on both sides of the $2-4$ move, as shown in the table 2. The term $Z_{\text{remainder}}$ denotes the part of the state sum that is identical on both sides of the move, as before. The proof that $Z_{\text{left}} = Z_{\text{right}}$ is given in the appendix B.

4.3 Pachner move $3 \leftrightarrow 3$



$3 \leftrightarrow 3$

In order to verify the state sum invariance under $3-3$ Pachner move, we order the vertices in such a way that on the l.h.s. of the $3-3$ move, we have three 4-simplices $M_4^{\text{left}} = \{(23456), (13456), (12456)\}$, whereas on the r.h.s. we have the 4-simplices $M_4^{\text{right}} = \{(12356), (12346), (12345)\}$. On the l.h.s. there are tetrahedrons $M_3^{\text{left}} = \{(1456), (2456), (3456)\}$, and on the r.h.s. $M_3^{\text{right}} = \{(1234), (1235), (1236)\}$. One notices that the six tetrahedrons form the common boundary of both sides of the move, whereas on each side there are three tetrahedrons shared by two 4-simplices. On the l.h.s. one has the triangle $M_2^{\text{left}} = \{(456)\}$ and on the r.h.s. the triangle $M_3^{\text{right}} = \{(123)\}$. All other triangles appear on both sides of the move.

Therefore on the l.h.s. there is the state sum,

$$
\begin{aligned}
Z^{3\leftrightarrow 3}_{\text{left}} = \int_H dh_{456} \int_{L^3} & dl_{1456} dl_{2456} dl_{3456} \delta_G(g_{456})\, \delta_H(h_{3456}) \delta_H(h_{2456}) \delta_H(h_{1456}) \\
& \delta_L(l_{23456}) \delta_L(l_{13456}) \delta_L(l_{12456}) Z_{\text{remainder}}\,,
\end{aligned} \tag{4.18}
$$

whereas on the r.h.s. the state sum reads

$$
\begin{aligned}
Z^{3\leftrightarrow 3}_{\text{right}} = \int_H dh_{123} \int_{L^3} & dl_{1234} dl_{1235} dl_{1236} \delta_G(g_{123})\, \delta_H(h_{1234}) \delta_H(h_{1235}) \delta_H(h_{1236}) \\
& \delta_L(l_{12356}) \delta_L(l_{12346}) \delta_L(l_{12345}) Z_{\text{remainder}}\,.
\end{aligned} \tag{4.19}
$$

The numbers of k-simplices agree on both sides of the $3-3$ move for all k, and the prefactors play no role in this case, therefore they are part of the $Z_{\text{remainder}}$. The proof that $Z_{\text{left}} = Z_{\text{right}}$ is given in the appendix B.

We obtain that the state sum given by the definition 4.1 is invariant under all three Pachner moves, and thus independent of triangulation of the underlying 4-dimensional manifold (see appendix B for the proof).

5 Conclusions

Let us summarize the results of the paper. In section 2 we reviewed the pure the constrained $2BF$ actions describing the Yang-Mills field and Einstein-Cartan gravity, and constrained $3BF$ actions describing the Klein-Gordon and Dirac fields coupled to Yang-Mills fields and gravity in the standard way. In section 3, we reviewed the relevant algebraic tools involved in the description of higher gauge theory, 2-crossed modules, and 3-gauge theory and generalized the integral picture of an ordinary gauge theory to a 3-gauge theory that involves curves, surfaces, and volumes labeled with elements of non-Abelian groups. We have also proved three key results, stated in Lemmas 3.1, 3.2, and 3.3, which are crucial for the construction of the invariant state sum. In section 4, we have presented the two main results of the paper. First, we constructed a triangulation independent state sum Z of a topological higher gauge theory for a general 3-group and a 4-dimensional spacetime manifold $\mathcal{M}_4$. Second, we proved the theorem that the constructed state sum is indeed independent of the choice of triangulation, i.e., that it is a genuine topological invariant.

The constructed state sum coincides with Porter's TQFT [33, 34] for $d = 4$ and $n = 3$. The proof that the state sum is invariant under the local changes of triangulation called the Pachner moves and thus independent of the chosen triangulation is presented in appendix B. It is obtained that the state sum is invariant under all five different Pachner moves: the $3-3$ move, $4-2$ move, and $5-1$ move, and their inverses. The state sum constructed this way can be thought of as a combinatorial construction of a topological quantum field theory (TQFT) in the sense of Atiyah's axioms, a topic that is beyond the scope of this paper and will be studied in a future work.

In order to finish the second step of the spinfoam quantization procedure, however, the generalizations of the Peter-Weyl and Plancharel theorems to 2-groups and 3-groups are required, which so far represent open problems. Namely, these theorems should provide

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a decomposition of a function on a 3-group into a sum over the corresponding irreducible representations of a 3-group. In this way, the spectrum of labels for the simplices, i.e. , the domain of values of the fields living on the simplices of the triangulation, would be specified. Nonetheless, one can still try to guess the irreducible representations of 3-groups, as was done for example in the case of 2-groups in the spincube model of quantum gravity [30], or obtain the state sum using other techniques, see for example [50–52]).

However, if one wants to describe a real physical theory, i.e. , the theory which contains local propagating degrees of freedom, one needs to construct the nontopological state sum, with the non-trivial dynamics. To do so, once the topological state sum is constructed, the final third step of the spinfoam quantization procedure is to impose the constraints that deform the topological theory into a realistic theory of gravity coupled to matter fields (as defined in [31]) at the quantum level. We leave the construction of the constrained state sum model for future work.

In addition to the above topics, there are also many other possible applications of the invariant state sum, both in physics and mathematics.

Acknowledgments

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A Proof of the invariance identity

Let us prove the identity (3.16). Using the definitions of the upward composition (3.14) and the vertical composition (3.15) of the 3-morphisms, one obtains that the left-hand side of the equation (3.16) is equal to:

$$\begin{aligned}((g_2,h'_2,l'_2)\#_3(g_2,h_2,l_2))\#_2((g_1,h'_1,l'_1)\#_3(g_1,h_1,l_1)) &= (g_2,h_2,l'_2l_2)\#_2(g_1,h_1,l'_1l_1)\\ &= (g_1,h_2h_1,l'_2l_2\,h_2\rhd'(l'_1l_1))\,.\end{aligned} \tag{A.1}$$

The right-hand side of the equation (3.16) is equal to:

$$\begin{aligned}((g_2,h'_2,l'_2)\#_2(g_1,h'_1,l'_1))\#_3((g_2,h_2,l_2)\#_2(g_1,h_1,l_1)) &= (g_1,h'_2h'_1,l'_2h'_2\rhd' l'_1)\#_3(g_1,h_2h_1,l_2h_2\rhd' l_1)\\ &= (g_1,h_2h_1,l'_2\,h'_2\rhd' l'_1\,l_2\,h_2\rhd' l_1)\quad (h'_2=\delta(l_2)h_2)\\ &= (g_1,h_2h_1,l'_2\,(\delta(l_2)h_2)\rhd' l'_1\,l_2\,h_2\rhd' l_1)\quad \text{eq. (A.3)}\\ &= (g_1,h_2h_1,l'_2\,\delta(l_2)\rhd'(h_2\rhd' l'_1)\,l_2\,h_2\rhd' l_1)\quad \text{(Peiffer identity)}\\ &= (g_1,h_2h_1,l'_2\,l_2(h_2\rhd' l'_1)l_2^{-1}\,l_2\,h_2\rhd' l_1)\quad (l_2^{-1}l_2=e)\\ &= (g_1,h_2h_1,l'_2\,l_2h_2\rhd' l'_1\,h_2\rhd' l_1)\quad \text{eq. (A.4)}\\ &= (g_1,h_2h_1,l'_2\,l_2h_2\rhd'(l'_1l_1))\,,\end{aligned} \tag{A.2}$$

where in the third and sixth line we use the identities

$$(h_1h_2) \rhd' l = h_1 \rhd' (h_2 \rhd' l), \qquad \forall h_1,h_2 \in H, \qquad \forall l \in L\,, \tag{A.3}$$

$$h \rhd' (l_1l_2) = h \rhd' l_1 \; h \rhd' l_2, \qquad \forall h \in H, \qquad \forall l_1,l_2 \in L\,. \tag{A.4}$$

This proves the equation (3.16).

B Proof of Pachner move invariance

In this section, a self contained proof in terms of Pachner moves that the partition function (4.13) is independent of the chosen triangulation is presented.

B.1 Pachner move $1 \leftrightarrow 5$

On the *left hand side of the move* there is the integrand $\delta_L(l_{23456})$:

$$\delta_L(l_{23456}) = \delta_L(l_{2346}{}^{-1}(h_{236} \rhd' l_{3456})l_{2356}h_{256} \rhd' (g_{56} \rhd l_{2345})l_{2456}{}^{-1}h_{246} \rhd' \{h_{456},(g_{56}g_{45}) \rhd h_{234}\}_{\mathrm{p}}). \tag{B.1}$$

Let us examine the *right hand side of the move*, given by the equation (4.14). First, one integrates out g_{12} using $\delta_G(g_{123})$, g_{13} using $\delta_G(g_{134})$, g_{14} using $\delta_G(g_{145})$, and g_{15} using $\delta_G(g_{156})$, and obtains:

$$\begin{aligned}
g_{12} &= g_{23}^{-1}\,\partial(h_{123})^{-1}\,g_{13}\,,\\
g_{13} &= g_{34}^{-1}\,\partial(h_{134})^{-1}\,g_{14}\,,\\
g_{14} &= g_{45}^{-1}\,\partial(h_{145})^{-1}\,g_{15}\,,\\
g_{15} &= g_{56}^{-1}\,\partial(h_{156})^{-1}\,g_{16}\,.
\end{aligned} \tag{B.2}$$

One integrates out h_{123} using $\delta_H(h_{1234})$, h_{124} using $\delta_H(h_{1245})$, h_{125} using $\delta_H(h_{1256})$, h_{134} using $\delta_H(h_{1345})$, h_{135} using $\delta_H(h_{1356})$, and h_{145} using $\delta_H(h_{1456})$, and obtains:

$$\begin{aligned}
h_{123} &= g_{34}^{-1} \rhd h_{134}^{-1}\, g_{34}^{-1} \rhd \delta(l_{1234})^{-1}\; g_{34}^{-1} \rhd h_{124}\; g_{34}^{-1} \rhd h_{234}\,,\\
h_{124} &= g_{45}^{-1} \rhd h_{145}^{-1}\, g_{45}^{-1} \rhd \delta(l_{1245})^{-1}\; g_{45}^{-1} \rhd h_{125}\; g_{45}^{-1} \rhd h_{245}\,,\\
h_{125} &= g_{56}^{-1} \rhd h_{156}^{-1}\, g_{56}^{-1} \rhd \delta(l_{1256})^{-1}\; g_{56}^{-1} \rhd h_{126}\; g_{56}^{-1} \rhd h_{256}\,,\\
h_{134} &= g_{45}^{-1} \rhd h_{145}^{-1}\, g_{45}^{-1} \rhd \delta(l_{1345})^{-1}\; g_{45}^{-1} \rhd h_{135}\; g_{45}^{-1} \rhd h_{345}\,,\\
h_{135} &= g_{56}^{-1} \rhd h_{156}^{-1}\, g_{56}^{-1} \rhd \delta(l_{1356})^{-1}\; g_{56}^{-1} \rhd h_{136}\; g_{56}^{-1} \rhd h_{356}\,,\\
h_{145} &= g_{56}^{-1} \rhd h_{156}^{-1}\, g_{56}^{-1} \rhd \delta(l_{1456})^{-1}\; g_{56}^{-1} \rhd h_{146}\; g_{56}^{-1} \rhd h_{456}\,.
\end{aligned} \tag{B.3}$$

The δ-functions on the group G now read $\delta_G(e)^6$. Let us show this. First, for $\delta_G(g_{124})$ one obtains

$$\begin{aligned}
\delta_G(g_{124}) &= \delta_G\Big(\partial(h_{124})\,g_{24}\,g_{12}\,g_{14}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{124})\,g_{24}\,g_{23}^{-1}\,\partial(h_{123})^{-1}\,g_{13}\,g_{14}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{124})\,g_{24}\,g_{23}^{-1}\,g_{34}^{-1}\,\partial(h_{234})^{-1}\partial(h_{124})^{-1}\partial(h_{134})\,g_{34}\,g_{13}\,g_{14}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{124})\,g_{24}\,g_{23}^{-1}\,g_{34}^{-1}\,(g_{34}\,g_{23}^{-1}\,g_{24}^{-1})\,\partial(h_{124})^{-1}\,e\Big)\\
&= \delta_G(e)\,,
\end{aligned} \tag{B.4}$$

Next, for δ-function $\delta_G(g_{125})$ one obtains,

$$\begin{aligned}
\delta_G(g_{125}) &= \delta_G\Big(\partial(h_{125})\, g_{25}\, g_{12}\, g_{15}^{-1}\Big)\,,\\
&= \delta_G\Big(\partial(h_{125})\, g_{25}\, g_{23}^{-1}\, \partial(h_{123})^{-1}\, g_{13}\, g_{15}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{125})\, g_{25}\, g_{23}^{-1}\, g_{34}^{-1}\, \partial(h_{234})^{-1}\partial(h_{124})^{-1}\partial(h_{134})\, g_{34}\, g_{13}\, g_{15}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{125})\, g_{25}\, g_{23}^{-1}\, g_{34}^{-1}\, \partial(h_{234})^{-1} g_{45}^{-1}(\partial(h_{245})^{-1}\partial(h_{125})^{-1}\partial(h_{145}))\, g_{45} g_{14}\, g_{15}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{125})\, g_{25}\, g_{23}^{-1}\, g_{34}^{-1}\, (g_{34}\, g_{23}^{-1}\, g_{24}^{-1}) g_{45}^{-1}(g_{45}\, g_{24}^{-1}\, g_{25}^{-1})\partial(h_{125})^{-1} e\Big)\\
&= \delta_G(e)\,.
\end{aligned} \tag{B.5}$$

Similarly, $\delta_G(g_{126})$ becomes

$$\begin{aligned}
\delta_G(g_{126}) &= \delta_G(\partial(h_{126}) g_{26} g_{12} g_{16}^{-1})\\
&= \delta_G(\partial(h_{126}) g_{26} g_{23}^{-1} \partial(h_{123})^{-1} g_{13} g_{16}^{-1})\\
&= \delta_G(\partial(h_{126}) g_{26} g_{23}^{-1} g_{34}^{-1} \partial(h_{234})^{-1} \partial(h_{124})^{-1} \partial(h_{134}) g_{34} g_{13} g_{16}^{-1})\\
&= \delta_G(\partial(h_{126}) g_{26} g_{23}^{-1} g_{34}^{-1} \partial(h_{234})^{-1} g_{45}^{-1} (\partial(h_{245})^{-1} \partial(h_{125})^{-1} \partial(h_{145})) g_{45} \partial(h_{134}) g_{34} g_{13} g_{16}^{-1})\\
&= \delta_G(\partial(h_{126}) g_{26} g_{23}^{-1} g_{34}^{-1} \partial(h_{234})^{-1} g_{45}^{-1} (\partial(h_{245})^{-1} g_{56}^{-1} \partial(h_{256})^{-1} \partial(h_{126})^{-1} \partial(h_{156}) g_{56}\\
&\quad \partial(h_{145})) g_{45} g_{14} g_{16}^{-1})\\
&= \delta_G(\partial(h_{126}) g_{26} g_{23}^{-1} g_{34}^{-1} (g_{34} g_{23}^{-1} g_{24}^{-1}) g_{45}^{-1} (g_{45} g_{24}^{-1} g_{25}^{-1}) g_{56}^{-1} (g_{56} g_{25}^{-1} g_{26}^{-1}) \partial(h_{126})^{-1}\\
&\quad (g_{16} g_{15}^{-1} g_{56}^{-1}) g_{56} g_{15} g_{16}^{-1})\\
&= \delta_G(e),
\end{aligned} \tag{B.6}$$

and $\delta_G(g_{135})$ now reads,

$$\begin{aligned}
\delta_G(g_{135}) &= \delta_G\Big(\partial(h_{135})\, g_{35}\, g_{13}\, g_{15}^{-1}\Big)\,,\\
&= \delta_G\Big(\partial(h_{135})\, g_{35}\, g_{34}^{-1}\, \partial(h_{134})^{-1}\, g_{14}\, g_{15}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{135})\, g_{35}\, g_{34}^{-1}\, g_{45}^{-1}\, \partial(h_{345})^{-1}\partial(h_{135})^{-1}\partial(h_{145})\, g_{45}\, g_{14}\, g_{15}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{135})\, g_{35}\, g_{34}^{-1}\, g_{45}^{-1}\, \partial(h_{345})^{-1}\partial(h_{135})^{-1}\, \partial(h_{145})\, g_{45}\, g_{45}^{-1}\, \partial(h_{145})^{-1}\, g_{15}\, g_{15}^{-1}\Big)\\
&= \delta_G\Big(\partial(h_{135})\, g_{35}\, g_{34}^{-1}\, g_{45}^{-1}\, (g_{45}\, g_{34}^{-1}\, g_{35}^{-1})\partial(h_{135})^{-1}\Big)\\
&= \delta_G(e)\,,
\end{aligned} \tag{B.7}$$

while $\delta_G(g_{136})$ reads:

$$
\begin{aligned}
\delta_G(g_{136}) &= \delta_G(\partial(h_{136})\, g_{36}\, g_{13}\, g_{16}^{-1}) \\
&= \delta_G(\partial(h_{136})\, g_{36}\, g_{34}^{-1}\, \partial(h_{134})^{-1}\, g_{14}\, g_{16}^{-1}) \\
&= \delta_G(\partial(h_{136})\, g_{36}\, g_{34}^{-1}\, g_{45}^{-1}\, \partial(h_{345})^{-1}\partial(h_{135})^{-1}\partial(h_{145})\, g_{45}\, g_{14}\, g_{16}^{-1}) \\
&= \delta_G(\partial(h_{136})\, g_{36}\, g_{34}^{-1}\, g_{45}^{-1}\, \partial(h_{345})^{-1} g_{56}^{-1}(\partial(h_{356})^{-1}\partial(h_{136})^{-1}\partial(h_{156}))\, g_{56}\partial(h_{145})\, g_{45}\, g_{14}\, g_{16}^{-1}) \\
&= \delta_G(\partial(h_{136})\, g_{36}\, g_{34}^{-1}\, g_{45}^{-1}\, (g_{45}\, g_{34}^{-1}\, g_{35}^{-1}) g_{56}^{-1}(g_{56}\, g_{35}^{-1}\, g_{36}^{-1})\partial(h_{136})^{-1} e) \\
&= \delta_G(e)\,.
\end{aligned} \tag{B.8}
$$

Finally, the δ-function $\delta_G(g_{146})$ reads:

$$
\begin{aligned}
\delta_G(g_{146}) &= \delta_G\Big(\partial(h_{146})\, g_{46}\, g_{14}\, g_{16}^{-1}\Big) \\
&= \delta_G\Big(\partial(h_{146})\, g_{46}\, (g_{45}^{-1}\, \partial(h_{145})^{-1}\, g_{15})\, g_{16}^{-1}\Big) \\
&= \delta_G\Big(\partial(h_{146})\, g_{46}\, g_{45}^{-1}\, \partial(h_{145})^{-1}\, (g_{56}^{-1}\, \partial(h_{156})^{-1}\, g_{16})\, g_{16}^{-1}\Big) \\
&= \delta_G\Big(\partial(h_{146})\, g_{46}\, g_{45}^{-1}\, g_{56}^{-1}\partial(h_{456})^{-1}\partial(h_{146})^{-1}\partial(h_{156}) g_{56}\, (g_{56}^{-1}\, \partial(h_{156})^{-1}\, g_{16})\, g_{16}^{-1}\Big) \\
&= \delta_G(e)\,.
\end{aligned} \tag{B.9}
$$

Next, one integrates out l_{1235} using $\delta_L(l_{12345})$, l_{1236} using $\delta_L(l_{12346})$, l_{1246} using $\delta_L(l_{12456})$, and l_{1346} using $\delta_L(l_{13456})$, and obtains

$$l_{1235} = (h_{125} \rhd' l_{2345}) l_{1245} h_{145} \rhd' (g_{45} \rhd l_{1234}) l_{1345}^{-1}\, h_{135} \rhd' \{h_{345}, (g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}\,, \tag{B.10}$$

$$l_{1236} = (h_{126} \rhd' l_{2346}) l_{1246} h_{146} \rhd' (g_{46} \rhd l_{1234}) l_{1346}^{-1}\, h_{136} \rhd' \{h_{346}, (g_{46} g_{34}) \rhd h_{123}\}_{\mathrm{p}}\,, \tag{B.11}$$

$$l_{1246} = (h_{126} \rhd' l_{2456}) l_{1256} h_{156} \rhd' (g_{56} \rhd l_{1245}) {l_{1456}}^{-1}\, h_{146} \rhd' \{h_{456}, (g_{56} g_{45}) \rhd h_{124}\}_{\mathrm{p}}\,, \tag{B.12}$$

$$l_{1346} = (h_{136} \rhd' l_{3456}) l_{1356} h_{156} \rhd' (g_{56} \rhd l_{1345}) {l_{1456}}^{-1}\, h_{146} \rhd' \{h_{456}, (g_{56} g_{45}) \rhd h_{134}\}_{\mathrm{p}}\,. \tag{B.13}$$

Let us now show that the remaining δ-functions on the group H equal $\delta_H(e)^4$. First, $\delta_H(h_{1235})$ becomes:

$$
\begin{aligned}
\delta_H(h_{1235}) =& \delta_H(\delta(l_{1235}) h_{135} (g_{35} \rhd h_{123}) h_{235}^{-1} h_{125}^{-1}) \\
=& \delta_H\Big(\delta((h_{125} \rhd' l_{2345}) l_{1245} h_{145} \rhd' (g_{45} \rhd l_{1234}) l_{1345}^{-1} h_{135} \rhd' \{h_{345}, (g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}) h_{135} (g_{35} \rhd h_{123}) h_{235}^{-1} h_{125}^{-1}\Big) \\
=& \delta_H\Big((h_{125} \delta(l_{2345}) h_{125}^{-1} \delta(l_{1245}) h_{145} (g_{45} \rhd \delta(l_{1234})) h_{145}^{-1} \delta(l_{1345})^{-1} h_{135} \delta(\{h_{345}, (g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}) h_{135}^{-1}) \\
& h_{135} (g_{35} \rhd h_{123}) h_{235}^{-1} h_{125}^{-1}\Big) \\
=& \delta_H\Big(h_{235} h_{345} (g_{45} \rhd h_{234}^{-1}) h_{245}^{-1} h_{125}^{-1} h_{125} h_{245} (g_{45} \rhd h_{124}^{-1}) h_{145}^{-1} h_{145} (g_{45} \rhd (h_{124} h_{234} (g_{34} \rhd h_{123}^{-1}) h_{134}^{-1})) \\
& h_{145}^{-1} (h_{145} (g_{45} \rhd h_{134}) h_{345}^{-1} h_{135}^{-1}) h_{135} \delta(\{h_{345}, (g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}) h_{135}^{-1} h_{135} (g_{35} \rhd h_{123}) h_{235}^{-1}\Big) \\
=& \delta_H(h_{345} ((g_{45} g_{34}) \rhd h_{123}^{-1}) h_{345}^{-1} \delta(\{h_{345}, (g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}) (g_{35} \rhd h_{123}).
\end{aligned} \tag{B.14}
$$

Here, one uses the following identity

$$\delta\{h_1\,, h_2\}_{\mathrm{p}} (\partial(h_1) \rhd h_2) h_1 h_2^{-1} h_1^{-1} = e\,. \tag{B.15}$$

Substituting $g_{35} = \partial(h_{345})g_{45}g_{34}$, and applying the (B.15) identity for $h_1 = h_{345}$ and $h_2 = (g_{45}g_{34}) \triangleright h_{123}$, one obtains

$$\delta_H(h_{1235}) = \delta_H(e). \tag{B.16}$$

Similarly, one obtains for $\delta_H(h_{1236})$:

$$\begin{aligned}
\delta_H(h_{1236}) =& \delta_H(\delta(l_{1236})h_{136}(g_{36}\triangleright h_{123})h_{236}^{-1}h_{126}^{-1}) \\
=& \delta_H\Big(\delta((h_{126}\triangleright' l_{2346})l_{1246}h_{146}\triangleright'(g_{46}\triangleright l_{1236}l_{1346}^{-1}h_{136}\triangleright'\{h_{346},(g_{46}g_{34})\triangleright h_{123}\}_{\mathrm{p}})h_{136}(g_{36}\triangleright h_{123})h_{236}^{-1}h_{126}^{-1}\Big) \\
=& \delta_H\Big((h_{126}\delta(l_{2346})h_{126}^{-1}\delta(l_{1246})h_{146}(g_{46}\triangleright\delta(l_{1234}))h_{146}^{-1}\delta(l_{1346})^{-1}h_{136}\delta(\{h_{346},(g_{46}g_{34})\triangleright h_{123}\}_{\mathrm{p}})h_{136}^{-1}) \\
& h_{136}(g_{36}\triangleright h_{123})h_{236}^{-1}h_{126}^{-1}\Big) \\
=& \delta_H\Big(h_{236}h_{346}(g_{46}\triangleright h_{234}^{-1})h_{246}^{-1}h_{126}^{-1}h_{126}h_{246}(g_{46}\triangleright h_{124}^{-1})h_{146}^{-1}h_{146}(g_{46}\triangleright(h_{124}h_{234}(g_{34}\triangleright h_{123}^{-1})h_{134}^{-1})) \\
& h_{146}^{-1}(h_{146}(g_{46}\triangleright h_{134})h_{346}^{-1}h_{136}^{-1})h_{136}\delta(\{h_{346},(g_{46}g_{34})\triangleright h_{123}\}_{\mathrm{p}})h_{136}^{-1}h_{136}(g_{36}\triangleright h_{123})h_{236}^{-1}\Big) \\
=& \delta_H(h_{346}((g_{46}g_{34})\triangleright h_{123}^{-1})h_{346}^{-1}\delta(\{h_{346},(g_{46}g_{34})\triangleright h_{123}\}_{\mathrm{p}})(g_{36}\triangleright h_{123}).
\end{aligned} \tag{B.17}$$

Substituting $g_{36} = \partial(h_{346})g_{46}g_{34}$, and applying the (B.15) identity for $h_1 = h_{346}$ and $h_2 = (g_{46}g_{34}) \triangleright h_{123}$, one obtains

$$\delta_H(h_{1236}) = \delta_H(e)\,. \tag{B.18}$$

Similarly, one obtains that $\delta_H(h_{1246}) = \delta_H(h_{1346}) = \delta_H(e)$. The remaining δ-function on the group L $\delta_L(l_{12356})$ reads:

$$\delta_L(l_{12356}) = \delta_L\big({l_{1236}}^{-1}(h_{126}\triangleright' l_{2356})l_{1256}h_{156}\triangleright'(g_{56}\triangleright l_{1235}){l_{1356}}^{-1}h_{136}\triangleright'\{h_{356},(g_{56}g_{35})\triangleright h_{123}\}_{\mathrm{p}}\big)\,. \tag{B.19}$$

After substituting the equations (B.10), (B.11), (B.12), and (B.13), one obtains:

$$\begin{aligned}
&\delta_L(l_{12356}) = \delta_L\Big(h_{136}\triangleright'\{h_{346},(g_{46}g_{34})\triangleright h_{123}\}_{\mathrm{p}}^{-1}(h_{136}\triangleright' l_{3456})l_{1356}h_{156}\triangleright'(g_{56}\triangleright l_{1345}){l_{1456}}^{-1} \\
&h_{146}\triangleright'\{h_{456},(g_{56}g_{45})\triangleright h_{134}\}_{\mathrm{p}}h_{146}\triangleright'(g_{46}\triangleright l_{1234})^{-1}h_{146}\triangleright'\{h_{456},(g_{56}g_{45})\triangleright h_{124}\}_{\mathrm{p}}^{-1}l_{1456} \\
&h_{156}\triangleright'(g_{56}\triangleright l_{1245})^{-1}l_{1256}^{-1}(h_{126}\triangleright' l_{2456})^{-1}(h_{126}\triangleright' {l_{2346}}^{-1})(h_{126}\triangleright' l_{2356})l_{1256} \\
&h_{156}\triangleright'(g_{56}\triangleright((h_{125}\triangleright' l_{2345})l_{1245}h_{145}\triangleright'(g_{45}\triangleright l_{1234})l_{1345}^{-1}h_{135}\triangleright'\{h_{345},(g_{45}g_{34})\triangleright h_{123}\}_{\mathrm{p}})) \\
&{l_{1356}}^{-1}h_{136}\triangleright'\{h_{356},(g_{56}g_{35})\triangleright h_{123}\}_{\mathrm{p}}\Big)\,.
\end{aligned} \tag{B.20}$$

Using the identity (3.4) the delta function $\delta_L(l_{12356})$ becomes:

$$\begin{aligned}
&\delta_L(l_{12356}) = \delta_L\Big((h_{136}\triangleright' l_{3456})l_{1356}h_{156}\triangleright'(g_{56}\triangleright l_{1345}){l_{1456}}^{-1} \\
&h_{146}\triangleright'\{h_{456},(g_{56}g_{45})\triangleright h_{134}\}_{\mathrm{p}}h_{146}\triangleright'(g_{46}\triangleright l_{1234})^{-1}h_{146}\triangleright'\{h_{456},(g_{56}g_{45})\triangleright h_{124}\}_{\mathrm{p}}^{-1}l_{1456} \\
&\delta(h_{156}\triangleright'(g_{56}\triangleright l_{1245})^{-1})\triangleright'\Big((\delta(l_{1256})^{-1}h_{126})\triangleright'(l_{2456}^{-1}l_{2346}^{-1}l_{2356})h_{156}\triangleright'(g_{56}\triangleright(h_{125}\triangleright' l_{2345}))\Big) \\
&h_{156}\triangleright'(g_{56}\triangleright(h_{145}\triangleright'(g_{45}\triangleright l_{1234})l_{1345}^{-1})){l_{1356}}^{-1}(h_{136}h_{346})\triangleright'\{h_{346}^{-1}h_{356}g_{56}\triangleright h_{345}, \\
&(g_{56}g_{45}g_{34})\triangleright h_{123}\}_{\mathrm{p}}\Big)\,.
\end{aligned} \tag{B.21}$$

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Commuting the elements, one obtains

$$\delta_L(l_{12356}) = \delta_L\Big((h_{156} \triangleright' (g_{56} \triangleright \delta(l_{1245})^{-1})\delta(l_{1256})^{-1}h_{126}) \triangleright' (l_{2456}^{-1}l_{2346}^{-1}l_{2356}h_{256} \triangleright' (g_{56} \triangleright l_{2345}))$$
$$h_{156} \triangleright' (g_{56} \triangleright (h_{145} \triangleright' (g_{45} \triangleright l_{1234})l_{1345}^{-1}))l_{1356}{}^{-1}(h_{136}h_{346}) \triangleright' \{h_{346}^{-1}h_{356}g_{56} \triangleright h_{345}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}}$$
$$h_{136} \triangleright' l_{3456}l_{1356}h_{156} \triangleright' (g_{56} \triangleright l_{1345})(\delta(l_{1456})^{-1}h_{146}) \triangleright' (\{h_{456}, (g_{56}g_{45}) \triangleright h_{134}\}_{\mathrm{p}})$$
$$(\delta(l_{1456})^{-1}h_{146}) \triangleright' ((g_{46} \triangleright l_{1234})^{-1})(\delta(l_{1456})^{-1}h_{146}) \triangleright' \{h_{456}, (g_{56}g_{45}) \triangleright h_{124}\}_{\mathrm{p}}^{-1}\Big). \tag{B.22}$$

The tetrahedron (3456) is part of the integrand on both sides of the move, so using the condition (4.9) for $\delta_H(h_{3456})$ one can write $h_{346}^{-1}h_{356}g_{56} \triangleright h_{345} = h_{346}^{-1} \triangleright' \delta(l_{3456})^{-1}h_{456}$. Then, using the identity (3.4) one obtains that

$$\begin{aligned}\{h_{346}^{-1}h_{356}g_{56} \triangleright h_{345}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}} &= \{h_{346}^{-1} \triangleright' \delta(l_{3456})^{-1}h_{456}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}} \\ &= (h_{346}^{-1} \triangleright' \delta(l_{3456})^{-1}) \triangleright' \{h_{456}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}} \\ &\quad \{h_{346}^{-1} \triangleright' \delta(l_{3456})^{-1}, (g_{46}g_{34}) \triangleright h_{123}\}_{\mathrm{p}} \\ &= h_{346}^{-1} \triangleright' l_{3456}^{-1}\{h_{456}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}} \\ &\quad ((g_{46}g_{34}) \triangleright h_{123}h_{346}^{-1}) \triangleright' l_{3456}\,,\end{aligned} \tag{B.23}$$

where in the last row the definition of the action $\triangleright'$ is used. Substituting the equation (B.23) in the equation (B.22) one obtains

$$\delta_L(l_{12356}) = \delta_L\Big((h_{156} \triangleright' (g_{56} \triangleright \delta(l_{1245})^{-1})\delta(l_{1256})^{-1}h_{126}\delta(l_{2456})^{-1}) \triangleright' \Big(l_{2346}^{-1}l_{2356}h_{256} \triangleright' (g_{56} \triangleright l_{2345})l_{2456}^{-1}\Big)$$
$$h_{156} \triangleright' (g_{56} \triangleright (h_{145} \triangleright' (g_{45} \triangleright l_{1234})))(h_{156} \triangleright' (g_{56} \triangleright \delta(l_{1345})^{-1})\delta(l_{1356})^{-1}h_{136}\delta(l_{3456})^{-1}h_{346}) \triangleright'$$
$$(\{h_{456}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}}((g_{46}g_{34}) \triangleright h_{123}) \triangleright' l_{3456})(\delta(l_{1456})^{-1}h_{146}) \triangleright' (\{h_{456}, (g_{56}g_{45}) \triangleright h_{134}\}_{\mathrm{p}})$$
$$(\delta(l_{1456})^{-1}h_{146}) \triangleright' ((g_{46} \triangleright l_{1234})^{-1})(\delta(l_{1456})^{-1}h_{146}) \triangleright' \{h_{456}, (g_{56}g_{45}) \triangleright h_{124}\}_{\mathrm{p}}^{-1}\Big). \tag{B.24}$$

Commuting the element l_{3456} to the end of the expression, one obtains

$$\delta_L(l_{12356}) = \delta_L((h_{156} \triangleright' (g_{56} \triangleright \delta(l_{1245})^{-1})\delta(l_{1256})^{-1}h_{126}\delta(l_{2456})^{-1}) \triangleright' (l_{2346}^{-1}l_{2356}h_{256} \triangleright' (g_{56} \triangleright l_{2345})l_{2456}^{-1})$$
$$h_{156} \triangleright' (g_{56} \triangleright (h_{145} \triangleright' (g_{45} \triangleright l_{1234})))(h_{156} \triangleright' (g_{56} \triangleright \delta(l_{1345})^{-1})\delta(l_{1356})^{-1}h_{136}\delta(l_{3456})^{-1}h_{346}) \triangleright'$$
$$(\{h_{456}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}})(\delta(l_{1456})^{-1}h_{146}) \triangleright' (\{h_{456}, (g_{56}g_{45}) \triangleright h_{134}\}_{\mathrm{p}})$$
$$(\delta(l_{1456})^{-1}h_{146}) \triangleright' ((g_{46} \triangleright l_{1234})^{-1})(\delta(l_{1456})^{-1}h_{146}) \triangleright' \{h_{456}, (g_{56}g_{45}) \triangleright h_{124}\}_{\mathrm{p}}^{-1}$$
$$(h_{156}g_{56} \triangleright h_{145}h_{246}g_{46} \triangleright h_{234}h_{346}^{-1}) \triangleright' l_{3456})). \tag{B.25}$$

Acting to the whole expression with $(h_{156} \triangleright' (g_{56} \triangleright \delta(l_{1245})^{-1})\delta(l_{1256})^{-1}h_{126}\delta(l_{2456})^{-1})^{-1} \triangleright'$, one obtains,

$$\delta_L(l_{12356}) = \delta_L(l_{2346}^{-1}l_{2356}h_{256} \triangleright' (g_{56} \triangleright l_{2345})l_{2456}^{-1}(h_{246}h_{456}(g_{56}g_{45}) \triangleright h_{124}^{-1}) \triangleright'$$
$$\Big((g_{56}g_{45}) \triangleright l_{1234}((g_{56}g_{45}) \triangleright h_{134}h_{456}^{-1}) \triangleright' \{h_{456}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}}$$
$$h_{456}^{-1} \triangleright' \{h_{456}, (g_{56}g_{45}) \triangleright h_{134}\}_{\mathrm{p}}h_{456}^{-1} \triangleright g_{46} \triangleright l_{1234}^{-1}(h_{456}^{-1}g_{46} \triangleright h_{124}) \triangleright' \{h_{456}, (g_{56}g_{45}) \triangleright h_{124}^{-1}\}_{\mathrm{p}}\Big)$$
$$(h_{246}g_{46} \triangleright h_{234}h_{346}^{-1}) \triangleright' l_{3456}. \tag{B.26}$$

Using the identity (3.5) for $\{h_{456}, (g_{56}g_{45}) \triangleright (h_{134}g_{34} \triangleright h_{123})\}_{\mathrm{p}}$,

$$\{h_{456}, (g_{56}g_{45}) \triangleright (h_{134}g_{34} \triangleright h_{123})\}_{\mathrm{p}} = \{h_{456}, (g_{56}g_{45}) \triangleright h_{134}\}_{\mathrm{p}}(g_{46} \triangleright h_{134}) \triangleright' \{h_{456}, (g_{56}g_{45}g_{34}) \triangleright h_{123}\}_{\mathrm{p}}\,, \tag{B.27}$$

one obtains:

$$\begin{aligned}\delta_L(l_{12356}) = \delta_L\big(& l_{2346}^{-1} l_{2356} h_{256} \rhd' (g_{56} \rhd l_{2345}) l_{2456}^{-1} h_{246} \rhd' \Big((h_{456}(g_{56}g_{45}) \rhd h_{124}^{-1}) \rhd' \\ & \Big((g_{56}g_{45}) \rhd l_{1234} h_{456}^{-1} \rhd' \{h_{456}, (g_{56}g_{45}) \rhd (h_{134} g_{34} \rhd h_{123})\}_{\mathrm{p}} \\ & h_{456}^{-1} \rhd g_{46} \rhd l_{1234}^{-1} \Big) \{h_{456}, (g_{56}g_{45}) \rhd h_{124}^{-1}\}_{\mathrm{p}} \Big) (h_{246} g_{46} \rhd h_{234} h_{346}^{-1}) \rhd' l_{3456} \big) .\end{aligned} \tag{B.28}$$

Using the identity (3.5) for $\{h_{456}, (g_{56}g_{45}) \rhd (h_{124}^{-1} \delta(l_{1234}) h_{134} g_{34} \rhd h_{123})\}_{\mathrm{p}}$ one obtains the terms featuring l_{1234} cancel, i.e. ,

$$\begin{aligned}\delta_L(l_{12356}) =& \delta_L\big(l_{2346}^{-1} l_{2356} h_{256} \rhd' (g_{56} \rhd l_{2345}) l_{2456}^{-1} \\ & h_{246} \rhd' \{h_{456}, (g_{56}g_{45}) \rhd (h_{124}^{-1} \delta(l_{1234}) h_{134} g_{34} \rhd h_{123})\}_{\mathrm{p}} (h_{246} g_{46} \rhd h_{234} h_{346}^{-1}) \rhd' l_{3456} \\ =& \delta_L\big({l_{2346}}^{-1} l_{2356} h_{256} \rhd' (g_{56} \rhd l_{2345}) {l_{2456}}^{-1} h_{246} \rhd' \{h_{456}, (g_{56}g_{45}) \rhd h_{234}\}_{\mathrm{p}} (\delta(l_{2346})^{-1} h_{236}) \rhd' l_{3456})\big) \\ =& \delta_L(l_{23456}),\end{aligned} \tag{B.29}$$

the delta function $\delta_L(l_{12356})$ on the r.h.s. reduces to the delta function $\delta_L(l_{23456})$ of the l.h.s. The integrations over l_{1234}, l_{1245}, l_{1256}, l_{1345}, l_{1356}, and l_{1456} are trivial, and finally one obtains,

$$r.h.s. = \delta_G(e)^6 \delta_H(e)^4 \delta_L(l_{23456}) = |G|^6 |H|^4 \delta_L(l_{23456}) . \tag{B.30}$$

The prefactors $|G|^{-11}|H|^{-4}|L|^{-1}$ on the r.h.s. and $|G|^{-5}|H|^{0}|L|^{-1}$ on the l.h.s., compensate for left-over factors.

B.2 Pachner move $2 \leftrightarrow 4$

On the left hand side of the move one has the following integrals and the integrand,

$$\int_L dl_{2345} \delta_H(h_{2345}) \delta_L(l_{23456}) \delta_L(l_{12345}). \tag{B.31}$$

Integrating out l_{2345} using $\delta_L(l_{12345})$, one obtains

$$l_{2345} = {h_{125}}^{-1} \rhd' \left(l_{1235} h_{135} \rhd' \{h_{345}, (g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1} l_{1345} h_{145} \rhd' (g_{45} \rhd l_{1234})^{-1} l_{1245}^{-1}\right) . \tag{B.32}$$

The δ-function $\delta_H(h_{2345})$ now reads,

$$\begin{aligned}\delta_H(h_{2345}) =& \delta_H\big(\delta(l_{2345}) h_{245} \, (g_{45} \rhd h_{234}) \, h_{345}^{-1} \, h_{235}^{-1}\big) \\ =& \delta_H\Big({h_{125}}^{-1} \delta(l_{1235}) h_{135} \delta(\{h_{345}, (g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1}) h_{135}^{-1} \delta(l_{1345}) h_{145} (g_{45} \rhd \delta(l_{1234}))^{-1} h_{145}^{-1} \\ & \delta(l_{1245})^{-1} h_{125} h_{245} \, (g_{45} \rhd h_{234}) \, h_{345}^{-1} \, h_{235}^{-1}\big) .\end{aligned} \tag{B.33}$$

Using the identity (4.9) for the tetrahedrons (1235), (1345), (1234), and (1245), the equation (B.33) reduces to:

$$\begin{aligned}\delta_H(h_{2345}) =& \delta_H\Big({h_{125}}^{-1} h_{125} \, h_{235} \, (g_{35} \rhd h_{123}^{-1}) \, h_{135}^{-1} h_{135} \delta(\{h_{345}, (g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1}) h_{135}^{-1} h_{135} \, h_{345} \, (g_{45} \rhd h_{134}^{-1}) \\ & h_{145}^{-1} h_{145} g_{45} \rhd (h_{134}(g_{34} \rhd h_{123}) h_{234}^{-1} h_{124}^{-1}) h_{145}^{-1} h_{145} (g_{45} \rhd h_{124}) h_{245}^{-1} h_{125}^{-1} h_{125} h_{245} \, (g_{45} \rhd h_{234}) \, h_{345}^{-1} \, h_{235}^{-1}\big) \\ =& \delta_H\Big((g_{35} \rhd h_{123}^{-1}) \, \delta(\{h_{345}, (g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1}) \, h_{345} \, (g_{45}g_{34}) \rhd h_{123}) \, h_{345}^{-1}\big) .\end{aligned} \tag{B.34}$$

Here, one uses the following identity

$$\delta\{h_1\,,h_2\}_{\rm p}(\partial(h_1)\rhd h_2)h_1h_2^{-1}h_1^{-1}=e\,, \tag{B.35}$$

for $h_1=h_{345}$ and $h_2=(g_{45}g_{34})\rhd h_{123}$, and the identity $g_{35}=\partial(h_{345})g_{45}g_{34}$, and obtains

$$\delta_H(h_{2345})=\delta_H(e)\,. \tag{B.36}$$

The remaining δ-function $\delta_L(l_{23456})$, reads

$$\delta_L(l_{23456})=\delta_L(l_{2346}{}^{-1}(h_{236}\rhd' l_{3456})l_{2356}h_{256}\rhd'(g_{56}\rhd l_{2345})l_{2456}{}^{-1}h_{246}\rhd'\{h_{456},(g_{56}g_{45})\rhd h_{234}\}_{\rm p})\,. \tag{B.37}$$

Substituting the equation (B.33), one obtains

$$\begin{aligned}\delta_L(l_{23456})=\delta_L\Big(&l_{2346}{}^{-1}(h_{236}\rhd' l_{3456})l_{2356}h_{256}\rhd'\Big(g_{56}\rhd(h_{125}{}^{-1}\rhd'(l_{1235}h_{135}\rhd'\{h_{345},(g_{45}g_{34})\rhd h_{123}\}_{\rm p}^{-1}\\&l_{1345}h_{145}\rhd'(g_{45}\rhd l_{1234})^{-1}l_{1245}^{-1}))\Big)l_{2456}{}^{-1}h_{246}\rhd'\{h_{456},(g_{56}g_{45})\rhd h_{234}\}_{\rm p}\Big)\,.\end{aligned} \tag{B.38}$$

Commuting the elements one obtains

$$\begin{aligned}\delta_L(l_{23456})=\delta_L\Big(&l_{2456}{}^{-1}l_{2346}{}^{-1}l_{2356}(h_{256}g_{56}\rhd h_{125}{}^{-1})\rhd' g_{56}\rhd l_{1235}(h_{256}g_{56}\rhd h_{125}{}^{-1}g_{56}\rhd h_{135})\rhd'\\&\Big((g_{35}\rhd h_{123}h_{356}^{-1})\rhd' l_{3456})\{g_{56}\rhd h_{345},(g_{56}g_{45}g_{34})\rhd h_{123}\}_{\rm p}^{-1}\\&(g_{56}\rhd h_{345}(g_{56}g_{45})\rhd(h_{123}h_{234}^{-1})h_{456}^{-1})\rhd'\{h_{456},(g_{56}g_{45})\rhd h_{234}\}_{\rm p}\Big)\\&(h_{256}g_{56}\rhd h_{125}{}^{-1})\rhd' g_{56}\rhd l_{1345}(h_{256}g_{56}\rhd h_{125}{}^{-1}g_{56}\rhd h_{145})\rhd'((g_{56}g_{45})\rhd l_{1234})^{-1}\\&(h_{256}g_{56}\rhd h_{125}{}^{-1})\rhd' g_{56}\rhd l_{1245}^{-1}\Big)\,.\end{aligned} \tag{B.39}$$

Finally, the l.h.s. reads:

$$\text{l.h.s.}=\delta_H(e)\delta_L(l_{23456})=|H|\delta_L(l_{23456})\,. \tag{B.40}$$

Let us now examine the right hand side of the move, i.e., the integral (4.17). First, one integrates out g_{16} using $\delta_G(g_{126})$, and obtains

$$g_{16}=\partial(h_{126})\,g_{26}\,g_{12}\,. \tag{B.41}$$

Next, one integrates out h_{126} using $\delta_H(h_{1236})$, h_{136} using $\delta_H(h_{1346})$, and h_{146} using $\delta_H(h_{1456})$, and obtains

$$\begin{aligned}h_{126}&=\delta(l_{1236})h_{136}\,(g_{36}\rhd h_{123})\,h_{236}^{-1}\,,\\h_{136}&=\delta(l_{1346})h_{146}\,(g_{46}\rhd h_{134})\,h_{346}^{-1}\,,\\h_{146}&=\delta(l_{1456})h_{156}\,(g_{56}\rhd h_{145})\,h_{456}^{-1}\,.\end{aligned} \tag{B.42}$$

The remaining δ-functions on the group G reduces to $\delta_G(e)^3$. The δ-function $\delta_G(g_{136})$

$$\delta_G(g_{136})=\delta_G(\partial(h_{136})\,g_{36}\,g_{13}\,g_{16}^{-1})\,, \tag{B.43}$$

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after substituting the equation (B.41) reads:

$$\delta_G(g_{136}) = \delta_G\big(\partial(h_{136})\, g_{36}\, g_{13}\, g_{12}^{-1} g_{26}^{-1}\partial(h_{126})^{-1}\big)\,. \tag{B.44}$$

Using the equations (B.42) for h_{126}, and h_{136}, and h_{146}, and the identity $\partial(\delta l) = 0$ for every element $l \in L$, the δ-function $\delta_G(g_{136})$ reduces to $\delta_G(e)$ after implementing the identity (4.7) for the triangles (156), (145), (456) (134), (346), (236), and (123). Similarly, one obtains $\delta_G(g_{146}) = \delta_G(g_{156}) = \delta_G(e)$.

One integrates out l_{1236} using $\delta_L(l_{12346})$ and obtains

$$l_{1236} = (h_{126} \rhd' l_{2346}) l_{1246} h_{146} \rhd' (g_{46} \rhd l_{1234}) l_{1346}^{-1}\, h_{136} \rhd' \{h_{346}, (g_{46}g_{34}) \rhd h_{123}\}_{\mathrm{p}}, \tag{B.45}$$

l_{1246} using $\delta_L(l_{12456})$ and obtains

$$l_{1246} = (h_{126} \rhd' l_{2456}) l_{1256} h_{156} \rhd' (g_{56} \rhd l_{1245}) {l_{1456}}^{-1}\, h_{146} \rhd' \{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_{\mathrm{p}}, \tag{B.46}$$

and l_{1346} using $\delta_L(l_{13456})$ and obtains

$$l_{1346} = (h_{136} \rhd' l_{3456}) l_{1356} h_{156} \rhd' (g_{56} \rhd l_{1345}) {l_{1456}}^{-1}\, h_{146} \rhd' \{h_{456}, (g_{56}g_{45}) \rhd h_{134}\}_{\mathrm{p}}. \tag{B.47}$$

The remaining δ-functions on H reduce on $\delta_H(e)^3$, similarly as in the case of $1-5$ Pachner move, i.e. , one obtains $\delta_H(h_{1256}) = \delta_H(h_{1356}) = \delta_H(h_{1456}) = \delta_H(e)$. For the remaining δ-function $\delta_L(l_{12356})$,

$$\delta_L(l_{12356}) = \delta_L\Big({l_{1236}}^{-1}(h_{126} \rhd' l_{2356}) l_{1256} h_{156} \rhd' (g_{56} \rhd l_{1235}) {l_{1356}}^{-1} h_{136} \rhd' \{h_{356}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}}\Big)\,, \tag{B.48}$$

one obtains, after substituting the equations (B.45), (B.46), and (B.47), the following

$$\begin{aligned}
\delta_L(l_{12356}) = \delta_L\Big(& h_{136} \rhd' \{h_{346}, (g_{46}g_{34}) \rhd h_{123}\}_{\mathrm{p}}{}^{-1} l_{1346} h_{146} \rhd' (g_{46} \rhd l_{1234})^{-1} l_{1246}^{-1} (h_{126} \rhd' l_{2346})^{-1} \\
& (h_{126} \rhd' l_{2356}) l_{1256} h_{156} \rhd' (g_{56} \rhd l_{1235}) {l_{1356}}^{-1} h_{136} \rhd' \{h_{356}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}}\Big) \\
= \delta_L\Big(& (h_{126} \rhd' l_{2456})^{-1} (h_{126} \rhd' l_{2346})^{-1} (h_{126} \rhd' l_{2356}) (h_{256} g_{56} \rhd {h_{125}}^{-1}) \rhd' l_{1235} \\
& \delta(l_{1256}) \rhd' \Big(\delta(l_{1356})^{-1} \rhd' (h_{136} \rhd' \{h_{356}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}} (h_{136}h_{346}) \rhd' \{h_{346}^{-1}, g_{36} \rhd h_{123}\}_{\mathrm{p}} \\
& (h_{136} \rhd' l_{3456})) h_{156} \rhd' (g_{56} \rhd l_{1345}) {l_{1456}}^{-1}\, h_{146} \rhd' \{h_{456}, (g_{56}g_{45}) \rhd h_{134}\}_{\mathrm{p}} h_{146} \rhd' (g_{46} \rhd l_{1234})^{-1} \\
& h_{146} \rhd' \{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_{\mathrm{p}}^{-1} l_{1456} h_{156} \rhd' (g_{56} \rhd l_{1245})^{-1}\Big)\Big)\,.
\end{aligned} \tag{B.49}$$

Commuting the elements in order to match the l.h.s. of the move, i.e. , the δ-function given by the equation (B.39), and using the identity (3.4), i.e. ,

$$\{h_{346}^{-1} h_{356}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}} = h_{346}^{-1} \rhd' \{h_{356}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}} \{h_{346}^{-1}, g_{36} \rhd h_{123}\}_{\mathrm{p}}\,, \tag{B.50}$$

one obtains

$$\begin{aligned}
\delta_L(l_{12356}) = \delta_L\Big(& (h_{126} \rhd' l_{2456})^{-1} (h_{126} \rhd' l_{2346})^{-1} (h_{126} \rhd' l_{2356}) (h_{126} h_{256} g_{56} \rhd {h_{125}}^{-1}) \rhd' l_{1235} \\
& \delta(l_{1256}) \rhd' \Big(\delta(l_{1356})^{-1} \rhd' ((h_{136}h_{346}) \rhd' \{h_{346}^{-1} h_{356}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}} (h_{136} \rhd' l_{3456})) \\
& h_{156} \rhd' (g_{56} \rhd l_{1345}) (\delta(l_{1456})^{-1}\, h_{146}) \rhd' (\{h_{456}, (g_{56}g_{45}) \rhd h_{134}\}_{\mathrm{p}} (g_{46} \rhd l_{1234})^{-1} \\
& \{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_{\mathrm{p}}^{-1}) h_{156} \rhd' (g_{56} \rhd l_{1245})^{-1}\Big)\Big)\,.
\end{aligned} \tag{B.51}$$

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Using the identity (3.4) again one rewrites the following term as

$$\begin{aligned}
&(h_{136}h_{346}) \rhd' \{h_{346}^{-1}h_{356}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}}(h_{136} \rhd' l_{3456}) = \\
&(h_{136}h_{346}) \rhd' \{h_{346}^{-1} \rhd' \delta(l_{3456})^{-1}h_{456}g_{56} \rhd h_{345}^{-1}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}}(h_{136} \rhd' l_{3456}) = \\
&(h_{136} \rhd' \delta(l_{3456})^{-1}h_{136}h_{346}) \rhd' (\{h_{456}g_{56} \rhd h_{345}^{-1}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}}((g_{46}g_{34}) \rhd h_{123}h_{346}^{-1}) \rhd' l_{3456}^{-1})\,,
\end{aligned} \tag{B.52}$$

and substituting it in the equation (B.51) the δ-function becomes:

$$\begin{aligned}
\delta_L(l_{12356}) = \delta_L\Big(&(h_{126} \rhd' l_{2456})^{-1}(h_{126} \rhd' l_{2346})^{-1}(h_{126} \rhd' l_{2356})(h_{126}h_{256}g_{56} \rhd h_{125}{}^{-1}) \rhd' l_{1235} \\
&\delta(l_{1256}) \rhd' \Big((\delta(l_{1356})^{-1}h_{136} \rhd' \delta(l_{3456})^{-1}h_{136}h_{346})\rhd' \\
&(\{h_{456}g_{56} \rhd h_{345}^{-1}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}}((g_{46}g_{34}) \rhd h_{123}h_{346}^{-1}) \rhd' l_{3456})) \\
&(h_{156}g_{56} \rhd h_{135}g_{56} \rhd (h_{345}g_{45} \rhd h_{134}^{-1})h_{456}^{-1}) \rhd' (\{h_{456}, (g_{56}g_{45}) \rhd h_{134}\}_{\mathrm{p}}(g_{46} \rhd l_{1234})^{-1} \\
&\{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_{\mathrm{p}}^{-1})\Big)(h_{126}h_{256}g_{56} \rhd h_{125}{}^{-1}) \rhd' (h_{156} \rhd' (g_{56} \rhd l_{1345})(g_{56} \rhd l_{1245})^{-1})\Big)\,.
\end{aligned} \tag{B.53}$$

Commuting the elements l_{3456} and $\{h_{456}g_{56} \rhd h_{345}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}}$, and using the identity (3.4) to rewrite this Peiffer lifting, one obtains

$$\begin{aligned}
\delta_L(l_{12356}) = \delta_L\Big(&(h_{126} \rhd' l_{2456})^{-1}(h_{126} \rhd' l_{2346})^{-1}(h_{126} \rhd' l_{2356})(h_{126}h_{256}g_{56} \rhd h_{125}{}^{-1}) \rhd' l_{1235} \\
&(h_{126}h_{256}g_{56} \rhd h_{125}{}^{-1}h_{135}(g_{56}g_{35}) \rhd h_{123}g_{56} \rhd h_{356}^{-1}) \rhd' g_{56} \rhd l_{3456} \\
&(h_{126}h_{256}g_{56} \rhd h_{125}^{-1}g_{56} \rhd h_{135}g_{56} \rhd h_{345}) \rhd' \Big(\{g_{56} \rhd h_{345}^{-1}, (g_{56}g_{35}) \rhd h_{123}\}_{\mathrm{p}} \\
&h_{456}^{-1} \rhd' \{h_{456}, (g_{56}g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}((g_{56}g_{45}) \rhd h_{134}^{-1}h_{456}^{-1}) \rhd' (\{h_{456}, (g_{56}g_{45}) \rhd h_{134}\}_{\mathrm{p}}(g_{46} \rhd l_{1234})^{-1} \\
&\{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_{\mathrm{p}}^{-1})\Big)(h_{126}h_{256}g_{56} \rhd h_{125}{}^{-1}) \rhd' (h_{156} \rhd' (g_{56} \rhd l_{1345})(g_{56} \rhd l_{1245})^{-1})\Big)\,.
\end{aligned} \tag{B.54}$$

After the similar transformations as in the case of $1-5$ move, commuting the element l_{1234} so that the order of the elements matches the order in the expression (B.39), and acting to the whole expression with h_{126}^{-1} one obtains

$$\begin{aligned}
\delta_L(l_{12356}) = \delta_L\Big(&l_{2456}{}^{-1}l_{2346}{}^{-1}l_{2356}(h_{256}g_{56} \rhd h_{125}{}^{-1}) \rhd' g_{56} \rhd l_{1235}(h_{256}g_{56} \rhd h_{125}{}^{-1}g_{56} \rhd h_{135})\rhd' \\
&\Big((g_{35} \rhd h_{123}h_{356}^{-1}) \rhd' l_{3456})\{g_{56} \rhd h_{345}, (g_{56}g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1}(g_{56} \rhd h_{345}(g_{56}g_{45}) \rhd (h_{123}h_{234}^{-1})h_{456}^{-1})\rhd' \\
&\{h_{456}, (g_{56}g_{45}) \rhd h_{234}\}_{\mathrm{p}}\Big)(h_{256}g_{56} \rhd h_{125}{}^{-1}) \rhd' g_{56} \rhd l_{1345} \\
&(h_{256}g_{56} \rhd h_{125}{}^{-1}g_{56} \rhd h_{145}) \rhd' ((g_{56}g_{45}) \rhd l_{1234})^{-1}(h_{256}g_{56} \rhd h_{125}{}^{-1}) \rhd' g_{56} \rhd l_{1245}^{-1}\Big)\,.
\end{aligned} \tag{B.55}$$

which is precisely the equation (B.39). The remaining integration over the element h_{156} of the group H and remaining integration over the three elements of the group L, l_{1246}, l_{1256}, and l_{1356}, are trivial, yielding the result on the r.h.s. to:

$$\text{r.h.s.} = \delta_G(e)^3\,\delta_H(e)^3\,\delta_L(l_{12356}) = |G|^3\,|H|^3\,\delta_L(l_{12356})\,. \tag{B.56}$$

The prefactors are $|G|^{-8}|H|^{-1}|L|^{-1}$ on the l.h.s., and $|G|^{-11}|H|^{-3}|L|^{-1}$ on the r.h.s. compensate for the left-over factors.

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B.3 Pachner move $3 \leftrightarrow 3$

Let us first investigate the r.h.s. of the move. First, one integrates out the l_{1235}, exploiting $\delta_L(l_{12345})$ and obtains

$$l_{1235} = (h_{125} \triangleright' l_{2345}) l_{1245} h_{145} \triangleright' (g_{45} \triangleright l_{1234}) l_{1345}{}^{-1}\, h_{135} \triangleright' \{h_{345}, (g_{45} g_{34}) \triangleright h_{123}\}_{\mathrm{p}}, \tag{B.57}$$

and one integrates out l_{1236}, exploiting $\delta_L(l_{12356})$ and obtains

$$l_{1236} = (h_{126} \triangleright' l_{2356}) l_{1256} h_{156} \triangleright' (g_{56} \triangleright l_{1235}) l_{1356}{}^{-1} h'_{136} \triangleright \{h_{356}, (g_{56} g_{35}) \triangleright h_{123}\}_{\mathrm{p}}. \tag{B.58}$$

Next, one integrates out h_{123}, exploiting $\delta_H(l_{1234})$ and obtains:

$$h_{123} = g_{34}^{-1} \triangleright h_{134}^{-1}\, g_{34}^{-1} \triangleright \delta(l_{1234})^{-1}\, g_{34}^{-1} \triangleright h_{124}\, g_{34}^{-1} \triangleright h_{234}. \tag{B.59}$$

The δ-function $\delta_G(g_{123})$, when using the equation (B.59) reads

$$\delta_G(g_{123}) = \delta_G\big(g_{34}^{-1} \triangleright \partial(h_{134})^{-1}\, g_{34}^{-1} \triangleright \partial(\delta(l_{1234}))^{-1}\, g_{34}^{-1} \triangleright \partial(h_{124})\, g_{34}^{-1} \triangleright \partial(h_{234})\, g_{23}\, g_{12}\, g_{13}^{-1}\big)\,, \tag{B.60}$$

which then using the condition $\partial\delta = 0$, reduces to

$$\delta_G(g_{123}) = \delta_G\big(\partial(h_{134})^{-1}\, \partial(h_{124})\, \partial(h_{234})\, g_{34}^{-1} g_{23}\, g_{12}\, g_{13}^{-1} g_{34}\big)\,. \tag{B.61}$$

Using the condition (4.7) for the triangles (134), (124), and (234), it finally reduces to

$$\delta_G(g_{123}) = \delta_G(e)\,. \tag{B.62}$$

For the δ-function $\delta_H(h_{1235})$, one obtains, after using the equation (B.57):

$$\begin{aligned}\delta_H(h_{1235}) = \delta_H\Big(&(h_{125}\delta(l_{2345})h_{125}^{-1})\delta(l_{1245})(h_{145}(g_{45} \triangleright \delta(l_{1234}))h_{145}^{-1})\delta(l_{1345})^{-1} \\ &h_{135} \triangleright' \{h_{345}, g_{35} \triangleright h_{123}\}_{\mathrm{p}}\, h_{135}((g_{35} g_{34}{}^{-1}) \triangleright (h_{134}^{-1}\, \delta(l_{1234})^{-1}\, h_{124}\, h_{234}))\, h_{235}^{-1}\, h_{125}^{-1}\Big)\,.\end{aligned} \tag{B.63}$$

Using the δ-functions $\delta_L(h_{2345})$, $\delta_L(h_{1245})$, and $\delta_L(h_{1345})$, that appear on both sides of the move, and are thus part of the integrand,

$$\begin{aligned}\delta(l_{2345}) &= h_{235}\, h_{345}\, (g_{45} \triangleright h_{234}^{-1})\, h_{245}^{-1}\,, \\ \delta(l_{1245}) &= h_{125}\, h_{245}\, (g_{45} \triangleright h_{124}^{-1})\, h_{145}^{-1}\,, \\ \delta(l_{1345})^{-1} &= h_{145}\, (g_{45} \triangleright h_{134})\, h_{345}^{-1}\, h_{135}^{-1}\,,\end{aligned} \tag{B.64}$$

one obtains:

$$\begin{aligned}\delta_H(h_{1235}) = \delta_H\Big(&h_{125} h_{235}\, h_{345}\, (g_{45} \triangleright h_{234}^{-1})\, h_{245}^{-1} h_{125}^{-1} h_{125}\, h_{245}\, (g_{45} \triangleright h_{124}^{-1})\, h_{145}^{-1} h_{145}(g_{45} \triangleright \delta(l_{1234}))h_{145}^{-1} \\ &h_{145}\, (g_{45} \triangleright h_{134})\, h_{345}^{-1}\, h_{135}^{-1} h_{135} \triangleright \delta(\{h_{345}, (g_{45} g_{34}) \triangleright h_{123}\}_{\mathrm{p}}) \\ &h_{135}\, ((g_{35} g_{34}{}^{-1}) \triangleright (h_{134}^{-1} \delta(l_{1234})^{-1}\, h_{124}\, h_{234}))\, h_{235}^{-1}\, h_{125}^{-1}\Big) \\ = \delta_H\Big(&h_{345}(g_{45} g_{34}) \triangleright h_{123}^{-1}\, h_{345}^{-1} \delta(\{h_{345}, (g_{45} g_{34}) \triangleright h_{123}\}_{\mathrm{p}})\, (g_{35} \triangleright h_{123})\Big)\,.\end{aligned} \tag{B.65}$$

Substituting $g_{35} = \partial(h_{345}) g_{45} g_{34}$, and applying the identity

$$\delta\{h_1\,, h_2\}_{\mathrm{p}}(\partial(h_1) \rhd h_2) h_1 h_2^{-1} h_1^{-1} = e\,, \tag{B.66}$$

for $h_1 = h_{345}$ and $h_2 = (g_{45} g_{34}) \rhd h_{123}$, one obtains

$$\delta_H(h_{1235}) = \delta_H(e). \tag{B.67}$$

Similarly, one obtains that $\delta_H(h_{1236}) = \delta_H(e)$. The remaining δ-function $\delta_H(l_{12346})$ reads

$$\delta_L(l_{12346}) = \delta_L(l_{1236}{}^{-1}(h_{126} \rhd' l_{2346}) l_{1246} h_{146} \rhd' (g_{46} \rhd l_{1234}) l_{1346}{}^{-1}\, h_{136} \rhd' \{h_{346}, (g_{46} g_{34}) \rhd h_{123}\}_{\mathrm{p}})\,. \tag{B.68}$$

After substituting the equation (B.58), and then the equation (B.57), one obtains:

$$\begin{aligned}
\delta_L(l_{12346}) = {} & \delta_L(h_{136} \rhd' \{h_{356}, (g_{56} g_{35}) \rhd h_{123}\}_{\mathrm{p}}^{-1} l_{1356} h_{156} \rhd' (g_{56} \rhd l_{1235})^{-1} l_{1256}^{-1} h_{126} \rhd' l_{2356}^{-1} \\
& (h_{126} \rhd' l_{2346}) l_{1246} h_{146} \rhd' (g_{46} \rhd l_{1234}) l_{1346}{}^{-1} h_{136} \rhd' \{h_{346}, (g_{46} g_{34}) \rhd h_{123}\}_{\mathrm{p}}) \\
= {} & \delta_L(h_{136} \rhd' \{h_{356}, (g_{56} g_{35}) \rhd h_{123}\}_{\mathrm{p}}^{-1} l_{1356} \\
& h_{156} \rhd' (g_{56} \rhd ((h_{125} \rhd' l_{2345}) l_{1245} h_{145} \rhd' (g_{45} \rhd l_{1234}) l_{1345}{}^{-1}\, h_{135} \rhd' \{h_{345}, (g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}))^{-1} \\
& l_{1256}^{-1} h_{126} \rhd' l_{2356}^{-1} (h_{126} \rhd' l_{2346}) l_{1246} h_{146} \rhd' (g_{46} \rhd l_{1234}) l_{1346}{}^{-1} h_{136} \rhd' \{h_{346}, (g_{46} g_{34}) \rhd h_{123}\}_{\mathrm{p}})\,.
\end{aligned} \tag{B.69}$$

After commuting the elements, i.e. , using the Peiffer identity for the crossed module $(L \xrightarrow{\delta} H, \rhd')$, one obtains

$$\begin{aligned}
\delta_L(l_{12346}) = {} & \delta_L(h_{136} \rhd' \{h_{356}, (g_{56} g_{35}) \rhd h_{123}\}_{\mathrm{p}}^{-1} \\
& (\delta(l_{1356}) h_{156} g_{56} \rhd h_{135}) \rhd' g_{56} \rhd \{h_{345}, (g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1} l_{1356} h_{156} \rhd' (g_{56} \rhd l_{1345}) \\
& (h_{156} g_{56} \rhd h_{145}) \rhd' ((g_{56} g_{45}) \rhd l_{1234})^{-1} h_{156} \rhd' (g_{56} \rhd l_{1245})^{-1} (h_{156} g_{56} \rhd h_{125}) \rhd' (g_{56} \rhd l_{2345}^{-1}) l_{1256}^{-1} \\
& h_{126} \rhd' l_{2356}^{-1} (h_{126} \rhd' l_{2346}) l_{1246} h_{146} \rhd' (g_{46} \rhd l_{1234}) l_{1346}{}^{-1} h_{136} \rhd' \{h_{346}, (g_{46} g_{34}) \rhd h_{123}\}_{\mathrm{p}}) \\
= {} & \delta_L((\delta(l_{1346})^{-1} h_{136}) \rhd' \{h_{346}, (g_{46} g_{34}) \rhd h_{123}\}_{\mathrm{p}} (\delta(l_{1346})^{-1} h_{136}) \rhd' \{h_{356}, (g_{56} g_{35}) \rhd h_{123}\}_{\mathrm{p}}^{-1} \\
& ((\delta(l_{1346})^{-1} \delta(l_{1356}) h_{156} g_{56} \rhd h_{135}) \rhd' g_{56} \rhd \{h_{345}, (g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1} \\
& (\delta(l_{1346})^{-1} \delta(l_{1356}) h_{156} \rhd' (g_{56} \rhd \delta(l_{1345})) h_{156} g_{56} \rhd h_{145}) \rhd' ((g_{56} g_{45}) \rhd l_{1234})^{-1} l_{1346}^{-1} \\
& l_{1356} h_{156} \rhd' (g_{56} \rhd l_{1345}) h_{156} \rhd' (g_{56} \rhd l_{1245})^{-1} (h_{156} g_{56} \rhd h_{125}) \rhd' (g_{56} \rhd l_{2345}^{-1}) \\
& l_{1256}^{-1} h_{126} \rhd' l_{2356}^{-1} (h_{126} \rhd' l_{2346}) l_{1246} h_{146} \rhd' (g_{46} \rhd l_{1234}))\,.
\end{aligned} \tag{B.70}$$

Using the identity (3.7) one obtains that

$$\{h_{346}, (g_{46} g_{34}) \rhd h_{123}\}_{\mathrm{p}} = h_{346} \rhd' \{h_{346}^{-1}, g_{36} \rhd h_{123}\}_{\mathrm{p}}^{-1}\,. \tag{B.71}$$

Using a variant of the identity (3.4), i.e. , that

$$\{h_1 h_2 h_3, h_4\}_{\mathrm{p}}^{-1} = \{h_1, \partial(h_2 h_3) \rhd h_4\}_{\mathrm{p}}^{-1} h_1 \rhd' \{h_2, \partial(h_2) \rhd h_4\}_{\mathrm{p}}^{-1} (h_1 h_2) \rhd' \{h_3, h_4\}_{\mathrm{p}}^{-1}\,, \tag{B.72}$$

one obtains that

$$\begin{aligned}
\{h_{346}^{-1}\, h_{356}\, (g_{56} \rhd h_{345}), (g_{56} g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1} = {} & \{h_{346}^{-1}, (g_{46} g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1} h_{346}^{-1} \rhd' \{h_{356}, (g_{56} g_{35}) \rhd h_{123}\}_{\mathrm{p}}^{-1} \\
& (h_{346}^{-1} h_{356}) \rhd' \{g_{56} \rhd h_{345}, (g_{56} g_{45} g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1}\,,
\end{aligned} \tag{B.73}$$

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rendering the expression (B.70) to

$$\delta_L(l_{12346}) = \delta_L\big((h_{146}g_{46} \rhd h_{134}) \rhd' \{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1} \\ (\delta(l_{1346})^{-1}\delta(l_{1356})h_{156} \rhd' (g_{56} \rhd \delta(l_{1345}))h_{156}g_{56} \rhd h_{145}) \rhd' ((g_{56}g_{45}) \rhd l_{1234})^{-1} \\ l_{1346}^{-1}l_{1356}h_{156} \rhd' (g_{56} \rhd l_{1345})h_{156} \rhd' (g_{56} \rhd l_{1245})^{-1}(h_{156}g_{56} \rhd h_{125}) \rhd' (g_{56} \rhd l_{2345}^{-1})l_{1256}^{-1} \\ h_{126} \rhd' l_{2356}^{-1}(h_{126} \rhd' l_{2346})l_{1246}h_{146} \rhd' (g_{46} \rhd l_{1234})\big)\,. \tag{B.74}$$

Substituting the equation (B.59), and using the identity (3.5), one obtains that the expression,

$$\{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1} = \{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}) \rhd ((h_{134}^{-1} \rhd' \delta(l_{1234})^{-1})h_{134}^{-1}h_{124}h_{234}\}_{\mathrm{p}}^{-1} \\ = (g_{46} \rhd (h_{134}^{-1} \rhd' \delta(l_{1234})^{-1})) \rhd' \{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}) \rhd \\ (h_{134}^{-1}h_{124}h_{234})\}_{\mathrm{p}}^{-1}\{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}) \rhd (h_{134}^{-1} \rhd' \delta(l_{1234})^{-1})\}_{\mathrm{p}}^{-1}\,, \tag{B.75}$$

using the identity (3.9), i.e. , that

$$\{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}) \rhd (h_{134}^{-1} \rhd' \delta(l_{1234})^{-1})\}_{\mathrm{p}}^{-1} = g_{46} \rhd (h_{134}^{-1} \rhd' l_{1234}^{-1})(h_{346}^{-1}\, h_{356} \\ (g_{56} \rhd h_{345})) \rhd' ((g_{56}g_{45}) \rhd (h_{134}^{-1} \rhd' l_{1234}))\,, \tag{B.76}$$

reduces to

$$\{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}g_{34}) \rhd h_{123}\}_{\mathrm{p}}^{-1} = g_{46} \rhd (h_{134}^{-1} \rhd' \delta(l_{1234})^{-1}) \\ \{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}) \rhd (h_{134}^{-1}h_{124}h_{234})\}_{\mathrm{p}}^{-1} \\ (h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345})) \rhd' ((g_{56}g_{45}) \rhd (h_{134}^{-1} \rhd' l_{1234}))\,. \tag{B.77}$$

Substituting this result in the expression (B.74) the terms featuring l_{1234} cancel, and finally the delta function $\delta_L(l_{12346})$ reads:

$$\delta_L(l_{12346}) = \delta_L\big((h_{146}g_{46} \rhd h_{134}) \rhd' \{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}) \rhd (h_{134}^{-1}h_{124}h_{234})\}_{\mathrm{p}}^{-1}l_{1346}^{-1}l_{1356} \\ h_{156} \rhd' (g_{56} \rhd l_{1345})h_{156} \rhd' (g_{56} \rhd l_{1245})^{-1}(h_{156}g_{56} \rhd h_{125}) \rhd' (g_{56} \rhd l_{2345}^{-1}) \\ l_{1256}^{-1}h_{126} \rhd' l_{2356}^{-1}(h_{126} \rhd' l_{2346})l_{1246}\big)\,. \tag{B.78}$$

One obtains that the integration over l_{1234} is trivial, and the r.h.s. of the move finally reads

$$\text{r.h.s.} = \delta_G(e)\delta_H(e)^2\delta_L\big(h_{156} \rhd' (g_{56} \rhd l_{1245})^{-1}\, h_{156} \rhd' (g_{56} \rhd (h_{125} \rhd' l_{2345}))^{-1}\, l_{1256}^{-1} \\ h_{126} \rhd' l_{2356}^{-1}(h_{126} \rhd' l_{2346})l_{1246}(h_{146}g_{46} \rhd h_{134}) \rhd' \\ \{h_{346}^{-1}\, h_{356}\,(g_{56} \rhd h_{345}), (g_{56}g_{45}) \rhd (h_{134}^{-1}h_{124}h_{234})\}_{\mathrm{p}}^{-1}l_{1346}^{-1}l_{1356}h_{156} \rhd' (g_{56} \rhd l_{1345}\big)\,. \tag{B.79}$$

The integral of the l.h.s. reads

$$\textstyle\int_H dh_{456} \int_{L^3} dl_{1456}dl_{2456}dl_{3456}\delta_G(g_{456})\,\delta_H(h_{3456})\delta_H(h_{2456})\delta_H(h_{1456})\delta_L(l_{23456})\delta_L(l_{13456})\delta_L(l_{12456})\,. \tag{B.80}$$

First, one integrates out the l_{1456}, exploiting $\delta_L(l_{13456})$ and obtains

$$l_{1456} = h_{146} \rhd \{h_{456}, (g_{56}g_{45}) \rhd h_{134}\}{l_{1346}}^{-1}(h_{136} \rhd' l_{3456})l_{1356}h_{156} \rhd' (g_{56} \rhd l_{1345}). \tag{B.81}$$

Next, one integrates out the l_{2456}, exploiting $\delta_L(l_{23456})$ and obtains

$$l_{2456} = h_{246} \rhd \{h_{456}, (g_{56}g_{45}) \rhd h_{234}\} {l_{2346}}^{-1}(h_{236} \rhd' l_{3456}) l_{2356} h_{256} \rhd' (g_{56} \rhd l_{2345}) \,. \quad \text{(B.82)}$$

Next, one integrates out h_{456}, exploiting $\delta_H(h_{3456})$ and obtains

$$h_{456} = h_{346}^{-1}\, \delta(l_{3456}) h_{356}\, (g_{56} \rhd h_{345}) \,. \quad \text{(B.83)}$$

Using the equation (B.83), one obtains that

$$\delta_G(g_{456}) = \delta_G\big(\partial(h_{346})^{-1}\, \partial(h_{356})\, g_{56} \rhd \partial(h_{345})\, g_{56}\, g_{45}\, g_{46}^{-1}\big) \,, \quad \text{(B.84)}$$

which, using the identity (4.7) for triangles (346), (356), and (345), reduces to:

$$\delta_G(g_{456}) = \delta_G(e) \,. \quad \text{(B.85)}$$

Similarly as done for the right-hand side of the move, one shows that $\delta_H(h_{1456})$, when using the equation (B.81), and $\delta_H(h_{2456})$, when using the equation (B.82), reduce to $\delta_H(e)^2$. The remaining $\delta_L(l_{12456})$ now reads

$$\delta_L(l_{12456}) = \delta_L({l_{1246}}^{-1}(h_{126} \rhd' l_{2456}) l_{1256} h_{156} \rhd' (g_{56} \rhd l_{1245}) {l_{1456}}^{-1}\, h_{146} \rhd \{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_\mathrm{p}) \,. \quad \text{(B.86)}$$

Substituting the equations (B.81) and (B.82), one obtains

$$\begin{aligned}\delta_L(l_{12456}) = \delta_L\big({l_{1246}}^{-1}&(h_{126} \rhd' (h_{246} \rhd \{h_{456},(g_{56}g_{45}) \rhd h_{234}\}_\mathrm{p} {l_{2346}}^{-1}(h_{236} \rhd' l_{3456}) l_{2356} \\ &h_{256} \rhd' (g_{56} \rhd l_{2345}))) l_{1256} h_{156} \rhd' (g_{56} \rhd l_{1245}) h_{156} \rhd' (g_{56} \rhd l_{1345})^{-1} l_{1356}^{-1} (h_{136} \rhd' l_{3456})^{-1} \\ &l_{1346} h_{146} \rhd \{h_{456},(g_{56}g_{45}) \rhd h_{134}\}_\mathrm{p}^{-1} h_{146} \rhd \{h_{456},(g_{56}g_{45}) \rhd h_{124}\}_\mathrm{p}\big).\end{aligned} \quad \text{(B.87)}$$

After commuting the elements, i.e. , using the Peiffer identity for the crossed module $(L \xrightarrow{\delta} H, \rhd')$, one obtains

$$\begin{aligned}\delta_L(l_{12456}) = \delta_L\big(&(\delta(l_{1246})^{-1} h_{126} h_{246}) \rhd \{h_{456}, (g_{56}g_{45}) \rhd h_{234}\}_\mathrm{p} (\delta(l_{1246})^{-1} h_{126} \rhd \delta(l_{2346})^{-1} h_{126} h_{236}) \rhd' l_{3456} \\ &l_{1246}^{-1} h_{126} \rhd' {l_{2346}}^{-1} h_{126} \rhd' l_{2356} (h_{126} h_{256}) \rhd' (g_{56} \rhd l_{2345})\,) \\ &l_{1256} h_{156} \rhd' (g_{56} \rhd l_{1245}) h_{156} \rhd' (g_{56} \rhd l_{1345})^{-1} l_{1356}^{-1} l_{1346} (\delta(l_{1346})^{-1} h_{136}) \rhd' {l_{3456}}^{-1} \\ &h_{146} \rhd \{h_{456}, (g_{56}g_{45}) \rhd h_{134}\}_\mathrm{p}^{-1}\, h_{146} \rhd \{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_\mathrm{p}\big) \,.\end{aligned} \quad \text{(B.88)}$$

Using the identity (3.10) for the inverse of the element $\{h_{456}, (g_{56}g_{45}) \rhd h_{134}\}_\mathrm{p}^{-1}$, and then the variant of the identity (3.5), i.e. , that is,

$$\{h_1, h_2h_3h_4\}_\mathrm{p} = \{h_1, h_2\}_\mathrm{p} (\partial(h_1) \rhd h_2) \rhd' \{h_1, h_3\}_\mathrm{p} (\partial(h_1) \rhd (h_2h_3)) \rhd' \{h_1, h_4\}_\mathrm{p} \,, \quad \text{(B.89)}$$

one obtains

$$\begin{aligned}\{h_{456}, (g_{56}g_{45}) \rhd (h_{134}^{-1} h_{124} h_{234})\}_\mathrm{p} = \{&h_{456}, (g_{56}g_{45}) \rhd h_{134}^{-1}\}_\mathrm{p} (g_{46} \rhd h_{134}^{-1}) \rhd' \{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_\mathrm{p} \\ &(g_{46} \rhd (h_{134}^{-1} h_{124})) \rhd' \{h_{456}, (g_{56}g_{45}) \rhd h_{124}\}_\mathrm{p} \,,\end{aligned} \quad \text{(B.90)}$$

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rendering the equation (B.88) to

$$\begin{aligned}\delta_L(l_{12456}) = \delta_L\big((\delta(l_{1246})^{-1}h_{126} \triangleright \delta(l_{2346})^{-1}h_{126}h_{236}) \triangleright' l_{3456} \\ l_{1246}^{-1}h_{126} \triangleright' l_{2346}{}^{-1}h_{126} \triangleright' l_{2356}(h_{126}h_{256}) \triangleright' (g_{56} \triangleright l_{2345})\big) \\ l_{1256}h_{156} \triangleright' (g_{56} \triangleright l_{1245})h_{156} \triangleright' (g_{56} \triangleright l_{1345})^{-1}l_{1356}^{-1}l_{1346}(\delta(l_{1346})^{-1}h_{136}) \triangleright' l_{3456}{}^{-1} \\ (h_{146}g_{46} \triangleright h_{134}) \triangleright' \{h_{456}, (g_{56}g_{45}) \triangleright (h_{134}^{-1}h_{124}h_{234})\}_{\mathrm{p}}\big)\,.\end{aligned} \tag{B.91}$$

Using the equation (B.83), and the identities (3.4) and (3.6), similarly as for the r.h.s. of the move, one obtains that the terms featuring l_{3456} cancel, i.e. , the delta function $\delta_L(l_{12456})$ reads

$$\begin{aligned}\delta_L(l_{12456}) = \delta_L\big(l_{1246}^{-1}h_{126} \triangleright' l_{2346}{}^{-1}h_{126} \triangleright' l_{2356}(h_{126}h_{256}) \triangleright' (g_{56} \triangleright l_{2345}))l_{1256}h_{156} \triangleright' (g_{56} \triangleright l_{1245}) \\ h_{156} \triangleright' (g_{56} \triangleright l_{1345})^{-1}l_{1356}^{-1}l_{1346}(h_{146}g_{46} \triangleright h_{134}) \triangleright' \{h_{456}, (g_{56}g_{45}) \triangleright (h_{134}^{-1}h_{124}h_{234})\}_{\mathrm{p}}\big)\,.\end{aligned} \tag{B.92}$$

It follows that the integral over l_{3456} is now trivial and l.h.s. of the move finally reduces to:

$$\begin{aligned}\text{l.h.s.} = \delta_G(e)\delta_H(e)^2\delta_L\big(h_{126} \triangleright' l_{2346}l_{1246}(h_{146}g_{46} \triangleright h_{134}) \triangleright' \{h_{456}, (g_{56}g_{45}) \triangleright (h_{134}^{-1}h_{124}h_{234})\}_{\mathrm{p}}^{-1} \\ l_{1346}^{-1}\, l_{1356}\, h_{156} \triangleright' (g_{56} \triangleright l_{1345})\, h_{156} \triangleright' (g_{56} \triangleright l_{1245})^{-1}(h_{156}g_{56} \triangleright h_{125}) \triangleright' (g_{56} \triangleright l_{2345})^{-1} \\ l_{1256}^{-1}\, h_{126} \triangleright' l_{2356}^{-1}\big)\,.\end{aligned} \tag{B.93}$$

The expressions (B.79) and (B.86) are the same, which proves the invariance of the state sum (4.1) under the Pachner move $3-3$. The numbers of k-simplices agree on both sides of the $3-3$ move for all k, and the prefactors play no role in this case.

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Gauge symmetry of the 3*BF* theory for a generic semistrict Lie three-group

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Abstract

The higher category theory can be employed to generalize the *BF* action to the so-called 3*BF* action, by passing from the notion of a gauge group to the notion of a gauge three-group. In this work we determine the full gauge symmetry of the 3*BF* action. To that end, the complete Hamiltonian analysis of the 3*BF* action for an arbitrary semistrict Lie three-group is performed, by using the Dirac procedure. The Hamiltonian analysis is the first step towards a canonical quantization of a 3*BF* theory. This is an important stepping-stone for the quantization of the complete standard model of elementary particles coupled to Einstein–Cartan gravity, formulated as a 3*BF* action with suitable simplicity constraints. We show that the resulting gauge symmetry group consists of the familiar *G*-, *H*-, and *L*-gauge transformations, as well as additional *M*- and *N*-gauge transformations, which have not been discussed in the existing literature.

Keywords: quantum gravity, higher gauge theory, higher category theory, three-group, *BF* action, 3*BF* action, gauge symmetry

Contents

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1. Introduction

Among the most important open problems in contemporary theoretical physics is the problem of quantization of the gravitational field. Within the framework of loop quantum gravity (LQG), one of the most prominent candidates for the quantum theory of gravity, the study of nonperturbative quantization has evolved in two directions: the canonical and the covariant approach. See [1–4] for an overview and a comprehensive introduction to the theory.

The *covariant quantization* approach focuses on defining the gravitational path integral of the theory:

$$Z_{\text{gr}} = \int \mathcal{D}g\, e^{iS_{\text{gr}}[g]}. \tag{1}$$

In order to give the rigorous definition of the path integral, the classical action of the theory S_{gr} is written as a sum of the topological *BF* action, i.e. the action with no propagating degrees of freedom, and the part featuring the simplicity constraints, i.e. sum of products of Langrange multipliers and the corresponding simplicity constraints imposed on the variables of the topological part of the action. Next, one defines the path-integral of the topological theory given by the *BF* action, using the topological quantum field theory (TQFT) formalism. Once a path-integral is defined for the topological sector, it is deformed into a non-topological theory, by imposing the simplicity constraints. This quantization technique is known as the *spinfoam quantization* method.

The spinfoam quantization procedure has been successfully employed in various theories, including the three-dimensional topological Ponzano–Regge model of quantum gravity [5], the four-dimensional topological Ooguri model [6], the Barrett–Crane model of gravity in four dimensions [7–9], and others. The most successful among these is the renowned EPRL/FK model [10, 11], which had been specifically formulated to correspond to the quantum theory of gravity obtained by the *canonical loop quantization*, where a state of the gravitational field is described by the so-called *spin network*.

However, note that all mentioned models, formulated as constrained *BF* actions, are theories of pure gravity, without matter fields. Recently, as an endeavor to formulate a theory that unifies all the known interactions, one interesting new avenue of research has been opened, based on a categorical generalization of the *BF* action in the context of higher gauge theory (HGT) formalism [12]. One novel candidate discussed in the literature [13], uses the three-group structure to formulate the 3*BF* action as a categorical generalization of the *BF* theory. Then, modifying the pure 3*BF* action by adding the appropriate simplicity constraints, one obtains the *constrained* 3*BF* action, describing the theory of all the fields present in the standard model coupled in a standard way to Einstein–Cartan gravity.

Once the appropriate classical theory has been constructed, one needs to quantize it by constructing a topological state sum Z using the algebraic structure underlying the topological sector of the constrained 3*BF* action, i.e. the underlying two-crossed module. This construction has been recently carried out in [14], where a triangulation independent state sum Z of a topological HGT for an arbitrary two-crossed module and a four-dimensional closed and orientable spacetime manifold $\mathcal{M}_4$ is defined. Once the topological state sum is formulated, one could proceed to modify the amplitudes of the state sum in order to impose the simplicity constraints and obtain the state sum describing the full theory. In this way one would finally arrive at the rigorous definition of a path integral given by the equation (1).

In addition to the covariant approach, one can also study the constrained 3*BF* action, using the *canonical quantization*. This approach focuses on defining the quantum theory via a triple $(\mathcal{H}, \mathcal{A}, W)$, i.e. the Hilbert space of states $\mathcal{H}$, the algebra of observables $\mathcal{A}$, and the dynamics W given by the transition amplitudes. Specifically, in canonical LQG, the algebra of fields that are promoted to the quantum operators is chosen to be the algebra based on the holonomies of the gravitational connection. However, in the case of the 3*BF* theory, the notion of connection is generalized to the notion of three-connection, which makes its canonical quantization approach an interesting avenue of research. The first step toward the canonical quantization of the theory is the Hamiltonian analysis, resulting in the algebra of first-class and second-class constraints. The first-class constraints become conditions on the physical states determining the Hilbert space, while the Hamiltonian constraint determines the dynamics.

The results presented in this paper are the natural continuation of the results presented in [13]. The main result is the calculation of the full symmetry group of the pure 3*BF* action. To that end, the complete Hamiltonian analysis of the 3*BF* action for a semistrict Lie three-group is performed by using the Dirac procedure (see [15] for an overview and a comprehensive introduction to the Hamiltonian analysis). It is a generalization of the Hamiltonian analysis of a 2*BF* action performed in [16–19], and of the Hamiltonian analysis for the special case of a two-crossed module corresponding to the theory of scalar electrodynamics, carried out in [20]. The analysis of the Hamiltonian structure of the theory gives us the algebra of first-class and second-class constraints present in the theory. As usual, the first-class constraints generate gauge transformations, which do not change the physical state of the system. Using the Castellani's procedure, one can find the generator of the gauge transformations in the theory on a spatial hypersurface. Then, the results obtained by this method are generalized to the whole spacetime. The complete gauge symmetry, consisting of five types of finite gauge transformations, along with the proofs that they are indeed the gauge symmetries of 3*BF* action, is presented. With these results in hand, the structure of the full gauge symmetry group is analyzed, and its corresponding Lie algebra is determined.

The obtained results give rise to a connection between the gauge symmetry group of the 3*BF* action, and its underlining three-group structure, establishing a *duality* between the two. This analysis is an important step towards the study of the gauge symmetry group of the theory of gravity with matter, formulated as the constrained 3*BF* action [13], as well as its canonical quantization. Furthermore, it is important for the overall understanding of the physical meaning of the three-group structure and its interpretation as the underlining symmetry of the pure 3*BF* action, which represents a basis for the constrained 3*BF* action describing the physical theory.

The layout of the paper is as follows. In section 2, we give a brief overview of *BF* and 2*BF* theories, and introduce the 3*BF* action. Section 3 contains the Hamiltonian analysis for the 3*BF* theory. In subsection 3.1, the canonical structure of the theory is obtained, while in subsection 3.2 the resulting first-class and second-class constraints present in the theory, as well as the algebra of constraints, are presented. In the subsection 3.3 we analyze the Bianchi identities (BI) that the first-class constraints satisfy, which enforce restrictions in the sense of Hamiltonian analysis, and reduce the number of independent first-class constraints present in the theory. We then proceed with the counting of the physical degrees of freedom. Finally, this section concludes with the subsection 3.4 where we construct the generator of the gauge symmetries for the topological theory, based on the calculations done in section 3.2.

Section 4 contains the main results of our paper and is devoted to the analysis of the symmetries of the 3*BF* action. Having results of the subsection 3.4 in hand, we find the form variations of all variables and their canonical momenta, and use that result to determine all gauge transformations of the theory. This is done in four steps. The subsection 4.1 deals with the gauge group G, and the corresponding G-gauge transformations. In subsection 4.2 we discuss the gauge group $\tilde{H}_L$ which consists of the H-gauge and L-gauge transformations (familiar from [21]), while the subsection 4.3 examines the novel M-gauge and N-gauge transformations which also arise in the theory. The results of the subsections 4.1–4.3 are summarized in subsection 4.4, where the complete structure of the symmetry group is presented, including its Lie algebra. Our concluding remarks are given in section 5, containing a summary and a discussion of the obtained results, as well as possible future lines of investigation. The appendices contain various technical details concerning three-groups, additional relations of the constraint algebra, the computation of the generator of gauge symmetries, form-variations of all fields and momenta, and some other technical details.

Our notation and conventions are as follows. Spacetime indices, denoted by the mid-alphabet Greek letters $\mu, \nu, \ldots$, are raised and lowered by the spacetime metric $g_{\mu\nu}$. The spatial part of these is denoted with lowercase mid-alphabet Latin indices $i, j, \ldots$, and the time component is denoted with 0. The indices that are counting the generators of groups G, H, and L are denoted with initial Greek letters $\alpha, \beta, \ldots$, lowercase initial Latin letters $a, b, c, \ldots$, and uppercase Latin indices $A, B, C, \ldots$, respectively. The antisymmetrization over two indices is denoted as $A_{[a_1|a_2\ldots a_{n-1}|a_n]} = \frac{1}{2}\left(A_{a_1a_2\ldots a_{n-1}a_n} - A_{a_na_2\ldots a_{n-1}a_1}\right)$, while the total antisymmetrization is denoted as $A_{[a_1\ldots a_n]} = \frac{1}{n!}\sum_{\sigma\in S_n}(-1)^{\mathrm{sgn}(\sigma)}A_{a_{\sigma(1)}\ldots a_{\sigma(n)}}$. Likewise, the symmetrization over two indices is denoted as $A_{(a_1|a_2\ldots a_{n-1}|a_n)} = \frac{1}{2}\left(A_{a_1a_2\ldots a_{n-1}a_n} + A_{a_na_2\ldots a_{n-1}a_1}\right)$, while the total symmetrization is denoted as $A_{(a_1\ldots a_n)} = \frac{1}{n!}\sum_{\sigma\in S_n}A_{a_{\sigma(1)}\ldots a_{\sigma(n)}}$. We work in the natural system of units, defined by $c = \hbar = 1$ and $G = l_{\mathrm{p}}^2$, where l_{p} is the Planck length. All additional notation and conventions used throughout the paper are explicitly defined in the text where they appear.

2. The 3*BF* theory

Given a Lie group G and its corresponding Lie algebra $\mathfrak{g}$, one can introduce the so-called *BF* action as

$$S_{BF} = \int_{\mathcal{M}_4} \langle B \wedge F \rangle_{\mathfrak{g}}, \tag{2}$$

where $F \equiv \mathrm{d}\alpha + \alpha \wedge \alpha$ is the curvature two-form for the algebra-valued connection one-form $\alpha \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{g})$ on a trivial principal G-bundle over a four-dimensional compact and orientable spacetime manifold $\mathcal{M}_4$, and $B \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{g})$ is a Lagrange multiplier two-form. The $\langle \_, \_ \rangle_{\mathfrak{g}}$ denotes the G-invariant bilinear symmetric nondegenerate form on $\mathfrak{g}$. For more details see [22–24].

Varying the action (2) with respect to the Lagrange multiplier B and the connection α, one obtains the equations of motion,

$$F = 0, \qquad \nabla B \equiv \mathrm{d}B + \alpha \wedge B = 0. \tag{3}$$

These equations of motion imply that α is a flat connection, while the Lagrange multiplier B is a constant field. Therefore, the theory given by the *BF* action has no local propagating degrees of freedom, i.e. the theory is topological.

Within the framework of HGT, one can define the categorical generalization of the *BF* action to the so-called 2*BF* action, by passing from the notion of a gauge group to the notion of a gauge two-group, see [25–27]. In the category theory, a two-group is defined as a two-category consisting of only one object, where all the morphisms and two-morphisms are invertible. It has been shown that every strict two-group is equivalent to a crossed module $(H \xrightarrow{\partial} G, \triangleright)$, where G and H are groups, δ is a homomorphism from H to G, while $\triangleright : G \times H \to H$ is an action of G on H. Given a crossed-module $(H \xrightarrow{\partial} G, \triangleright)$, one can introduce a generalization of the *BF* action, the so-called 2*BF* action [25, 26]:

$$S_{2BF} = \int_{\mathcal{M}_4} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} + \langle C \wedge \mathcal{G} \rangle_{\mathfrak{h}}, \tag{4}$$

where the two-form $B \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{g})$ and the one-form $C \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{h})$ are Lagrange multipliers, and $\mathfrak{h}$ is a Lie algebra of the Lie group H. The variables $\mathcal{F} \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{g})$ and $\mathcal{G} \in \mathcal{A}^3(\mathcal{M}_4, \mathfrak{h})$ define the *fake* two-*curvature* $(\mathcal{F}, \mathcal{G})$ for the two-connection (α, β) on a trivial principal two-bundle over a four-dimensional compact and oriented spacetime manifold $\mathcal{M}_4$. See [28] for a rigorous definition. Here the two-connection (α, β) is given by $\mathfrak{g}$-valued one-form $\alpha \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{g})$ and an $\mathfrak{h}$-valued two-form $\beta \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{h})$:

$$\mathcal{F} = \mathrm{d}\alpha + \alpha \wedge \alpha - \partial\beta, \qquad \mathcal{G} = \mathrm{d}\beta + \alpha \wedge^{\triangleright} \beta. \tag{5}$$

The two-curvature $(\mathcal{F}, \mathcal{G})$ is called *fake*, because of the additional term $\partial\beta$, see [12]. Also, $\langle \_, \_ \rangle_{\mathfrak{g}}$ and $\langle \_, \_ \rangle_{\mathfrak{h}}$ denote the G-invariant bilinear symmetric nondegenerate forms for the algebras $\mathfrak{g}$ and $\mathfrak{h}$, respectively. See [25, 26] for review and references. Varying the 2*BF* action (4) with respect to variables B and C one obtains the equations of motion

$$\mathcal{F} = 0, \qquad \mathcal{G} = 0, \tag{6}$$

while varying with respect to α and β one obtains

$$\mathrm{d}B_\alpha - f_{\alpha\beta}{}^{\gamma} B_\gamma \wedge \alpha^\beta - \triangleright_{\alpha a}{}^{b} C_b \wedge \beta^a = 0, \tag{7}$$

$$\mathrm{d}C_a - \partial_a{}^{\alpha} B_{\alpha} + \triangleright_{\alpha a}{}^{b} C_b \wedge \alpha^{\alpha} = 0. \tag{8}$$

Here, the coefficients $f_{\alpha\beta}{}^{\gamma}$ are the structure constants of the algebra $\mathfrak{g}$, $\triangleright_{\alpha a}{}^{b}$ are the coefficients of the action $\triangleright$ of the algebra $\mathfrak{g}$ on $\mathfrak{h}$, while $\partial_a{}^{\alpha}$ are the coefficients of the map ∂, given in the bases of algebras $\mathfrak{g}$ and $\mathfrak{h}$ (see the equations (10)–(12) below). Similarly to the case of the *BF* action, the 2*BF* action defines a topological theory, i.e. a theory with no propagating degrees of freedom, see [16, 19].

Continuing the categorical generalization one step further, one can generalize the notion of a two-group to the notion of a three-group. Similarly to the definition of a group and a two-group within the category theory formalism, a three-group is defined as a three-category with only one object, where all morphisms, two-morphisms, and three-morphisms are invertible. Moreover, analogously as a strict two-group is equivalent to a crossed-module, it has been proved that a semistrict three-group is equivalent to a two-crossed module [29].

A Lie two-crossed module, denoted as $(L \xrightarrow{\delta} H \xrightarrow{\partial} G, \triangleright, \{\_,\_\}_{\mathrm{pf}})$ (see appendix A for the precise definition), is an algebraic structure specified by three Lie groups G, H, and L, together with the homomorphisms $\delta : L \to H$ and $\partial : H \to G$, an action $\triangleright$ of the group G on all three groups, and a G-equivariant map, called the Peiffer lifting:

$$\{\_,\_\}_{\mathrm{pf}} : H \times H \to L.$$

In order for this structure to be a three-group, the structure constants of algebras $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$, together with the maps ∂ and δ, the action $\triangleright$, and the Peiffer lifting, must satisfy certain axioms, see [13]. Here $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$ denote the Lie algebras corresponding to the Lie groups G, H, and L.

Analogously to the definition of a two-connection given in [28], one can define a three-connection as follows. Given a two-crossed module and a four-dimensional compact and orientable spacetime manifold $\mathcal{M}_4$, one can introduce a trivial principal three-bundle using the two-crossed module as a fiber over the base manifold $\mathcal{M}_4$. See [21, 29] for the precise definition of a corresponding three-holonomy. This gives rise to a three-connection, which can be represented as an ordered triple (α, β, γ), where α, β, and γ are algebra-valued differential forms, $\alpha \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{g})$, $\beta \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{h})$, and $\gamma \in \mathcal{A}^3(\mathcal{M}_4, \mathfrak{l})$. The corresponding fake three-curvature $(\mathcal{F}, \mathcal{G}, \mathcal{H})$ is defined as:

$$\mathcal{F} = \mathrm{d}\alpha + \alpha \wedge \alpha - \partial\beta, \quad \mathcal{G} = \mathrm{d}\beta + \alpha \wedge^{\triangleright} \beta - \delta\gamma, \quad \mathcal{H} = \mathrm{d}\gamma + \alpha \wedge^{\triangleright} \gamma + \{\beta \wedge \beta\}_{\mathrm{pf}}. \tag{9}$$

Similarly as in the case of the 2*BF* theory, the three-curvature $(\mathcal{F}, \mathcal{G}, \mathcal{H})$ is called *fake*, because of the additional terms $\partial\beta$, $\delta\gamma$, and $\{\beta \wedge \beta\}_{\mathrm{pf}}$. Fixing the bases in algebras $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$ as $\tau_\alpha \in \mathfrak{g}$, $t_a \in \mathfrak{h}$, and $T_A \in \mathfrak{l}$, one defines the structure constants

$$[\tau_\alpha, \tau_\beta] = f_{\alpha\beta}{}^{\gamma}\, \tau_\gamma, \qquad [t_a, t_b] = f_{ab}{}^{c}\, t_c, \qquad [T_A, T_B] = f_{AB}{}^{C}\, T_C, \tag{10}$$

maps $\partial : H \to G$ and $\delta : L \to H$ as

$$\partial(t_a) = \partial_a{}^{\alpha}\, \tau_\alpha, \qquad \delta(T_A) = \delta_A{}^{a}\, t_a, \tag{11}$$

and an action of $\mathfrak{g}$ on the generators of $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$ as

$$\tau_\alpha \triangleright \tau_\beta = f_{\alpha\beta}{}^{\gamma}\, \tau_\gamma, \qquad \tau_\alpha \triangleright t_a = \triangleright_{\alpha a}{}^{b}\, t_b, \qquad \tau_\alpha \triangleright T_A = \triangleright_{\alpha A}{}^{B}\, T_B, \tag{12}$$

respectively. To define the Peiffer lifting in a basis, one specifies the coefficients $X_{ab}{}^{A}$:

$$\{t_a,\, t_b\}_{\mathrm{pf}} = X_{ab}{}^{A} T_A. \tag{13}$$

Writing the curvature in the bases of the corresponding algebras and differential forms

$$\mathcal{F} = \frac{1}{2}\mathcal{F}^{\alpha}{}_{\mu\nu}\tau_{\alpha}\mathrm{d}x^{\mu}\wedge\mathrm{d}x^{\nu}, \quad \mathcal{G} = \frac{1}{3!}\mathcal{G}^{a}{}_{\mu\nu\rho}t_{a}\mathrm{d}x^{\mu}\wedge\mathrm{d}x^{\nu}\wedge\mathrm{d}x^{\rho},$$
$$\mathcal{H} = \frac{1}{4!}\mathcal{H}^{A}{}_{\mu\nu\rho\sigma}T_{A}\mathrm{d}x^{\mu}\wedge\mathrm{d}x^{\nu}\wedge\mathrm{d}x^{\rho}\wedge\mathrm{d}x^{\sigma},$$

one obtains the corresponding components:

$$\begin{aligned}
\mathcal{F}^{\alpha}{}_{\mu\nu} &= \partial_{\mu}\alpha^{\alpha}{}_{\nu} - \partial_{\nu}\alpha^{\alpha}{}_{\mu} + f_{\beta\gamma}{}^{\alpha}\alpha^{\beta}{}_{\mu}\alpha^{\gamma}{}_{\nu} - \beta^{a}{}_{\mu\nu}\partial_{a}{}^{\alpha},\\
\mathcal{G}^{a}{}_{\mu\nu\rho} &= \partial_{\mu}\beta^{a}{}_{\nu\rho} + \partial_{\nu}\beta^{a}{}_{\rho\mu} + \partial_{\rho}\beta^{a}{}_{\mu\nu}\\
&\quad + \alpha^{\alpha}{}_{\mu}\beta^{b}{}_{\nu\rho}\rhd_{\alpha b}{}^{a} + \alpha^{\alpha}{}_{\nu}\beta^{b}{}_{\rho\mu}\rhd_{\alpha b}{}^{a} + \alpha^{\alpha}{}_{\rho}\beta^{b}{}_{\mu\nu}\rhd_{\alpha b}{}^{a} - \gamma^{A}{}_{\mu\nu\rho}\delta_{A}{}^{a},\\
\mathcal{H}^{A}{}_{\mu\nu\rho\sigma} &= \partial_{\mu}\gamma^{A}{}_{\nu\rho\sigma} - \partial_{\nu}\gamma^{A}{}_{\rho\sigma\mu} + \partial_{\rho}\gamma^{A}{}_{\sigma\mu\nu} - \partial_{\sigma}\gamma^{A}{}_{\mu\nu\rho}\\
&\quad + 2\beta^{a}{}_{\mu\nu}\beta^{b}{}_{\rho\sigma}X_{(ab)}{}^{A} - 2\beta^{a}{}_{\mu\rho}\beta^{b}{}_{\nu\sigma}X_{(ab)}{}^{A} + 2\beta^{a}{}_{\mu\sigma}\beta^{b}{}_{\nu\rho}X_{(ab)}{}^{A}\\
&\quad + \alpha^{\alpha}{}_{\mu}\gamma^{B}{}_{\nu\rho\sigma}\rhd_{\alpha B}{}^{A} - \alpha^{\alpha}{}_{\nu}\gamma^{B}{}_{\rho\sigma\mu}\rhd_{\alpha B}{}^{A} + \alpha^{\alpha}{}_{\rho}\gamma^{B}{}_{\sigma\mu\nu}\rhd_{\alpha B}{}^{A}\\
&\quad - \alpha^{\alpha}{}_{\sigma}\gamma^{B}{}_{\mu\nu\rho}\rhd_{\alpha B}{}^{A}.
\end{aligned} \tag{14}$$

Then, similarly to the construction of BF and $2BF$ actions, one can define the gauge invariant topological $3BF$ action, with the underlying structure of a three-group. For the four-dimensional compact and orientable manifold $\mathcal{M}_4$ and the two-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G, \rhd, \{\_,\_\}_{\mathrm{pf}})$, that gives rise to three-curvature (9), one defines the $3BF$ action as

$$S_{3BF} = \int_{\mathcal{M}_4} \langle B\wedge\mathcal{F}\rangle_{\mathfrak{g}} + \langle C\wedge\mathcal{G}\rangle_{\mathfrak{h}} + \langle D\wedge\mathcal{H}\rangle_{\mathfrak{l}}, \tag{15}$$

where $B \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{g})$, $C \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{h})$, and $D \in \mathcal{A}^0(\mathcal{M}_4, \mathfrak{l})$ are Lagrange multipliers. The forms $\langle\_,\_\rangle_{\mathfrak{g}}$, $\langle\_,\_\rangle_{\mathfrak{h}}$, and $\langle\_,\_\rangle_{\mathfrak{l}}$ are G-invariant bilinear symmetric nondegenerate forms on $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$, respectively. Note that in the case of a semisimple Lie algebra, a natural choice for this bilinear form is the Killing form. However, one can also choose it differently, and moreover for a solvable Lie algebra one can introduce a non-trivial bilinear form, despite the fact that the Killing form is degenerate in this case. Fixing the basis in algebras $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$, as defined in (10), the forms $\langle\_,\_\rangle_{\mathfrak{g}}$, $\langle\_,\_\rangle_{\mathfrak{h}}$, and $\langle\_,\_\rangle_{\mathfrak{l}}$ map pairs of basis vectors of algebras $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$, to the metrics on their vector spaces, $g_{\alpha\beta}$, g_{ab}, and g_{AB}:

$$\langle\tau_\alpha, \tau_\beta\rangle_{\mathfrak{g}} = g_{\alpha\beta}, \qquad \langle t_a, t_b\rangle_{\mathfrak{h}} = g_{ab}, \qquad \langle T_A, T_B\rangle_{\mathfrak{l}} = g_{AB}. \tag{16}$$

As the symmetric maps are nondegenerate, the inverse metrics $g^{\alpha\beta}$, g^{ab}, and g^{AB} are well defined, and are used to raise and lower indices of the corresponding algebras.

Varying the action (15) with respect to Lagrange multipliers B^{α}, C^{a}, and D^{A} one obtains the equations of motion

$$\mathcal{F}^{\alpha} = 0, \qquad \mathcal{G}^{a} = 0, \qquad \mathcal{H}^{A} = 0, \tag{17}$$

while varying with respect to the three-connection variables α^α, β^a, and γ^A one gets:

$$\mathrm{d}B_\alpha - f_{\alpha\beta}{}^{\gamma} B_\gamma \wedge \alpha^\beta - \rhd_{\alpha a}{}^{b} C_b \wedge \beta^a + \rhd_{\alpha B}{}^{A} D_A \wedge \gamma^B = 0, \tag{18}$$

$$\mathrm{d}C_a - \partial_a{}^{\alpha} B_\alpha + \rhd_{\alpha a}{}^{b} C_b \wedge \alpha^\alpha + 2X_{(ab)}{}^{A} D_A \wedge \beta^b = 0, \tag{19}$$

$$\mathrm{d}D_A - \rhd_{\alpha A}{}^{B} D_B \wedge \alpha^\alpha + \delta_A{}^{a} C_a = 0. \tag{20}$$

For further details see [21, 29, 30] for the definition of the three-group, and [13] for the definition of the pure $3BF$ action.

Choosing the convenient underlying two-crossed module structure and imposing the appropriate simplicity constraints onto the degrees of freedom present in the $3BF$ action, one can obtain the non-trivial classical dynamics of the gravitational and matter fields. A reader interested in the construction of the constrained $2BF$ actions describing the Yang–Mills field and Einstein–Cartan gravity, and $3BF$ actions describing the Klein–Gordon, Dirac, Weyl and Majorana fields coupled to gravity in the standard way, is referred to [13, 27]. One can also introduce higher dimensional, nBF actions, see for example [31]. Various properties of these models have been studied in [32–34]. Naturally, if one is interested in theories defined on a four-dimensional spacetime manifold, there is an upper limit on the order of the differential forms one can use to construct a n-connection, and in four dimensions that is $n = 3$.

3. Hamiltonian analysis of the $3BF$ theory

In this section, the canonical structure of the theory is presented, with the resulting first-class and second-class constraints present in the theory. The algebra of Poisson brackets between all, the first-class and the second-class constraints, is obtained. We will use this result to calculate the total number of degrees of freedom in the theory, and in order to do that, we will have to analyse the BI that the first-class constraints satisfy, which enforce restrictions in the sense of Hamiltonian analysis. They reduce the number of independent first-class constraints present in the theory, thus increasing the number of degrees of freedom. We will obtain that the pure $3BF$ theory is topological, i.e. there are no local propagating degrees of freedom. Finally, we will finish this section with the construction of the generator of gauge symmetries of the $3BF$ action, which is used to calculate the form-variations of all the variables and their canonical momenta. This result will be crucial for finding the gauge symmetries of $3BF$ action, which will be a topic of section 4.

3.1. Canonical structure and Hamiltonian

Assuming that the spacetime manifold $\mathcal{M}_4$ is globally hyperbolic, the Lagrangian on a spatial foliation Σ_3 of spacetime $\mathcal{M}_4$ corresponding to the $3BF$ action (15) is given as:

$$L_{3BF} = \int_{\Sigma_3} \mathrm{d}^3\vec{x}\, \epsilon^{\mu\nu\rho\sigma} \left(\frac{1}{4} B^\alpha{}_{\mu\nu}\, \mathcal{F}^\beta{}_{\rho\sigma}\, g_{\alpha\beta} + \frac{1}{3!}\, C^a{}_\mu\, \mathcal{G}^b{}_{\nu\rho\sigma}\, g_{ab} + \frac{1}{4!} D^A \mathcal{H}^B{}_{\mu\nu\rho\sigma} g_{AB} \right). \tag{21}$$

For the Lagrangian (21), the canonical momenta corresponding to all variables $B^{\alpha}{}_{\mu\nu}$, $\alpha^{\alpha}{}_{\mu}$, $C^{a}{}_{\mu}$, $\beta^{a}{}_{\mu\nu}$, D^{A}, and $\gamma^{A}{}_{\mu\nu\rho}$ are:

$$
\begin{aligned}
\pi(B)_{\alpha}{}^{\mu\nu} &= \frac{\delta L}{\delta\partial_0 B^{\alpha}{}_{\mu\nu}} = 0,\\
\pi(\alpha)_{\alpha}{}^{\mu} &= \frac{\delta L}{\delta\partial_0 \alpha^{\alpha}{}_{\mu}} = \frac{1}{2}\epsilon^{0\mu\nu\rho}B_{\alpha\nu\rho},\\
\pi(C)_{a}{}^{\mu} &= \frac{\delta L}{\delta\partial_0 C^{a}{}_{\mu}} = 0,\\
\pi(\beta)_{a}{}^{\mu\nu} &= \frac{\delta L}{\delta\partial_0 \beta^{a}{}_{\mu\nu}} = -\epsilon^{0\mu\nu\rho}C_{a\rho},\\
\pi(D)_{A} &= \frac{\delta L}{\delta\partial_0 D^{A}} = 0,\\
\pi(\gamma)_{A}{}^{\mu\nu\rho} &= \frac{\delta L}{\delta\partial_0 \gamma^{A}{}_{\mu\nu\rho}} = \epsilon^{0\mu\nu\rho}D_{A}.
\end{aligned}
\tag{22}
$$

These momenta give rise to the six primary constraints of the theory, since none of them can be inverted for the time derivatives of the variables,

$$
\begin{aligned}
P(B)_{\alpha}{}^{\mu\nu} &\equiv \pi(B)_{\alpha}{}^{\mu\nu} \approx 0,\\
P(\alpha)_{\alpha}{}^{\mu} &\equiv \pi(\alpha)_{\alpha}{}^{\mu} - \frac{1}{2}\epsilon^{0\mu\nu\rho}B_{\alpha\nu\rho} \approx 0,\\
P(C)_{a}{}^{\mu} &\equiv \pi(C)_{a}{}^{\mu} \approx 0,\\
P(\beta)_{a}{}^{\mu\nu} &\equiv \pi(\beta)_{a}{}^{\mu\nu} + \epsilon^{0\mu\nu\rho}C_{a\rho} \approx 0,\\
P(D)_{A} &\equiv \pi(D)_{A} \approx 0,\\
P(\gamma)_{A}{}^{\mu\nu\rho} &\equiv \pi(\gamma)_{A}{}^{\mu\nu\rho} - \epsilon^{0\mu\nu\rho}D_{A} \approx 0.
\end{aligned}
\tag{23}
$$

Employing the following fundamental Poisson brackets,

$$
\begin{aligned}
\{\, B^{\alpha}{}_{\mu\nu}(\vec{x})\,,\, \pi(B)_{\beta}{}^{\rho\sigma}(\vec{y})\,\} &= 2\delta^{\alpha}_{\beta}\delta^{\rho}_{[\mu|}\delta^{\sigma}_{|\nu]}\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \alpha^{\alpha}{}_{\mu}(\vec{x})\,,\, \pi(\alpha)_{\beta}{}^{\nu}(\vec{y})\,\} &= \delta^{\alpha}_{\beta}\delta^{\nu}_{\mu}\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, C^{a}{}_{\mu}(\vec{x})\,,\, \pi(C)_{b}{}^{\nu}(\vec{y})\,\} &= \delta^{a}_{b}\delta^{\nu}_{\mu}\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \beta^{a}{}_{\mu\nu}(\vec{x})\,,\, \pi(\beta)_{b}{}^{\rho\sigma}(\vec{y})\,\} &= 2\delta^{a}_{b}\,\delta^{\rho}_{[\mu|}\delta^{\sigma}_{|\nu]}\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, D^{A}(\vec{x})\,,\, \pi(D)_{B}(\vec{y})\,\} &= \delta^{A}_{B}\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \gamma^{A}{}_{\mu\nu\rho}(\vec{x})\,,\, \pi(\gamma)_{B}{}^{\sigma\tau\xi}(\vec{y})\,\} &= 3!\delta^{A}_{B}\,\delta^{\sigma}_{[\mu}\delta^{\tau}_{\nu}\delta^{\xi}_{\rho]}\,\delta^{(3)}(\vec{x}-\vec{y}),
\end{aligned}
\tag{24}
$$

one obtains the *algebra of primary constraints*:

$$
\begin{aligned}
\{ P(B)_\alpha{}^{jk}(\vec{x})\,,\, P(\alpha)_\beta{}^{i}(\vec{y}) \} &= \epsilon^{0ijk}\, g_{\alpha\beta}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}),\\
\{ P(C)_a{}^{k}(\vec{x})\,,\, P(\beta)_b{}^{ij}(\vec{y}) \} &= -\epsilon^{0ijk}\, g_{ab}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}),\\
\{ P(D)_A(\vec{x})\,,\, P(\gamma)_B{}^{ijk}(\vec{y}) \} &= \epsilon^{0ijk}\, g_{AB}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}).
\end{aligned} \tag{25}
$$

Note that all other Poisson brackets vanish. The *canonical, on-shell Hamiltonian* is given by the following expression:

$$
\begin{aligned}
H_{\mathrm{c}} = \int_{\Sigma_3} \mathrm{d}^3\vec{x}\, \Bigg[&\frac{1}{2}\pi(B)_\alpha{}^{\mu\nu}\, \partial_0 B^\alpha{}_{\mu\nu} + \pi(\alpha)_\alpha{}^{\mu}\, \partial_0 \alpha^\alpha{}_\mu + \pi(C)_a{}^{\mu}\, \partial_0 C^a{}_\mu \\
&+ \frac{1}{2}\pi(\beta)_a{}^{\mu\nu}\, \partial_0 \beta^a{}_{\mu\nu} + \pi(D)_A\, \partial_0 D^A + \frac{1}{3!}\pi(\gamma)_A{}^{\mu\nu\rho}\, \partial_0 \gamma^A{}_{\mu\nu\rho} \Bigg] - L.
\end{aligned} \tag{26}
$$

Employing the definition of the curvature components (14), the Hamiltonian (26) can be written as the sum of terms that are equal to the product of the primary constraints and time derivatives of the variables, and the remainder. As the primary constraints are zero on-shell, the terms multiplying the time derivatives vanish, and the canonical Hamiltonian becomes:

$$
\begin{aligned}
H_{\mathrm{c}} = -\int_{\Sigma_3} \mathrm{d}^3\vec{x}\, \epsilon^{0ijk} \Bigg[&\frac{1}{2} B_{\alpha 0i}\, \mathcal{F}^\alpha{}_{jk} + \frac{1}{6} C_{a0}\, \mathcal{G}^a{}_{ijk} + \beta^a{}_{0i} \left(\nabla_j C_{ak} - \frac{1}{2}\partial_a{}^\alpha B_{\alpha\, jk} + \beta^b{}_{jk}\, D_A\, X_{(ab)}{}^A \right) \\
&+ \frac{1}{2}\alpha^\alpha{}_0 \left(\nabla_i B_{\alpha jk} - C_{ai} \rhd_{\alpha b}{}^a\, \beta^b{}_{jk} + \frac{1}{3} D_A \rhd_{\alpha B}{}^A\, \gamma^B{}_{ijk} \right) + \frac{1}{2}\gamma^A{}_{0ij} \left(\nabla_k D_A + C_{ak}\, \delta_A{}^a \right) \Bigg].
\end{aligned} \tag{27}
$$

Adding to the canonical Hamiltonian the product of the Lagrange multipliers λ and the primary constraints, for every primary constraint, one gets the *total, off-shell Hamiltonian*:

$$
\begin{aligned}
H_{\mathrm{T}} = H_{\mathrm{c}} + \int_{\Sigma_3} \mathrm{d}^3\vec{x}\, \Bigg[&\frac{1}{2}\lambda(B)^\alpha{}_{\mu\nu} P(B)_\alpha{}^{\mu\nu} + \lambda(\alpha)^\alpha{}_\mu P(\alpha)_\alpha{}^\mu + \lambda(C)^a{}_\mu P(C)_a{}^\mu + \frac{1}{2}\lambda(\beta)^a{}_{\mu\nu} P(\beta)_a{}^{\mu\nu} \\
&+ \lambda(D)^A P(D)_A + \frac{1}{3!}\lambda(\gamma)^A{}_{\mu\nu\rho} P(\gamma)_A{}^{\mu\nu\rho} \Bigg].
\end{aligned} \tag{28}
$$

3.2. Consistency conditions and algebra of constraints

In order for primary constraints to be preserved during the evolution of the system, they must satisfy the consistency conditions,

$$
\dot{P} \equiv \{ P\,,\, H_{\mathrm{T}} \} \approx 0, \tag{29}
$$

for every primary constraint P. Imposing this condition on primary constraints $P(B)_\alpha{}^{0i}$, $P(\alpha)_\alpha{}^0$, $P(C)_a{}^0$, $P(\beta)_a{}^{0i}$, and $P(\gamma)_A{}^{0ij}$, one obtains the secondary constraints $\mathcal{S}$,

$$
\begin{aligned}
\mathcal{S}(\mathcal{F})_\alpha{}^i &\equiv \frac{1}{2}\epsilon^{0ijk}\mathcal{F}_{\alpha jk} \approx 0,\\
\mathcal{S}(\nabla B)_\alpha &\equiv \frac{1}{2}\epsilon^{0ijk}\left(\nabla_{[i}B_{\alpha\, jk]} - C_{a[i}\rhd_{\alpha b}{}^a\,\beta^b{}_{jk]} + \frac{1}{3}D_A\rhd_{\alpha B}{}^A\,\gamma^B{}_{ijk}\right) \approx 0,\\
\mathcal{S}(\mathcal{G})_a &\equiv \frac{1}{6}\epsilon^{0ijk}\mathcal{G}_{aijk} \approx 0,\\
\mathcal{S}(\nabla C)_a{}^i &\equiv \epsilon^{0ijk}\left(\nabla_{[j|}C_{a|k]} - \frac{1}{2}\partial_a{}^\alpha B_{\alpha\, jk} + \beta^b{}_{jk}\,D_A\,X_{(ab)}{}^A\right) \approx 0,\\
\mathcal{S}(\nabla D)_A{}^{ij} &\equiv \epsilon^{0ijk}\left(\nabla_k D_A + C_{ak}\,\delta_A{}^a\right) \approx 0,
\end{aligned}
\tag{30}
$$

while in the case of the constraints $P(\alpha)_\alpha{}^k$, $P(B)_\alpha{}^{jk}$, $P(\beta)_a{}^{jk}$, $P(C)_a{}^k$, $P(\gamma)_A{}^{ijk}$, and $P(D)_A$ the corresponding consistency conditions determine the following Lagrange multipliers:

$$
\begin{aligned}
\lambda(B)_{\alpha ij} \approx\ & \nabla_i B_{\alpha 0j} - \nabla_j B_{\alpha 0i} + C_{a0}\beta^b{}_{ij}\rhd_{\alpha b}{}^a + C_{bi}\rhd_\alpha{}^b{}_a\beta^a{}_{0j}\\
& - C_{bj}\rhd_\alpha{}^b{}_a\beta^a{}_{0i} + g_{\beta\gamma}{}^\alpha\alpha^\beta{}_0 B^\gamma{}_{ij} + D_B\gamma^A{}_{0ij}\rhd_\alpha{}^B{}_A,\\
\lambda(\alpha)^\alpha{}_i \approx\ & \nabla_i\alpha^\alpha{}_0 + \partial_a{}^\alpha\beta^a{}_{0i},\\
\lambda(C)^a{}_i \approx\ & \nabla_i C^a{}_0 + C^b{}_i\rhd_\alpha{}^a{}_b\alpha^\alpha{}_0 - 2\beta_{b0i}D_A X^{(ba)A} + B_{\alpha 0i}\partial^{a\alpha},\\
\lambda(\beta)^a{}_{ij} \approx\ & \nabla_i\beta^a{}_{0j} - \nabla_j\beta^a{}_{0i} - \beta^b{}_{ij}\rhd_{\alpha b}{}^a\alpha^\alpha{}_0 + \gamma^A{}_{0ij}\delta_A{}^a,\\
\lambda(D)_A \approx\ & \alpha^\alpha{}_0 D_B\rhd_{\alpha A}{}^B - C_{a0}\delta_A{}^a,\\
\lambda(\gamma)^A{}_{ijk} \approx\ & -2\beta^a{}_{0i}\beta^b{}_{jk}X_{(ab)}{}^A + 2\beta^a{}_{0j}\beta^b{}_{ik}X_{(ab)}{}^A - 2\beta^a{}_{0k}\beta^b{}_{ij}X_{(ab)}{}^A\\
& - \alpha^\alpha{}_0\rhd_{\alpha B}{}^A\gamma^B{}_{ijk} + \nabla_i\gamma^A{}_{0jk} - \nabla_j\gamma^A{}_{0ik} + \nabla_k\gamma^A{}_{0ij}.
\end{aligned}
\tag{31}
$$

Note that the rest of the Lagrange multipliers

$$\lambda(B)^\alpha{}_{0i},\qquad \lambda(\alpha)^\alpha{}_0,\qquad \lambda(C)^a{}_0,\qquad \lambda(\beta)^a{}_{0i},\qquad \lambda(\gamma)^A{}_{0ij}, \tag{32}$$

remain undetermined.

Further, as the secondary constraints must also be preserved during the evolution of the system, the consistency conditions of secondary constraints must be enforced. However, no tertiary constraints arise from these conditions (see equation (B.1) in appendix B), leading the iterative procedure to an end. Finally, the total Hamiltonian can be written in the following form:

$$
\begin{aligned}
H_{\mathrm{T}} = \int_{\Sigma_3} \mathrm{d}^3\vec{x}\, \Big[& \lambda(B)^{\alpha}{}_{0i}\, \Phi(B)_{\alpha}{}^{i} + \lambda(\alpha)^{\alpha}\, \Phi(\alpha)_{\alpha} + \lambda(C)^{a}{}_{0}\, \Phi(C)_{a} + \lambda(\beta)^{a}{}_{0i}\, \Phi(\beta)_{a}{}^{i} \\
& + \frac{1}{2}\lambda(\gamma)^{A}{}_{0ij}\Phi(\gamma)_{A}{}^{ij} - B_{\alpha 0i}\, \Phi(\mathcal{F})^{ai} - \alpha_{\alpha 0}\, \Phi(\nabla B)^{\alpha} - C_{a0}\, \Phi(\mathcal{G})^{a} \\
& - \beta_{a0i}\, \Phi(\nabla C)^{ai} - \frac{1}{2}\gamma_{A0ij}\, \Phi(\nabla D)^{Aij} \Big],
\end{aligned}
\tag{33}
$$

where

$$
\begin{aligned}
\Phi(B)_{\alpha}{}^{i} &= P(B)_{\alpha}{}^{0i}, \\
\Phi(\alpha)_{\alpha} &= P(\alpha)_{\alpha}{}^{0}, \\
\Phi(C)_{a} &= P(C)_{a}{}^{0}, \\
\Phi(\beta)_{a}{}^{i} &= P(\beta)_{a}{}^{0i}, \\
\Phi(\gamma)_{A}{}^{ij} &= P(\gamma)_{A}{}^{0ij}, \\
\Phi(\mathcal{F})^{\alpha i} &= \mathcal{S}(\mathcal{F})^{\alpha i} - \nabla_{j} P(B)^{\alpha ij} - P(C)_{a}{}^{i}\partial^{a\alpha}, \\
\Phi(\mathcal{G})_{a} &= \mathcal{S}(\mathcal{G})_{a} + \nabla_{i} P(C)_{a}{}^{i} - \frac{1}{2}\beta_{bij} \rhd_{\alpha}{}^{b}{}_{a} P(B)^{\alpha ij} + P(D)^{A}\delta_{Aa}, \\
\Phi(\nabla C)_{a}{}^{i} &= \mathcal{S}(\nabla C)_{a}{}^{i} - \nabla_{j} P(\beta)_{a}{}^{ij} + C_{bj} \rhd_{\alpha}{}^{b}{}_{a} P(B)^{\alpha ij} \\
& \quad - \partial_{a}{}^{\alpha} P(\alpha)_{\alpha}{}^{i} + 2D_{A} X_{(ab)}{}^{A} P(C)^{bi} + \beta^{b}{}_{jk} X_{(ab)}{}^{A} P(\gamma)_{A}{}^{ijk}, \\
\Phi(\nabla B)_{\alpha} &= \mathcal{S}(\nabla B)_{\alpha} + \nabla_{i} P(\alpha)_{\alpha}{}^{i} - \frac{1}{2} f_{\alpha\gamma}{}^{\beta} B_{\beta ij} P(B)^{\gamma ij} - C_{bi} \rhd_{\alpha a}{}^{b} P(C)^{ai} \\
& \quad - \frac{1}{2}\beta_{bij} \rhd_{\alpha a}{}^{b} P(\beta)^{aij} - P(D)^{A} D_{B} \rhd_{\alpha A}{}^{B} + \frac{1}{3!} P(\gamma)_{A}{}^{ijk} \gamma^{B}{}_{ijk} \rhd_{\alpha B}{}^{A}, \\
\Phi(\nabla D)_{A}{}^{ij} &= \mathcal{S}(\nabla D)_{A}{}^{ij} + \nabla_{k} P(\gamma)_{A}{}^{ijk} - P(\beta)_{a}{}^{ij}\delta_{A}{}^{a} - P(B)^{\alpha ij} \rhd_{\alpha}{}^{B}{}_{A} D_{B},
\end{aligned}
\tag{34}
$$

are the first-class constraints. The second-class constraints in the theory are:

$$
\begin{aligned}
&\chi(B)_{\alpha}{}^{jk} = P(B)_{\alpha}{}^{jk}, \quad \chi(C)_{a}{}^{i} = P(C)_{a}{}^{i}, \quad \chi(D)_{A} = P(D)_{A}, \\
&\chi(\alpha)_{\alpha}{}^{i} = P(\alpha)_{\alpha}{}^{i}, \quad \chi(\beta)_{a}{}^{ij} = P(\beta)_{a}{}^{ij}, \quad \chi(\gamma)_{A}{}^{ijk} = P(\gamma)_{A}{}^{ijk}.
\end{aligned}
\tag{35}
$$

The PB algebra of the first-class constraints is given by

$$
\begin{aligned}
\{\, \Phi(\mathcal{F})^{\alpha i}(\vec{x})\,,\, \Phi(\nabla B)_{\beta}(\vec{y})\,\} &= f_{\beta\gamma}{}^{\alpha}\, \Phi(\mathcal{F})^{\gamma i}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \Phi(\nabla B)_{\alpha}(\vec{x})\,,\, \Phi(\nabla B)_{\beta}(\vec{y})\,\} &= f_{\alpha\beta}{}^{\gamma}\, \Phi(\nabla B)_{\gamma}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \Phi(\mathcal{G})^{a}(\vec{x})\,,\, \Phi(\nabla C)_{b}{}^{i}(\vec{y})\,\} &= -\rhd_{\alpha b}{}^{a}\, \Phi(\mathcal{F})^{\alpha i}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \Phi(\nabla C)_{a}{}^{i}(\vec{x})\,,\, \Phi(\nabla C)_{b}{}^{j}(\vec{y})\,\} &= -2X_{(ab)}{}^{A}\, \Phi(\nabla D)_{A}{}^{ij}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \Phi(\mathcal{G})^{a}(\vec{x})\,,\, \Phi(\nabla B)_{\alpha}(\vec{y})\,\} &= \rhd_{\alpha b}{}^{a}\, \Phi(\mathcal{G})^{b}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \Phi(\nabla C)^{ai}(\vec{x})\,,\, \Phi(\nabla B)_{\alpha}(\vec{y})\,\} &= \rhd_{\alpha b}{}^{a}\, \Phi(\nabla C)^{bi}(\vec{x})\, \delta^{(3)}(\vec{x}-\vec{y}),\\
\{\, \Phi(\nabla B)_{\alpha}(\vec{x})\,,\, \Phi(\nabla D)_{A}{}^{ij}(\vec{y})\,\} &= \rhd_{\alpha A}{}^{B}\Phi(\nabla D)_{B}{}^{ij}(\vec{x})\delta^{(3)}(\vec{x}-\vec{y}).
\end{aligned}
\tag{36}
$$

The algebra between the first and the second class constraints is given in the appendix B, equation (B.2).

With the algebra of the constraints in hand, one can proceed to calculate the generator of gauge symmetries of the action. The generator will be used to calculate the form-variations of all the variables and their canonical momenta, which will help us find the finite gauge symmetries of the action. Additionally, we can determine the number of independent parameters of gauge transformations, since usually all the first class constraints generate unphysical transformations of dynamical variables, i.e. that to each parameter of the gauge symmetry there corresponds one first-class constraint. However, before we embark on the construction of the symmetry generator, we will devote some attention to the number of local propagating degrees of freedom in the theory, in order to determine if the $3BF$ action is topological or not.

3.3. Number of degrees of freedom

In this subsection, we will show that the structure of the constraints implies that there are no local degrees of freedom in a $3BF$ theory. To that end, let us first specify all the BI present in the theory.

The two-form curvatures corresponding to one-forms α and C, given by

$$
F^{\alpha} = \mathrm{d}\alpha^{\alpha} + f_{\beta\gamma}{}^{\alpha}\, \alpha^{\beta}\wedge\alpha^{\gamma}, \qquad T^{a} = \mathrm{d}C^{a} + \rhd_{\alpha b}{}^{a}\, \alpha^{\alpha}\wedge C^{b}, \tag{37}
$$

satisfy the BI:

$$
\epsilon^{\lambda\mu\nu\rho}\, \nabla_{\mu} F^{\alpha}{}_{\nu\rho} = 0, \tag{38}
$$

$$
\epsilon^{\lambda\mu\nu\rho}\left(\nabla_{\mu} T^{a}{}_{\nu\rho} - \rhd_{\alpha b}{}^{a} F^{\alpha}{}_{\mu\nu} C^{b}{}_{\rho}\right) = 0. \tag{39}
$$

Similarly, the three-form curvatures corresponding to two-forms B and β, given by

$$
S^{\alpha} = \mathrm{d}B^{\alpha} + f_{\beta\gamma}{}^{\alpha}\, \alpha^{\beta}\wedge B^{\gamma}, \qquad G^{a} = \mathrm{d}\beta^{a} + \rhd_{\alpha b}{}^{a}\, \alpha^{\alpha}\wedge\beta^{\beta}, \tag{40}
$$

Table 1. The fields present in the $3BF$ theory.

$\alpha^{\alpha}{}_{\mu}$	$\beta^{a}{}_{\mu\nu}$	$\gamma^{A}{}_{\mu\nu\rho}$	$B^{\alpha}{}_{\mu\nu}$	$C^{a}{}_{\mu}$	D^{A}
$4p$	$6q$	$4r$	$6p$	$4q$	r

Table 2. Second-class constraints in the $3BF$ theory.

$\chi(B)_{\alpha}{}^{jk}$	$\chi(C)_{a}{}^{i}$	$\chi(D)_{A}$	$\chi(\alpha)_{\alpha}{}^{i}$	$\chi(\beta)_{a}{}^{ij}$	$\chi(\gamma)_{A}{}^{ijk}$
$3p$	$3q$	r	$3p$	$3q$	r

satisfy the BI:

$$\epsilon^{\lambda\mu\nu\rho}\left(\frac{2}{3}\nabla_{\lambda}S^{\alpha}{}_{\mu\nu\rho}-f_{\beta\gamma}{}^{\alpha}F^{\beta}{}_{\lambda\mu}B^{\gamma}{}_{\nu\rho}\right)=0, \tag{41}$$

$$\epsilon^{\lambda\mu\nu\rho}\left(\frac{2}{3}\nabla_{\lambda}G^{a}{}_{\mu\nu\rho}-\rhd_{\alpha b}{}^{a}F^{\alpha}{}_{\lambda\mu}\beta^{b}{}_{\nu\rho}\right)=0. \tag{42}$$

Finally, defining the one-form curvature for D,

$$Q^{A}=\mathrm{d}D^{A}+\rhd_{\alpha B}{}^{A}\alpha^{\alpha}\wedge D^{B}, \tag{43}$$

one can write the corresponding BI for Q^{A}:

$$\epsilon^{\lambda\mu\nu\rho}\left(\nabla_{\nu}Q^{A}{}_{\rho}-\frac{1}{2}\rhd_{\alpha B}{}^{A}F^{\alpha}{}_{\nu\rho}D^{B}\right)=0. \tag{44}$$

These BI play an important role in determining the number of degrees of freedom present in the theory.

As the general theory states, if there are N fields in the theory, F independent first-class constraints per space point, and S independent second-class constraints per space point, the number of independent field components, i.e. the number of the physical degrees of freedom present in the theory, is given by:

$$n=N-F-\frac{S}{2}. \tag{45}$$

Let p denote the dimensionality of the group G, q the dimensionality of the group H, and r the dimensionality of the group L. Determining the number of fields present in the $3BF$ theory, by counting the field components listed in table 1, one obtains $N=10(p+q)+5r$. Similarly, one determines the number of independent components of the second-class constraints by counting the components listed in table 2 and obtains $S=6(p+q)+2r$. However, when counting the number of the first-class constraints F one notes they are not all mutually independent. Namely, one can prove the following identities, as a consequence of the BI.

Taking the derivative of $\Phi(\mathcal{F})_{\alpha}{}^{i}$ one obtains

$$\nabla_{i}\Phi(\mathcal{F})^{\alpha i}+\partial_{a}{}^{\alpha}\Phi(\mathcal{G})^{a}=\frac{1}{2}\epsilon^{0ijk}\nabla_{i}F^{\alpha}{}_{jk}-\frac{1}{2}f_{\beta\gamma}{}^{\alpha}\mathcal{F}^{\beta}{}_{ij}P(B)^{ij}. \tag{46}$$

This relation gives

$$\nabla_{i}\Phi(\mathcal{F})^{\alpha i}+\partial_{a}{}^{\alpha}\Phi(\mathcal{G})^{a}=0, \tag{47}$$

since the first term on the right-hand side of (46) is zero off-shell because $\epsilon^{ijk}\nabla_i F^a{}_{jk} = 0$ are the $\lambda = 0$ components of BI (38), and the second term on the right-hand side is also zero off-shell, since it is a product of two constraints:

$$\frac{1}{2} f_{\beta\gamma}{}^{\alpha} \mathcal{F}^{\beta}{}_{ij} P(B)^{ij} = \frac{1}{2} f_{\beta\gamma}{}^{\alpha} \epsilon_{0ijk} \mathcal{S}(\mathcal{F})^{\beta k} P(B)^{ij} = 0. \tag{48}$$

The relation (47) means that p components of the first-class constraints $\Phi(\mathcal{F})^{\alpha i}$ and $\Phi(\mathcal{G})^a$ are not independent of the others. Furthermore, taking the derivative of $\Phi(\nabla C)_a{}^i$ one obtains

$$\begin{aligned} &\nabla_i \Phi(\nabla C)_a{}^i + C_{bi} \triangleright_{\alpha a}{}^b \Phi(\mathcal{F})^{\alpha i} + \partial_a{}^{\alpha} \Phi(\nabla B)_{\alpha} - \beta^b{}_{ij} X_{(ab)}{}^A \Phi(\nabla D)_A{}^{ij} - 2 D_A X_{(ab)}{}^A \, \Phi(\mathcal{G})^b \\ &\quad = \frac{1}{2} \epsilon^{0ijk} \left(\nabla_i T_{ajk} - \triangleright_{\alpha b}{}^a F^{\alpha}{}_{jk} C^b{}_i \right) - \frac{1}{2} \epsilon^{0ijk} \triangleright_{\alpha a}{}^b \, P(B)^{\alpha}{}_{ij} \, S(\nabla C)_{bk} \\ &\qquad + \epsilon^{0ijk} X_{(ab)}{}^A \, P(C)^b{}_i \, S(\nabla D)_{A\,jk} + \frac{1}{3} \epsilon^{0ijk} X_{(ab)}{}^A \, P(\gamma)^A{}_{ijk} \, S(\mathcal{G})^b + \frac{1}{2} \epsilon^{0ijk} \triangleright_{\alpha a}{}^b \, P(\beta)^b{}_{ij} \, S(\mathcal{F})^{\alpha}{}_k. \end{aligned} \tag{49}$$

Noting that the right-hand side of (49) is zero off-shell as the $\lambda = 0$ components of the BI (39), and the remaining terms on the right-hand side are zero off-shell as products of two constraints, one obtains the following relation:

$$\nabla_i \Phi(\nabla C)_a{}^i + C_{bi} \triangleright_{\alpha a}{}^b \Phi(\mathcal{F})^{\alpha i} + \partial_a{}^{\alpha} \Phi(\nabla B)_{\alpha} - \beta^b{}_{ij} X_{(ab)}{}^A \Phi(\nabla D)_A{}^{ij} - 2 D_A X_{(ab)}{}^A \Phi(\beta)^b = 0. \tag{50}$$

This relation means that q components of the constraints $\Phi(\nabla C)_a{}^i$, $\Phi(\mathcal{F})^{\alpha i}$, $\Phi(\nabla B)_{\alpha}$, $\Phi(\nabla D)_A{}^{ij}$, and $\Phi(\beta)^b$, are not independent of the others, further lowering the number of the independent first-class constraints. Finally, the following relation is satisfied

$$\begin{aligned} &\nabla^j \Phi(\nabla D)^A{}_{ij} - \triangleright_{\alpha B}{}^A D^B \Phi(\mathcal{F})_{\alpha i} - \delta^A{}_a \Phi(\nabla C)^a{}_i \\ &\quad = \epsilon_{0ijk} \left(\nabla^j Q_A{}^k + \frac{1}{2} \triangleright_{\alpha A}{}^B F^{\alpha jk} D_B \right) + \frac{1}{2} \epsilon^{0jkl} \triangleright_{\alpha B}{}^A \, P(\gamma)^B{}_{ijk} \, S(\mathcal{F})_{\alpha l} \\ &\qquad - \frac{1}{2} \epsilon^{0jkl} \triangleright_{\alpha B}{}^A \, P(B)^{\alpha}{}_{ij} \, S(\nabla D)^B{}_{kl}. \end{aligned} \tag{51}$$

Since the first term on the right-hand side is precisely the $\lambda = 0$ component of the BI (44), while the second and third terms are equal to zero as products of two constraints, this gives:

$$\nabla^j \Phi(\nabla D)^A{}_{ij} - \triangleright_{\alpha B}{}^A D^B \Phi(\mathcal{F})_{\alpha i} - \delta^A{}_a \Phi(\nabla C)^a{}_i = 0. \tag{52}$$

This relation suggests that $3r$ components of the primary constraints $\Phi(\nabla D)^A{}_{ij}$, $\Phi(\mathcal{F})_{\alpha i}$, and $\Phi(C)^a{}_i$ are not independent of the others. However, this is slightly misleading, since the covariant derivative of the BI (44) is automatically satisfied as a consequence of the BI (38),

$$\epsilon^{\lambda\mu\nu\rho} D^B \triangleright_{\alpha B}{}^A \nabla_{\mu} F^{\alpha}{}_{\nu\rho} = 0, \tag{53}$$

Table 3. First-class constraints in the 3*BF* theory.

$\Phi(B)_\alpha{}^i$	$\Phi(C)_a$	$\Phi(\alpha)_\alpha$	$\Phi(\beta)_a{}^i$	$\Phi(\gamma)_A{}^{ij}$	$\Phi(\mathcal{F})^{\alpha i}$	$\Phi(\mathcal{G})^a$	$\Phi(\nabla C)^{ai}$	$\Phi(\nabla B)^\alpha$	$\Phi(\nabla D)_A{}^{ij}$
$3p$	q	p	$3q$	$3r$	$3p-p$	q	$3q-q$	p	$3r-2r$

which means that there are in fact only $2r$ components of the constraint (52). A formal proof of this statement would involve evaluating the Wronskian of all first-class constraints, and is out of the scope of this paper.

The number of independent components of first-class constraints is determined by counting the components listed in table 3, and then subtracting the number of independent relations (47), (50) and (52).

Bearing the previous analysis in mind, one obtains the number of independent first-class constraints:

$$F = 8(p+q) + 6r - p - q - 2r = 7(p+q) + 4r.$$

Finally, using the definition (45), the number of degrees of freedom in the 3*BF* theory is:

$$n = 10(p+q) + 5r - 7(p+q) - 4r - \frac{6(p+q)+2r}{2} = 0. \tag{54}$$

Therefore, there are no local propagating degrees of freedom in a 3*BF* theory.

3.4. Symmetry generator

The unphysical transformations of dynamical variables are often referred to as gauge transformations. The gauge transformations are *local*, meaning that the parameters of the transformations are arbitrary functions of space and time. We shall now construct the generator of all gauge symmetries of the theory governed by the total Hamiltonian (33), using the Castellani's algorithm (see chapter 5 in [15] for a comprehensive overview of the procedure). The details of the construction are given in appendix C, and the following result is obtained

$$G = \int_{\Sigma_3} \mathrm{d}^3\vec{x} \left((\nabla_0 \epsilon_{\mathfrak{g}}{}^\alpha)\,(\tilde{G}_1)_\alpha + \epsilon_{\mathfrak{g}}{}^\alpha\,(\tilde{G}_0)_\alpha + (\nabla_0 \epsilon_{\mathfrak{h}}{}^a{}_i)\,(\tilde{H}_1)_a{}^i + \epsilon_{\mathfrak{h}}{}^a{}_i\,(\tilde{H}_0)_a{}^i + \frac{1}{2}(\nabla_0 \epsilon_{\mathfrak{l}}{}^A{}_{ij})\,(\tilde{L}_1)_A{}^{ij} \right.$$
$$\left. + \frac{1}{2}\epsilon_{\mathfrak{l}}{}^A{}_{ij}\,(\tilde{L}_0)_A{}^{ij} + (\nabla_0 \epsilon_{\mathfrak{m}}{}^\alpha{}_i)\,(\tilde{M}_1)_\alpha{}^i + \epsilon_{\mathfrak{m}}{}^\alpha{}_i\,(\tilde{M}_0)_\alpha{}^i + (\nabla_0 \epsilon_{\mathfrak{n}}{}^a)\,(\tilde{N}_1)_a + \epsilon_{\mathfrak{n}}{}^a (\tilde{N}_0)_a \right), \tag{55}$$

where

$$
\begin{aligned}
(\tilde{G}_1)_\alpha &= -\Phi(\alpha)_\alpha, \\
(\tilde{G}_0)_\alpha &= -\Big(f_{\alpha\gamma}{}^{\beta} B_{\beta 0i} \Phi(B)^{\gamma i} + C_{a0} \rhd_{\alpha b}{}^{a} \Phi(C)^{b0} + \beta_{a0i} \rhd_{\alpha b}{}^{a} \Phi(\beta)^{b0i} \\
&\quad - \frac{1}{2} \gamma^{A}{}_{0ij} \rhd_{\alpha A}{}^{B} \Phi(\gamma)_B{}^{ij} - \Phi(\nabla B)_\alpha \Big), \\
(\tilde{H}_1)_a{}^{i} &= -\Phi(\beta)_a{}^{i}, \\
(\tilde{H}_0)_a{}^{i} &= C_{b0} \rhd_{\alpha a}{}^{b} \Phi(B)^{\alpha i} - 2\beta^{b}{}_{0j} X_{(ab)}{}^{A} \Phi(\gamma)_A{}^{ij} + \Phi(\nabla C)_a{}^{i}, \\
(\tilde{L}_1)_a{}^{ij} &= \Phi(\gamma)_A{}^{ij}, \\
(\tilde{L}_0)_a{}^{ij} &= -\Phi(\nabla D)_A{}^{ij}, \\
(\tilde{M}_1)_\alpha{}^{i} &= -\Phi(B)_\alpha{}^{i}, \\
(\tilde{M}_0)_\alpha{}^{i} &= \Phi(\mathcal{F})_\alpha{}^{i}, \\
(\tilde{N}_1)_a &= -\Phi(C)_a, \\
(\tilde{N}_0)_a &= \beta_{b0i} \rhd_{\alpha a}{}^{b} \Phi(B)^{\alpha i} + \Phi(\mathcal{G})_a,
\end{aligned}
\tag{56}
$$

and $\epsilon_{\mathfrak{g}}{}^{\alpha}$, $\epsilon_{\mathfrak{h}}{}^{a}{}_{i}$, $\epsilon_{\mathfrak{l}}^{A}{}_{ij}$, $\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{i}$, and $\epsilon_{\mathfrak{n}}{}^{a}$ are the independent parameters of the gauge transformations.

The obtained gauge generator (55) is then employed to calculate the form variations of variables and their corresponding canonical momenta, denoted as $A(t,\vec{x})$, using the following equation,

$$
\delta_0 A(t,\vec{x}) = \{A(t,\vec{x}), G\}. \tag{57}
$$

The form variations of all fields and canonical momenta are given in appendix E, equation (E.2), while the algebra of the generators (56) is obtained in the appendix B, equations (B.4)–(B.10). However, one must bear in mind that the gauge generator (55) is the generator of the symmetry transformations on a slice of spacetime, i.e. on a hypersurface Σ_3. Having in hand all these results, specifically the form variations of all variables and their canonical momenta (E.2), we can determine the full gauge symmetry of the theory, which will be done in the next section.

4. Symmetries of the 3*BF* action

In order to systematically describe all gauge transformations of the 3*BF* action, we will discuss in turn each set of gauge parameters $\epsilon_{\mathfrak{g}}{}^{\alpha}$, $\epsilon_{\mathfrak{h}}{}^{a}{}_{i}$, $\epsilon_{\mathfrak{l}}^{A}{}_{ij}$, $\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{i}$, and $\epsilon_{\mathfrak{n}}{}^{a}$, appearing in (55). The subsection 4.1 deals with the gauge group G, and the G-gauge transformations, which are already familiar from the ordinary *BF* theory. In subsection 4.2 we discuss the gauge group $\tilde{H}_L$ which consists of the *H*-gauge and *L*-gauge transformations, familiar from the previous literature [21], while the subsection 4.3 examines the *M*-gauge and *N*-gauge transformations which are also present in the theory. Finally, the results of the subsections 4.1–4.3 will be summarized in the subsection 4.4, where we will present the complete structure of the gauge symmetry group.

4.1. Gauge group G

First, consider the infinitesimal transformation with the parameter ${\epsilon_{\mathfrak{g}}}^{\alpha}$, given by the form variations

$$
\begin{gathered}
\delta_0 {\alpha^{\alpha}}_{\mu} = -\partial_{\mu}{\epsilon_{\mathfrak{g}}}^{\alpha} - {f_{\beta\gamma}}^{\alpha}{\alpha^{\beta}}_{\mu}{\epsilon_{\mathfrak{g}}}^{\gamma}, \quad \delta_0 {B^{\alpha}}_{\mu\nu} = {f_{\beta\gamma}}^{\alpha}{\epsilon_{\mathfrak{g}}}^{\beta}{B^{\gamma}}_{\mu\nu}, \\
\delta_0 {\beta^{a}}_{\mu\nu} = {\rhd_{\alpha b}}^{a}{\epsilon_{\mathfrak{g}}}^{\alpha}{\beta^{b}}_{\mu\nu}, \quad \delta_0 {C^{a}}_{\mu} = {\rhd_{\alpha b}}^{a}{\epsilon_{\mathfrak{g}}}^{\alpha}{C^{b}}_{\mu}, \\
\delta_0 {\gamma^{A}}_{\mu\nu\rho} = {\rhd_{\alpha B}}^{A}{\epsilon_{\mathfrak{g}}}^{\alpha}{\gamma^{B}}_{\mu\nu\rho}, \quad \delta_0 D^{A} = {\rhd_{\alpha B}}^{A}{\epsilon_{\mathfrak{g}}}^{\alpha}D^{B},
\end{gathered}
\tag{58}
$$

which is analogous to writing the transformation as:

$$
\begin{gathered}
\alpha \to \alpha' = \alpha - \nabla\epsilon_{\mathfrak{g}}, \quad B \to B' = B - [B, \epsilon_{\mathfrak{g}}], \\
\beta \to \beta' = \beta + \epsilon_{\mathfrak{g}} \rhd \beta, \quad C \to C' = C + \epsilon_{\mathfrak{g}} \rhd C, \\
\gamma \to \gamma' = \gamma + \epsilon_{\mathfrak{g}} \rhd \gamma, \quad D \to D' = D + \epsilon_{\mathfrak{g}} \rhd D.
\end{gathered}
\tag{59}
$$

Based on these infinitesimal transformations, one can extrapolate the finite symmetry transformations, defined in the theorem 1.

Theorem 1 (G-gauge transformations). *In the* 3*BF theory for the two-crossed module* $(L \xrightarrow{\delta} H \xrightarrow{\partial} G, \rhd, \{\_,\_\}_{\mathrm{pf}})$, *the following transformation is a gauge symmetry,*

$$
\begin{gathered}
\alpha \to \alpha' = \mathrm{Ad}_g\alpha + g\mathrm{d}g^{-1}, \quad B \to B' = gBg^{-1}, \\
\beta \to \beta' = g \rhd \beta, \quad C \to C' = g \rhd C, \\
\gamma \to \gamma' = g \rhd \gamma, \quad D \to D' = g \rhd D,
\end{gathered}
\tag{60}
$$

where $g = \exp(\epsilon_{\mathfrak{g}} \cdot \hat{G}) = \exp({\epsilon_{\mathfrak{g}}}_{\alpha}\hat{G}^{\alpha}) \in G$, *and* $\epsilon_{\mathfrak{g}} : \mathcal{M}_4 \to \mathfrak{g}$ *is the parameter of the transformation.*

Proof. Note that if one considers an element of the group, $g \in G$, the transformations of the theorem 1 give rise to the following three-curvature transformation

$$
\mathcal{F} \to \mathcal{F}' = g\mathcal{F}g^{-1}, \qquad \mathcal{G} \to \mathcal{G}' = g \rhd \mathcal{G}, \qquad \mathcal{H} \to \mathcal{H}' = g \rhd \mathcal{H},
\tag{61}
$$

and the invariance of the $3BF$ action under this transformation follows from the G-invariance of the symmetric bilinear forms on $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$. _

Let us consider two subsequent infinitesimal G-gauge transformations, determined by the small parameters $\epsilon_{\mathfrak{g}1}^{\alpha}$ and $\epsilon_{\mathfrak{g}2}^{\beta}$. To calculate the commutator between the generators of the G-gauge transformations, we will make use of the Baker–Campbell–Hausdorff (BCH) formula in the case when the parameters of the transformations are small

$$
\mathrm{e}^{\epsilon_{\mathfrak{g}}{}^{\alpha}{}_{1}\hat{G}_{\alpha}}\mathrm{e}^{\epsilon_{\mathfrak{g}}{}^{\beta}{}_{2}\hat{G}_{\beta}} = \mathrm{e}^{\epsilon_{\mathfrak{g}}{}^{\alpha}{}_{1}\hat{G}_{\alpha}+\epsilon_{\mathfrak{g}}{}^{\beta}{}_{2}\hat{G}_{\beta}+\frac{1}{2}\epsilon_{\mathfrak{g}}{}^{\alpha}{}_{1}\,\epsilon_{\mathfrak{g}}{}^{\beta}{}_{2}\,[\hat{G}_{\alpha},\hat{G}_{\beta}]+O(\epsilon_{\mathfrak{g}}{}^{3})}, \tag{62}
$$

from which it follows:

$$
\mathrm{e}^{\epsilon_{\mathfrak{g}}{}^{\alpha}{}_{1}\hat{G}_{\alpha}}\mathrm{e}^{\epsilon_{\mathfrak{g}}{}^{\beta}{}_{2}\hat{G}_{\beta}} - \mathrm{e}^{\epsilon_{\mathfrak{g}}{}^{\beta}{}_{2}\hat{G}_{\beta}}\mathrm{e}^{\epsilon_{\mathfrak{g}}{}^{\alpha}{}_{1}\hat{G}_{\alpha}} = \epsilon_{\mathfrak{g}}{}^{\alpha}{}_{1}\,\epsilon_{\mathfrak{g}}{}^{\beta}{}_{2}\,[\hat{G}_{\alpha},\hat{G}_{\beta}] + O(\epsilon_{\mathfrak{g}}{}^{3}). \tag{63}
$$

Using the equation (63), we obtain that the generators of the G-gauge transformations defined in the theorem 1 satisfy the following commutation relations:

$$
[\hat{G}_{\alpha},\hat{G}_{\beta}] = f_{\alpha\beta}{}^{\gamma}\hat{G}_{\gamma}, \tag{64}
$$

where $f_{\alpha\beta}{}^{\gamma}$ are the structure constants of the algebra $\mathfrak{g}$. By noting that there exists an isomorphism between generators $\hat{G}_{\alpha} \cong \tau_{\alpha}$, one establishes that the group of the G-gauge transformations from the theorem 1 is the same as the group G of the two-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G, \triangleright, \{\_,\_\}_{\mathrm{pf}})$. This is an important result, which will not be true for the remaining symmetry transformations, as we shall see below.

4.2. The gauge group $\tilde{H}_L$

Let us now consider the form variations of the variables corresponding to the parameter $\epsilon_{\mathfrak{h}}{}^{a}{}_{i}$. For example, one can see from the equation (E.2) that the form-variation of the variables $\alpha^{\alpha}{}_{0}$ and $\alpha^{\alpha}{}_{i}$ are:

$$
\delta_0\alpha^{\alpha}{}_{o} = 0, \qquad \delta_0\alpha^{\alpha}{}_{i} = -\partial_a{}^{\alpha}\epsilon_{\mathfrak{h}}{}^{a}{}_{i}. \tag{65}
$$

Taking into account that the action of the generator (55) gives the symmetry transformations on one hypersurface Σ_3 with the time component of the parameter equal to zero, $\epsilon_{\mathfrak{h}}{}^{a}{}_{0} = 0$, one can extrapolate that for parameter of the spacetime gauge transformations $\epsilon_{\mathfrak{h}}{}^{a}{}_{\mu}$, the form-variation of the variable $\alpha^{\alpha}{}_{\mu}$ is given as:

$$
\delta_0\alpha^{\alpha}{}_{\mu} = -\partial_a{}^{\alpha}\epsilon_{\mathfrak{h}}{}^{a}{}_{\mu}, \tag{66}
$$

and similarly for the rest of the variables. Thus, the infinitesimal symmetry transformations in the whole spacetime corresponding to the parameter $\epsilon_{\mathfrak{h}}{}^{a}{}_{\mu}$ are given by the form variations:

$$
\begin{aligned}
&\delta_0\alpha^{\alpha}{}_{\mu} = -\partial_a{}^{\alpha}\epsilon_{\mathfrak{h}}{}^{a}{}_{\mu}, \quad \delta_0 B^{\alpha}{}_{\mu\nu} = 2C_{a[\mu|}\epsilon_{\mathfrak{h}}{}^{b}{}_{|\nu]}\triangleright_{\beta b}{}^{a}g^{\alpha\beta},\\
&\delta_0\beta^{a}{}_{\mu\nu} = -2\nabla_{[\mu|}\epsilon_{\mathfrak{h}}{}^{a}{}_{|\nu]}, \quad \delta_0 C^{a}{}_{\mu} = 2D_A X_{(ab)}{}^{A}\epsilon_{\mathfrak{h}}{}^{b}{}_{\mu},\\
&\delta_0\gamma^{A}{}_{\mu\nu\rho} = 3!\beta^{a}{}_{[\mu\nu}\epsilon_{\mathfrak{h}}{}^{b}{}_{\rho]}X_{(ab)}{}^{A}, \quad \delta_0 D = 0.
\end{aligned} \tag{67}
$$

For these infinitesimal transformations one obtains the finite symmetry transformations given in theorem 2.

Theorem 2 (H-gauge transformations). *In the 3BF theory for the two-crossed module* $(L \xrightarrow{\delta} H \xrightarrow{\partial} G, \triangleright, \{\_,\_\}_{\mathrm{pf}})$*, the following transformation is a symmetry:*

$$
\begin{aligned}
&\alpha \to \alpha' = \alpha - \partial\epsilon_{\mathfrak{h}}, \quad \beta \to \beta' = \beta - \nabla'\epsilon_{\mathfrak{h}} - \epsilon_{\mathfrak{h}} \wedge \epsilon_{\mathfrak{h}}, \\
&\gamma \to \gamma' = \gamma + \{\beta', \epsilon_{\mathfrak{h}}\}_{\mathrm{pf}} + \{\epsilon_{\mathfrak{h}}, \beta\}_{\mathrm{pf}}, \;\; B \to B' = B - C' \wedge^{\mathcal{T}} \epsilon_{\mathfrak{h}} - \epsilon_{\mathfrak{h}} \wedge^{\mathcal{D}} \epsilon_{\mathfrak{h}} \wedge^{\mathcal{D}} D, \\
&C \to C' = C - D \wedge^{\mathcal{X}_1} \epsilon_{\mathfrak{h}} - D \wedge^{\mathcal{X}_2} \epsilon_{\mathfrak{h}}, \quad D \to D' = D.
\end{aligned}
\tag{68}
$$

where $\epsilon_{\mathfrak{h}} \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{h})$ *is an arbitrary* $\mathfrak{h}$*-valued one-form, and* ∇' *denotes the covariant derivative with respect to the connection* α'*. The maps* $\mathcal{T}$*,* $\mathcal{D}$*,* $\mathcal{X}_1$*, and* $\mathcal{X}_2$ *are defined in appendix* D.

Proof. Note that the three-curvature transforms as

$$
\begin{aligned}
&\mathcal{F} \to \mathcal{F}' = \mathcal{F}, \\
&\mathcal{G} \to \mathcal{G}' = \mathcal{G} - \mathcal{F} \wedge^{\triangleright} \epsilon_{\mathfrak{h}}, \\
&\mathcal{H} \to \mathcal{H}' = \mathcal{H} + \{\mathcal{G}', \epsilon_{\mathfrak{h}}\}_{\mathrm{pf}} - \{\epsilon_{\mathfrak{h}}, \mathcal{G}\}_{\mathrm{pf}}.
\end{aligned}
\tag{69}
$$

Taking into account the transformations of the three-curvature (69) and the transformations of the Lagrange multipliers, the action S_{3BF} transforms as:

$$
\begin{aligned}
S'_{3BF} = S_{3BF} + \int_{\mathcal{M}_4} \big(& -\langle C' \wedge^{\mathcal{T}} \epsilon_{\mathfrak{h}}, \mathcal{F} \rangle_{\mathfrak{g}} - \langle \epsilon_{\mathfrak{h}} \wedge^{\mathcal{D}} \epsilon_{\mathfrak{h}} \wedge^{\mathcal{D}} D, \mathcal{F} \rangle_{\mathfrak{g}} \\
& - \langle C', \mathcal{F} \wedge^{\triangleright} \epsilon_{\mathfrak{h}} \rangle_{\mathfrak{h}} - \langle D \wedge^{\mathcal{X}_1} \epsilon_{\mathfrak{h}}, \mathcal{G} \rangle_{\mathfrak{h}} - \langle D \wedge^{\mathcal{X}_2} \epsilon_{\mathfrak{h}}, \mathcal{G} \rangle_{\mathfrak{h}} \\
& + \langle D, \{\mathcal{G}, \epsilon_{\mathfrak{h}}\}_{\mathrm{pf}} \rangle_{\mathfrak{l}} - \langle D, \{\mathcal{F} \wedge^{\triangleright} \epsilon_{\mathfrak{h}}, \epsilon_{\mathfrak{h}}\}_{\mathrm{pf}} \rangle_{\mathfrak{l}} - \langle D, \{\epsilon_{\mathfrak{h}}, \mathcal{G}\}_{\mathrm{pf}} \rangle_{\mathfrak{l}} \big) .
\end{aligned}
\tag{70}
$$

Using the definitions of the maps $\mathcal{T}, \mathcal{D}$, $\mathcal{X}_1$, and $\mathcal{X}_2$, given in appendix D, one sees that the terms in the parentheses cancel, specifically the first term with the third, second with seventh, fourth with eighth, and fifth with the sixth term. _

The H-gauge transformations do not form a group. Namely, one can check that the two consecutive H-gauge transformations do not give a transformation of the same kind, i.e. the closure axiom of the group is not satisfied. This is analogous to the well-known structure of Lorentz group, where boost transformations are not closed, and thus do not form a group. Indeed, one must consider both rotations and boosts to obtain the set of transformations that forms the Lorentz group. In the case of the H-gauge transformations, we will show that together with the H-gauge transformations one needs to consider the transformations corresponding to the parameter $\epsilon_{\mathfrak{l}}{}^{A}{}_{ij}$. From the equation (E.2) one reads the form-variations on a space hypersurface Σ_3 corresponding to this parameter. Similarly as it is done in the case of the H-gauge transformations, one extrapolates that the form-variations for all the variables corresponding to the parameter $\epsilon_{\mathfrak{l}}{}^{A}{}_{\mu\nu}$ are given as:

$$\begin{aligned}
&\delta_0 \alpha^{\alpha}{}_{\mu} = 0, \\
&\delta_0 B^{\alpha}{}_{\mu\nu} = -D_A \rhd_{\beta B}{}^{A} \epsilon_{\mathfrak{l}}{}^{B}{}_{\mu\nu} g^{\alpha\beta}, \\
&\delta_0 \beta^{a}{}_{\mu\nu} = \delta_A{}^{a} \epsilon_{\mathfrak{l}}^{A}{}_{\mu\nu}, \\
&\delta_0 C^{a}{}_{\mu} = 0, \quad \delta_0 \gamma^{A}{}_{\mu\nu\rho} = \nabla_{\mu} \epsilon_{\mathfrak{l}}^{A}{}_{\nu\rho} - \nabla_{\nu} \epsilon_{\mathfrak{l}}^{A}{}_{\mu\rho} + \nabla_{\rho} \epsilon_{\mathfrak{l}}^{A}{}_{\mu\nu}, \\
&\delta_0 D^{A} = 0.
\end{aligned} \tag{71}$$

These infinitesimal transformations correspond to the finite symmetry transformations defined in theorem 3.

Theorem 3 (*L*-gauge transformations). *In the 3BF theory for the two-crossed module* $(L \xrightarrow{\delta} H \xrightarrow{\partial} G, \rhd, \{\_,\_\}_{\mathrm{pf}})$*, the following transformation is a symmetry*

$$\begin{array}{ll}
\alpha \to \alpha' = \alpha, & B \to B' = B + D \wedge^{\mathcal{S}} \epsilon_{\mathfrak{l}}, \\
\beta \to \beta' = \beta + \delta \epsilon_{\mathfrak{l}}, & C \to C' = C, \\
\gamma \to \gamma' = \gamma + \nabla \epsilon_{\mathfrak{l}}, & D \to D' = D,
\end{array} \tag{72}$$

where $\epsilon_{\mathfrak{l}} \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{l})$ *is an arbitrary* $\mathfrak{l}$*-valued two-form, and the map* $\mathcal{S}$ *is defined in appendix* D.

Proof. Note that the three-curvature transforms as

$$\begin{array}{l}
\mathcal{F} \to \mathcal{F}' = \mathcal{F}, \\
\mathcal{G} \to \mathcal{G}' = \mathcal{G}, \\
\mathcal{H} \to \mathcal{H}' = \mathcal{H} + \mathcal{F} \wedge^{\rhd} \epsilon_{\mathfrak{l}}.
\end{array} \tag{73}$$

Taking into account the transformations (73) and the transformations of the Lagrange multipliers, the action transforms as:

$$S'_{3BF} = S_{3BF} + \int_{\mathcal{M}_4} \left(\langle D \wedge^{\mathcal{S}} \epsilon_{\mathfrak{l}}, \mathcal{F} \rangle_{\mathfrak{g}} + \langle D, \mathcal{F} \wedge^{\rhd} \epsilon_{\mathfrak{l}} \rangle_{\mathfrak{l}} \right). \tag{74}$$

According to the definition of the map $\mathcal{S}$, the terms in the parentheses cancel. _

Let us denote the generators of the H-gauge transformations given by the theorem 2 and the L-gauge transformations given by the theorem 3 as $\hat{H}_a{}^{\mu}$ and $\hat{L}_A{}^{\mu\nu}$, respectively. As we have commented above, one can now check that the transformations defined in the theorem 2, i.e. the H-gauge transformations, do not form a group. If one performs two consecutive H-gauge transformations, defined with parameters $\epsilon_{\mathfrak{h}1}$ and $\epsilon_{\mathfrak{h}2}$, one obtains

$$\mathrm{e}^{\epsilon_{\mathfrak{h}1} \cdot \hat{H}} \mathrm{e}^{\epsilon_{\mathfrak{h}2} \cdot \hat{H}} - \mathrm{e}^{\epsilon_{\mathfrak{h}2} \cdot \hat{H}} \mathrm{e}^{\epsilon_{\mathfrak{h}1} \cdot \hat{H}} = 2 \left(\{\epsilon_{\mathfrak{h}1} \wedge \epsilon_{\mathfrak{h}2}\}_{\mathrm{pf}} - \{\epsilon_{\mathfrak{h}2} \wedge \epsilon_{\mathfrak{h}1}\}_{\mathrm{pf}} \right) \cdot \hat{L}, \tag{75}$$

where $\epsilon_{\mathfrak{h}} \cdot \hat{H} = \epsilon_{\mathfrak{h}}{}^{a}{}_{\mu} \hat{H}_a{}^{\mu}$ and $\epsilon_{\mathfrak{l}} \cdot \hat{L} = \frac{1}{2} \epsilon_{\mathfrak{l}}{}^{A}{}_{\mu\nu} \hat{L}_A{}^{\mu\nu}$. Using the equation analogous to BCH formula (63), one obtains that the commutator of the generators of two H-gauge transformations is the generator of an L-gauge transformation (see appendix F for the details of the calculation):

$$\left[\hat{H}_a{}^{\mu}, \hat{H}_b{}^{\nu}\right] = 2X_{(ab)}{}^{A}\hat{L}_A{}^{\mu\nu}. \tag{76}$$

Next, note that the transformations defined in theorem 3 are the linear transformations, and the two subsequent L-gauge transformations give one L-gauge transformation with the parameter $\epsilon_{\mathfrak{l}1} + \epsilon_{\mathfrak{l}2}$. Formally, one can write the previous statement as

$$\mathrm{e}^{\epsilon_{\mathfrak{l}1}\cdot\hat{L}}\mathrm{e}^{\epsilon_{\mathfrak{l}2}\cdot\hat{L}} = \mathrm{e}^{(\epsilon_{\mathfrak{l}1}+\epsilon_{\mathfrak{l}2})\cdot\hat{L}}, \tag{77}$$

which leads to the conclusion that the generators of the L-gauge transformations are mutually commuting:

$$\left[\hat{L}_A{}^{\mu\nu}, \hat{L}_B{}^{\rho\sigma}\right] = 0. \tag{78}$$

Thus, the L-gauge transformations form an abelian group, which will be denoted as $\tilde{L}$. According to the index structure of the parameters and generators, we can conclude that the group $\tilde{L}$ is isomorphic to $\mathbb{R}^{6r}$, where r is the dimension of the group L:

$$\tilde{L} \cong \mathbb{R}^{6r}. \tag{79}$$

Our analogy with the case of the Lorentz group can once again prove useful, since the closure of the L-gauge transformations resembles the fact that the composition of two rotations is a rotation. The abelian group $\tilde{L}$ should not be confused with the non-abelian group L of the two-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G, \triangleright, \{\_,\_\}_{\mathrm{pf}})$.

Let us now examine the relationship between H-gauge transformations and L-gauge transformations. The following result,

$$\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot\hat{H}}\mathrm{e}^{\epsilon_{\mathfrak{l}}\cdot\hat{L}} = \mathrm{e}^{\epsilon_{\mathfrak{l}}\cdot\hat{L}}\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot\hat{H}}, \tag{80}$$

leads to the conclusion that the commutator of generators of the H-gauge transformations and generators of the L-gauge transformations vanishes:

$$\left[\hat{H}_a{}^{\mu}, \hat{L}_A{}^{\nu\rho}\right] = 0. \tag{81}$$

From the closure of the algebra (76), (78) and (81), one can conclude that the H-gauge transformations together with the L-gauge transformations form a group, which will be denoted as $\tilde{H}_L$. Lastly, the action of the group G on the H-gauge and L-gauge transformations is examined by calculating the expressions:

$$[\epsilon_{\mathfrak{g}}\cdot\hat{G}, \epsilon_{\mathfrak{h}}\cdot\hat{H}] = (\epsilon_{\mathfrak{g}} \triangleright \epsilon_{\mathfrak{h}})\cdot\hat{H}, \qquad [\epsilon_{\mathfrak{g}}\cdot\hat{G}, \epsilon_{\mathfrak{l}}\cdot\hat{L}] = (\epsilon_{\mathfrak{g}} \triangleright \epsilon_{\mathfrak{l}})\cdot\hat{L}, \tag{82}$$

which lead to the following commutators:

$$\begin{aligned} \left[\hat{G}_\alpha, \hat{H}_a{}^{\mu}\right] &= \triangleright_{\alpha a}{}^{b}\,\hat{H}_b{}^{\mu}, \\ \left[\hat{G}_\alpha, \hat{L}_A{}^{\mu\nu}\right] &= \triangleright_{\alpha A}{}^{B}\,\hat{L}_B{}^{\mu\nu}. \end{aligned} \tag{83}$$

Theorems 1–3 represent the G-, H-, and L-gauge transformations, which are already familiar from the previous literature (see for example [21, 30]).

4.3. The gauge groups M and N

Next, consider the infinitesimal transformation with the parameter $\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{i}$, given by the form variations in appendix E. In a similar manner as done in the previous subsection, one establishes that the form variations obtained as a result of the Hamiltonian analysis are transformations on one hypersurface Σ_3, from which one can guess the symmetry in the whole spacetime. Keeping in mind that the variations on the hypersurface have the time component of the parameter set to $\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{0} = 0$, one extrapolates the form-variations of the whole spacetime for the parameter $\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu}$ to be:

$$\begin{aligned}
&\delta_0 \alpha^{\alpha}{}_{\mu} = 0, \\
&\delta_0 B^{\alpha}{}_{\mu\nu} = -2\nabla_{[\mu|}\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{|\nu]}, \\
&\delta_0 \beta^{a}{}_{\mu\nu} = 0, \\
&\delta_0 C^{a}{}_{\mu} = -\partial^{a}{}_{\alpha}\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu}, \\
&\delta_0 \gamma^{A}{}_{\mu\nu\rho} = 0, \\
&\delta_0 D^{A} = 0.
\end{aligned} \tag{84}$$

Based on this result, one obtains the finite symmetry transformations in the whole spacetime, as defined in theorem 4, which we will refer to as the *M*-gauge transformations.

Theorem 4 (M-gauge transformations). *In the* $3BF$ *theory for the two-crossed module* $(L \overset{\delta}{\longrightarrow} H \overset{\partial}{\longrightarrow} G, \triangleright, \{\_,\_\}_{\mathrm{pf}})$*, the following transformation is a symmetry*

$$\begin{aligned}
\alpha &\to \alpha' = \alpha, \\
B &\to B' = B - \nabla\epsilon_{\mathfrak{m}}, \\
\beta &\to \beta' = \beta, \\
C^{a} &\to C'^{a} = C^{a} - \partial^{a}{}_{\alpha}\epsilon_{\mathfrak{m}}{}^{\alpha}, \\
\gamma &\to \gamma' = \gamma, \\
D &\to D' = D,
\end{aligned} \tag{85}$$

where $\epsilon_{\mathfrak{m}} \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{g})$ *is an arbitrary* $\mathfrak{g}$*-valued one-form.*

Proof. Consider the transformation of the $3BF$ action under the transformations of the variables defined in the theorem 4. One obtains:

$$S'_{3BF} = S_{3BF} + \int_{\mathcal{M}_4} \mathrm{d}^4x\, \epsilon^{\mu\nu\rho\sigma} \left(-\frac{1}{2}(\nabla_{\mu}\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\nu})\mathcal{F}_{\alpha\rho\sigma} - \frac{1}{3!}\partial^{a}{}_{\alpha}\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu}\mathcal{G}_{a\nu\rho\sigma} \right). \tag{86}$$

Using the definition of three-curvature, given by the expressions (14), one obtains:

$$\begin{aligned}
S'_{3BF} = S_{3BF} + \int_{\mathcal{M}_4} \mathrm{d}^4x\, \epsilon^{\mu\nu\rho\sigma} &\left(-\frac{1}{2}(\nabla_{\mu}\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\nu}) \left(F_{\alpha\rho\sigma} - \partial^{a}{}_{\alpha}\beta_{a\rho\sigma}\right) \right. \\
&\left. - \frac{1}{3!}\partial^{a}{}_{\alpha}\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu} \left(3\nabla_{\nu}\beta_{a\rho\sigma} - \delta^{A}{}_{a}\gamma_{A\nu\rho\sigma}\right) \right).
\end{aligned} \tag{87}$$

Taking into account that the second and the third term cancel, while the last term is zero because of the identity (A.1), the expression reduces to:

$$S'_{3BF} = S_{3BF} - \frac{1}{2}\int_{\mathcal{M}_4} \mathrm{d}^4x\, \epsilon^{\mu\nu\rho\sigma} \epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu} \nabla_\nu F_{\alpha\rho\sigma}. \tag{88}$$

Finally, the term $\epsilon^{\mu\nu\rho\sigma}\nabla_\nu F_{\alpha\rho\sigma} = 0$ is the BI (38). One concludes that the action S_{3BF} is invariant under the transformation defined in theorem 4. □

Note that the transformations defined in theorem 4 are linear transformations, and the two subsequent M-gauge transformations give one M-gauge transformation with the parameter $\epsilon_{\mathfrak{m}1} + \epsilon_{\mathfrak{m}2}$. Denoting the generators of the M-gauge transformations as $\hat{M}_\alpha{}^\mu$, one can now write the previous statement formally as:

$$\mathrm{e}^{\epsilon_{\mathfrak{m}1}\cdot\hat{M}}\mathrm{e}^{\epsilon_{\mathfrak{m}2}\cdot\hat{M}} = \mathrm{e}^{(\epsilon_{\mathfrak{m}1}+\epsilon_{\mathfrak{m}2})\cdot\hat{M}}, \tag{89}$$

where $\epsilon_{\mathfrak{m}} \cdot \hat{M} = \epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu}\hat{M}_\alpha{}^\mu$, leading to the conclusion that:

$$\left[\hat{M}_\alpha{}^\mu, \hat{M}_\beta{}^\nu\right] = 0. \tag{90}$$

Thus, the M-gauge transformations form an abelian group, which will be denoted as $\tilde{M}$. According to the index structure of its parameters and generators, we see that this group is isomorphic to $\mathbb{R}^{4p}$, where p is the dimension of the group G:

$$\tilde{M} \cong \mathbb{R}^{4p}. \tag{91}$$

Next, one can examine the relationship of M-gauge transformations with the G, H, and L-gauge transformations defined in the previous subsections. Specifically, considering the G-gauge symmetry generators, one finds

$$[\epsilon_{\mathfrak{g}} \cdot \hat{G}, \epsilon_{\mathfrak{m}} \cdot \hat{M}] = (\epsilon_{\mathfrak{g}} \rhd \epsilon_{\mathfrak{m}}) \cdot \hat{M}, \tag{92}$$

obtaining the result:

$$\left[\hat{G}_\alpha, \hat{M}_\beta{}^\mu\right] = f_{\alpha\beta}{}^{\gamma}\hat{M}_\gamma{}^\mu. \tag{93}$$

Considering the H- and L-gauge transformations, one obtains

$$\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot\hat{H}}\mathrm{e}^{\epsilon_{\mathfrak{m}}\cdot\hat{M}} = \mathrm{e}^{\epsilon_{\mathfrak{m}}\cdot\hat{M}}\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot\hat{H}}, \tag{94}$$

$$\mathrm{e}^{\epsilon_{\mathfrak{l}}\cdot\hat{L}}\mathrm{e}^{\epsilon_{\mathfrak{m}}\cdot\hat{M}} = \mathrm{e}^{\epsilon_{\mathfrak{m}}\cdot\hat{M}}\mathrm{e}^{\epsilon_{\mathfrak{l}}\cdot\hat{L}}, \tag{95}$$

leading to the conclusion that the generators of the M-gauge transformations commute with both the generators of H-gauge transformations and the generators of the L-gauge transformations:

$$\left[\hat{H}_a, \hat{M}_\alpha{}^\mu\right] = 0, \qquad \left[\hat{L}_A{}^{\mu\nu}, \hat{M}_\alpha{}^\rho\right] = 0. \tag{96}$$

Finally, examining the infinitesimal transformation corresponding to the parameter $\epsilon_{\mathfrak{n}}{}^{a}$, given by the form-variations as calculated in (E.2),

$$
\begin{aligned}
&\delta_0 \alpha^{\alpha}{}_{\mu} = 0,\\
&\delta_0 B^{\alpha}{}_{\mu\nu} = \beta_{b\mu\nu} \rhd_{\alpha' a}{}^{b} \epsilon_{\mathfrak{n}}{}^{a} g^{\alpha\alpha'},\\
&\delta_0 \beta^{a}{}_{\mu\nu} = 0,\\
&\delta_0 C^{a}{}_{\mu} = -\nabla_{\mu}\epsilon_{\mathfrak{n}}{}^{a},\\
&\delta_0 \gamma^{A}{}_{\mu\nu\rho} = 0,\\
&\delta_0 D^{A} = \delta^{A}{}_{a}\epsilon_{\mathfrak{n}}{}^{a}.
\end{aligned}
\tag{97}
$$

one obtains the theorem 5, the symmetry transformations which will be referred to as *N*-gauge transformations. Note that the *N*-gauge transformations are simultaneously the transformations in the whole spacetime, since the parameter does not carry spacetime indices.

Theorem 5 (N-gauge transformations). *In the* 3*BF theory for the two-crossed module* $(L \overset{\delta}{\longrightarrow} H \overset{\partial}{\longrightarrow} G, \rhd, \{\_,\_\}_{\mathrm{pf}})$*, the following transformation is a symmetry*

$$
\begin{aligned}
\alpha &\to \alpha' = \alpha,\\
B &\to B' = B - \beta \wedge^{\mathcal{T}} \epsilon_{\mathfrak{n}},\\
\beta &\to \beta' = \beta,\\
C &\to C' = C - \nabla\epsilon_{\mathfrak{n}},\\
\gamma &\to \gamma' = \gamma,\\
D^{A} &\to D'^{A} = D^{A} + \delta^{A}{}_{a}\epsilon_{\mathfrak{n}}{}^{a},
\end{aligned}
\tag{98}
$$

where $\epsilon_{\mathfrak{n}} : \mathcal{M}_4 \to \mathfrak{h}$ *is an arbitrary* $\mathfrak{h}$*-valued zero-form.*

Proof. Under the transformations defined in theorem 5, the action is transformed as follows:

$$
\begin{aligned}
S'_{3BF} = S_{3BF} + \int_{\mathcal{M}_4} \mathrm{d}x^4 \epsilon^{\mu\nu\rho\sigma} \bigg(&\frac{1}{4}\beta_{b\mu\nu} \rhd_{\alpha a}{}^{b}\epsilon_{\mathfrak{n}}{}^{a}\mathcal{F}^{\alpha}{}_{\rho\sigma} - \frac{1}{3!}(\nabla_{\mu}\epsilon_{\mathfrak{n}}{}^{a})\mathcal{G}_{a\nu\rho\sigma}\\
&+ \frac{1}{4!}\delta^{A}{}_{a}\epsilon_{\mathfrak{n}}{}^{a}\mathcal{H}_{A\,\mu\nu\rho\sigma}\bigg).
\end{aligned}
\tag{99}
$$

Using the expressions for the three-curvature defined in (9), one obtains

$$
\begin{aligned}
S'_{3BF} = S_{3BF} + \int_{\mathcal{M}_4} \mathrm{d}x^4 \epsilon^{\mu\nu\rho\sigma} \bigg(&\frac{1}{4}\beta_{b\mu\nu} \rhd_{\alpha a}{}^{b}\epsilon_{\mathfrak{n}}{}^{a}\left(F^{\alpha}{}_{\rho\sigma} - \partial_{\mathrm{c}}{}^{\alpha}\beta^{c}{}_{\rho\sigma}\right)\\
&- \frac{1}{3!}(\nabla_{\mu}\epsilon_{\mathfrak{n}}{}^{a})\left(3\nabla_{\nu}\beta_{a\rho\sigma} - \delta^{A}{}_{a}\gamma_{A\,\nu\rho\sigma}\right)\\
&+ \frac{1}{4!}\delta^{A}{}_{a}\epsilon^{a}\left(4\nabla_{\mu}\gamma_{A\,\nu\rho\sigma} + 6X_{(bc)A}\beta^{b}{}_{\mu\nu}\beta^{c}{}_{\rho\sigma}\right)\bigg).
\end{aligned}
\tag{100}
$$

Here, after one partial integration the last term in the first row of the equation (100) cancels with the first term in the second row, while taking into account the identity

$$\frac{1}{2}\epsilon^{\mu\nu\rho\sigma}(\nabla_\nu\nabla_\mu\epsilon_{\mathfrak{n}}{}^a)\beta_{a\rho\sigma} = -\frac{1}{4}\epsilon^{\mu\nu\rho\sigma}\beta_{b\rho\sigma}\rhd_{\alpha a}{}^b\epsilon_{\mathfrak{n}}{}^a F^\alpha{}_{\mu\nu}, \tag{101}$$

the first term and the third term also cancel, leading to the following expression:

$$S'_{3BF} = S_{3BF} + \int_{\mathcal{M}_4} \mathrm{d}x^4 \epsilon^{\mu\nu\rho\sigma}\left(\frac{1}{4}\epsilon_{\mathfrak{n}a}\rhd_{\alpha(b|}{}^a\partial_{|c)}{}^\alpha\beta^b{}_{\mu\nu}\beta^c{}_{\rho\sigma} + \frac{1}{4}\epsilon_{\mathfrak{n}a}\delta_A{}^a X_{(bc)}{}^A\beta^b{}_{\mu\nu}\beta^c{}_{\rho\sigma}\right). \tag{102}$$

Here, the remaining two terms vanish because of the symmetrized form of the identity (A.6):

$$\rhd_{\alpha(b|}{}^a\partial_{|c)}{}^\alpha + \delta_A{}^a X_{(bc)}{}^A = f_{(bc)}{}^a = 0,$$

as a consequence of the antisymmetry of the structure constants. One concludes that the S_{3BF} action is invariant under the transformations defined in theorem 5. □

The N-gauge transformations defined in theorem 5 define the group which will be denoted as $\tilde{N}$. Note that these transformations are also linear, and the composition of two N-gauge transformations gives one N-gauge transformation with the parameter $\epsilon_{\mathfrak{n}1} + \epsilon_{\mathfrak{n}2}$. The generators of the group $\tilde{N}$ will be denoted with $\hat{N}_a$, and one can write these results as:

$$\mathrm{e}^{\epsilon_{\mathfrak{n}1}\cdot\hat{N}}\mathrm{e}^{\epsilon_{\mathfrak{n}2}\cdot\hat{N}} = \mathrm{e}^{(\epsilon_{\mathfrak{n}1}+\epsilon_{\mathfrak{n}2})\cdot\hat{N}}, \tag{103}$$

where $\epsilon_{\mathfrak{n}} \cdot \hat{N} = \epsilon_{\mathfrak{n}}^a \hat{N}_a$, leading to the conclusion that:

$$[\hat{N}_a, \hat{N}_b] = 0. \tag{104}$$

It follows that the group $\tilde{N}$ is abelian, and the index structure of parameters and generators indicates that it is isomorphic to $\mathbb{R}^q$, where q is the dimension of the group H. Therefore,

$$\tilde{N} \cong \mathbb{R}^q. \tag{105}$$

Next, one can examine the relationship of the N-gauge transformations with the G, H, L, and M-gauge transformations. First, considering the G-gauge transformations one obtains:

$$[\epsilon_{\mathfrak{g}} \cdot \hat{G}, \epsilon_{\mathfrak{n}} \cdot \hat{N}] = (\epsilon_{\mathfrak{g}} \rhd \epsilon_{\mathfrak{n}}) \cdot \hat{N}, \tag{106}$$

from which it follows:

$$[\hat{G}_\alpha, \hat{N}_a] = \rhd_{\alpha a}{}^b \hat{N}_b. \tag{107}$$

Let us now examine the relationship between N-gauge transformations and H-gauge transformations, calculating the following expression:

$$\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot\hat{H}}\mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot\hat{N}} - \mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot\hat{N}}\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot\hat{H}} = -(\epsilon_{\mathfrak{n}} \wedge^{\mathcal{T}} \epsilon_{\mathfrak{h}}) \cdot \hat{M}, \tag{108}$$

where the proof is given in appendix F. One obtains that the commutator between the generators of H-gauge transformation and N-gauge transformation is the generator of M-gauge transformation:

$$\left[\hat{H}_a{}^\mu, \hat{N}^b\right] = \rhd_{\alpha a}{}^b \hat{M}^{\alpha\mu}. \tag{109}$$

Analogously, one can check that the following is satisfied

$$e^{\epsilon_{\mathfrak{l}}\cdot\hat{L}}e^{\epsilon_{\mathfrak{n}}\cdot\hat{N}}=e^{\epsilon_{\mathfrak{n}}\cdot\hat{N}}e^{\epsilon_{\mathfrak{l}}\cdot\hat{L}},\qquad e^{\epsilon_{\mathfrak{m}}\cdot\hat{M}}e^{\epsilon_{\mathfrak{n}}\cdot\hat{N}}=e^{\epsilon_{\mathfrak{n}}\cdot\hat{N}}e^{\epsilon_{\mathfrak{m}}\cdot\hat{M}},\tag{110}$$

leading to the conclusion that the generators of *L*-gauge, *M*-gauge, and *N*-gauge transformations mutually commute, i.e.

$$\left[\hat{M}_{\alpha}{}^{\mu},\hat{N}_a\right]=0,\qquad \left[\hat{L}_A{}^{\mu\nu},\hat{N}_a\right]=0.\tag{111}$$

This concludes the calculation of the algebra of generators.

4.4. Structure of the symmetry group

Summarizing the results of the previous subsections, one can write the algebra of the generators of the full gauge symmetry group as follows.

- The algebra $\mathfrak{g}$ of the group G of the two-crossed module $(L\xrightarrow{\delta}H\xrightarrow{\partial}G,\triangleright,\{\_,\_\}_{\mathrm{pf}})$:

$$[\hat{G}_\alpha,\hat{G}_\beta]=f_{\alpha\beta}{}^{\gamma}\hat{G}_\gamma.\tag{112}$$

- The algebra of the group $\tilde{H}_L$ consisting of the generators of *H*- and *L*-gauge transformations:

$$\begin{aligned}&[\hat{H}_a{}^{\mu},\hat{H}_b{}^{\nu}]=2X_{(ab)}{}^{A}\hat{L}_A{}^{\mu\nu},\\&[\hat{L}_A{}^{\mu\nu},\hat{L}_B{}^{\rho\sigma}]=0,\\&[\hat{H}_a{}^{\mu},\hat{L}_A{}^{\nu\rho}]=0.\end{aligned}\tag{113}$$

- The algebra of the generators of *M*-gauge transformations:

$$[\hat{M}_\alpha{}^{\mu},\hat{M}_\beta{}^{\nu}]=0.\tag{114}$$

- The algebra of the generators of *N*-gauge transformations:

$$[\hat{N}_a,\hat{N}_b]=0.\tag{115}$$

- The commutators between the generators of the groups $\tilde{M}$ and $\tilde{N}$:

$$[\hat{M}_\alpha{}^{\mu},\hat{N}_a]=0.\tag{116}$$

- The action of the generators of the group $\tilde{H}_L$ on the generators of *M*- and *N*-gauge transformations:

$$\begin{aligned}&[\hat{H}_a{}^{\mu},\hat{N}^b]=\triangleright_{\alpha a}{}^{b}\hat{M}^{\alpha\mu},\\&[\hat{H}_a{}^{\mu},\hat{M}_\alpha{}^{\nu}]=0,\\&[\hat{L}_A{}^{\nu\rho},\hat{M}_\alpha{}^{\mu}]=0,\\&[\hat{L}_A{}^{\mu\nu},\hat{N}_a]=0.\end{aligned}\tag{117}$$

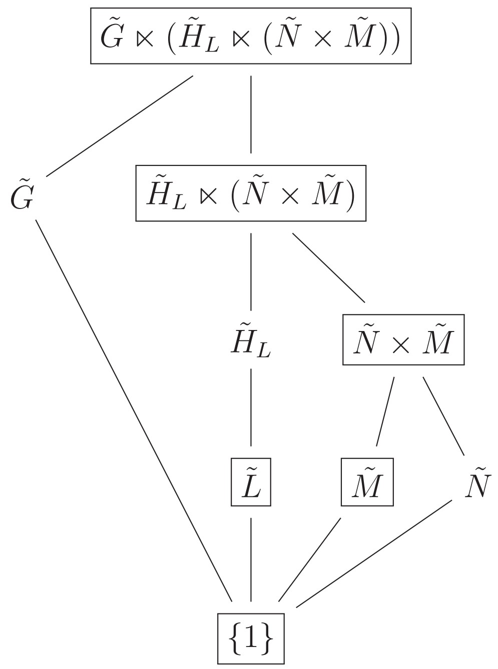

Figure 1. Relevant subgroups of the symmetry group $\mathcal{G}_{3BF}$. The invariant subgroups are boxed.

- The action of the generators of the group G on the generators of H-, L-, M-, and N-gauge transformations:

$$\begin{aligned}
\left[\hat{G}_\alpha, \hat{H}_a{}^{\mu}\right] &= \triangleright_{\alpha a}{}^{b}\, \hat{H}_b{}^{\mu}, \\
\left[\hat{G}_\alpha, \hat{L}_A{}^{\mu\nu}\right] &= \triangleright_{\alpha A}{}^{B} \hat{L}_B{}^{\mu\nu}, \\
\left[\hat{G}_\alpha, \hat{M}_\beta{}^{\mu}\right] &= f_{\alpha\beta}{}^{\gamma} \hat{M}_\gamma{}^{\mu}, \\
\left[\hat{G}_\alpha, \hat{N}_a\right] &= \triangleright_{\alpha a}{}^{b}\, \hat{N}_b.
\end{aligned} \tag{118}$$

Based on the equations (112)–(118), one can investigate the symmetry group structure. On the Hesse-like diagram shown in figure 1, we have included only the relevant subgroups of the whole symmetry group $\mathcal{G}_{3BF}$, where the invariant subgroups are boxed.

Let us remember that the subgroup is an *invariant subgroup*, or equivalently a *normal subgroup*, if it is invariant under conjugation by members of the group of which it is a subgroup. Formally, one says the group H is an invariant subgroup of the group G if H is a subgroup of G, i.e. $H \leqslant G$, and for all $h \in H$ and $g \in G$, the conjugation of the element of H with the element of G is an element of H, i.e. $\exists h' \in H$ such that $ghg^{-1} = h'$. On the level of algebra, the corresponding object is an *ideal*. Formally written, an algebra A is a subalgebra of an algebra L with respect to the multiplication in L, i.e. $[A, A] \subset A$. Then, a subalgebra A of L is an *ideal* in L if its elements, multiplied with any element of the algebra, give again an element of the subalgebra, i.e. $[A, L] \subset A$.

With the above definitions in mind, note first that the groups $\tilde{L}$, $\tilde{M}$, and $\tilde{N}$, are subgroups of the full symmetry group $\mathcal{G}_{3BF}$. The groups $\tilde{L}$ and $\tilde{M}$ are invariant subgroups, since the only nontrivial commutators between the generators $\hat{L}_A{}^{\mu\nu}$, and $\hat{M}_\alpha{}^{\mu}$, are with the generators of the group $\tilde{G}$, and are equal to some linear combinations of the generators of $\tilde{L}$, and $\tilde{M}$, respectively. The group $\tilde{N}$ is not an invariant subgroup, since the commutator between the generators $\hat{N}_a$ and $\hat{H}_a{}^{\mu}$ are linear combinations of the generators $\hat{M}_\alpha{}^{\mu}$. However, the generators of the groups $\tilde{N}$ and $\tilde{M}$ are mutually commuting, and the group $\tilde{N}$ is an invariant subgroup of the product of the groups $\tilde{M}$ and $\tilde{N}$, which makes this product a direct product. The obtained group $\tilde{N} \times \tilde{M}$ is an invariant subgroup of the whole symmetry group.

On the other hand, we saw that the H-gauge transformations together with the L-gauge transformations form the group $\tilde{H}_L$. This group is not an invariant subgroup of the whole symmetry group $\mathcal{G}_{3BF}$, because of the commutator of the generators $\hat{H}_a{}^{\mu}$ and $\hat{N}_b$. Similarly as before, one can join these two subgroups, of which one is invariant and one is not, using a semidirect product, to obtain a subgroup $\tilde{H}_L \ltimes (\tilde{N} \times \tilde{M})$, that will as a result be an invariant subgroup of the complete symmetry group $\mathcal{G}_{3BF}$. Here, the product is semidirect because the group $\tilde{H}_L$ is not an invariant subgroup of the group $\tilde{H}_L \ltimes (\tilde{N} \times \tilde{M})$, due to the commutator between the generators $\hat{H}_a{}^{\mu}$ and $\hat{N}_b$.

Finally, following the same line of reasoning, one adds the G-gauge transformations and obtains the complete gauge symmetry group $\mathcal{G}_{3BF}$ as:

$$\mathcal{G}_{3BF} = \tilde{G} \ltimes (\tilde{H}_L \ltimes (\tilde{N} \times \tilde{M})). \tag{119}$$

This concludes the analysis of the group of gauge symmetries for the 3BF action.

5. Conclusions

5.1. Summary of the results

Let us summarize the results of the paper. In section 2, we have introduced a generalization of the BF theory in the framework of higher category theory, the 3BF theory. Section 3 contains the Hamiltonian analysis for the 3BF theory. In subsection 3.1, the basic canonical structure and the total Hamiltonian are obtained, while in subsection 3.2 the complete Hamiltonian analysis of the 3BF theory is performed, resulting in the first-class and second-class constraints of the theory, as well as their Poisson brackets. In the subsection 3.3 we have discussed the BI and also the generalized BI, since they enforce restrictions and reduce the number of independent first-class constraints present in the theory, and having those identities in mind, the counting of the dynamical degrees of freedom has been performed. As expected, it was established that the considered 3BF action is a topological theory. Finally, this section concludes with the subsection 3.4 where we have constructed the generator of the gauge symmetries for the topological theory, based on the calculations done in section 3.2, and we have found the form-variations for all the variables and their canonical momenta, listed in the appendix E, equation (E.2).

In section 4, the main results of our paper are presented. With the material of the subsection 3.2 in hand, after obtaining the form variations of all variables and their canonical momenta, we proceeded to find all the gauge symmetries of the theory. The subsection 4.1 examined the gauge group G, and the G-gauge transformations. In subsection 4.2 we discussed the gauge group $\tilde{H}_L$ which gives the H-gauge and L-gauge transformations, while in the subsection 4.3 we analyzed the M-gauge and N-gauge transformations which represent a novel result. The results of the subsections 4.1–4.3 are summarized in subsection 4.4, where the complete structure of the symmetry group had been presented. The known G-, H-, and L-gauge transformations have been rigorously defined in theorems 1–3, while the two novel M- and N-gauge transformations, have been defined in theorems 4 and 5. The Lie algebra of the full gauge symmetry group $\mathcal{G}_{3BF}$ has also been obtained.

5.2. Discussion

One of the most important consequences of our results is the relationship between a two-crossed module and a symmetry group of the corresponding $3BF$ action, which we denoted as a *duality*. In particular, from the Lie algebra of the symmetry group $\mathcal{G}_{3BF}$ one sees that the structure constants depend on the choices of groups G, H, and L of the two-crossed module, on the action $\triangleright$, and on the symmetric part of the Peiffer lifting. However, $\mathcal{G}_{3BF}$ does not depend on the antisymmetric part of the Peiffer lifting, nor on the homomorphisms ∂ and δ. This means that in principle one can have several different two-crossed modules dual to the same symmetry group. Therefore, the term 'duality' is used in a loose sense, since there is no one-to-one correspondence between a two-crossed module and a symmetry group of the corresponding $3BF$ action. In addition, this result allows one to implement a strategy for the construction of a two-crossed module, by first specifying the choice of the group $\mathcal{G}_{3BF}$, and then supplying the additional information about the homomorphisms and the antisymmetric part of the Peiffer lifting, in a way that satisfies all axioms in the definition of a two-crossed module.

Another important topic for discussion is the following. From the fact that the $3BF$ action is formulated in a manifestly covariant way, using differential forms, it should be obvious that the diffeomorphisms are a symmetry of the theory. However, by looking at the structure of the gauge group $\mathcal{G}_{3BF}$, one does not immediately see whether $\mathrm{Diff}(\mathcal{M}_4, \mathbb{R})$ is its subgroup. In fact, this issue is subtle, and it deserves some discussion.

It is easy to see that every action, which depends on at least two fields $\phi_1(x)$ and $\phi_2(x)$, is invariant under the following transformation, determined by the Henneaux–Teitelboim (HT) parameter ϵ^{HT} (see [35] for details and naming),

$$\delta_0{}^{\mathrm{HT}}\phi_1 = \epsilon^{\mathrm{HT}}(x)\frac{\delta S}{\delta\phi_2}, \qquad \delta_0{}^{\mathrm{HT}}\phi_2 = -\epsilon^{\mathrm{HT}}(x)\frac{\delta S}{\delta\phi_1}, \tag{120}$$

which can be easily verified by calculating the variation of the action:

$$\delta^{\mathrm{HT}}S[\phi_1, \phi_2] = \frac{\delta S}{\delta\phi_1}\delta_0{}^{\mathrm{HT}}\phi_1 + \frac{\delta S}{\delta\phi_2}\delta_0{}^{\mathrm{HT}}\phi_2 = 0. \tag{121}$$

Since this invariance is present even in theories with no gauge symmetry, it is not associated with constraints, and thus not present in the generator of gauge symmetries (55), see [35] for details.

Now, let us consider the diffeomorphism transformation

$$x^\mu \to x'^\mu = x^\mu + \xi^\mu(x), \tag{122}$$

where the parameter $\xi^\mu(x)$ is an arbitrary function, which we will consider to be infinitesimal. Also, let us denote all parameters of the gauge group collectively as $\epsilon_i(x)$. If diffeomorphisms are a symmetry of the action, then for every field $\phi(x)$ in the theory, and every parameter of the diffeomorphisms $\xi^\mu(x)$, there should exist a choice of the parameters $\epsilon_i(x)$ and $\epsilon^{\mathrm{HT}}(x)$, such that:

$$(\delta_0{}^{\mathrm{gauge}} + \delta_0{}^{\mathrm{HT}} + \delta_0{}^{\mathrm{diff}})\,\phi = 0. \tag{123}$$

In other words, if the diffeomorphisms are a symmetry of the theory, their form variations should be expressible as gauge form variations combined with HT form variations:

$$\delta_0{}^{\mathrm{diff}}\,\phi = -\delta_0{}^{\mathrm{gauge}}\phi - \delta_0{}^{\mathrm{HT}}\phi. \tag{124}$$

In our case, the $3BF$ action depends on the fields $\alpha^\alpha{}_\mu$, $\beta^a{}_{\mu\nu}$, $\gamma^A{}_{\mu\nu\rho}$, $B^\alpha{}_{\mu\nu}$, $C^a{}_\mu$, and D^A. The HT parameters $\epsilon^{\mathrm{HT}\alpha\beta}{}_{\mu\nu\rho}$, $\epsilon^{\mathrm{HT}ab}{}_{\mu\nu\rho}$, and $\epsilon^{\mathrm{HT}AB}{}_{\mu\nu\rho}$ are defined via the following form variations, analogous to (120):

$$\begin{aligned}
\delta_0{}^{\mathrm{HT}}\alpha^\alpha{}_\mu &= \frac{1}{2}\epsilon^{\mathrm{HT}\alpha\beta}{}_{\mu\nu\rho}\frac{\delta S}{\delta B^\beta{}_{\nu\rho}},\\
\delta_0{}^{\mathrm{HT}}B^\alpha{}_{\mu\nu} &= -\epsilon^{\mathrm{HT}\alpha\beta}{}_{\rho\mu\nu}\frac{\delta S}{\delta\alpha^\beta{}_\rho},\\
\delta_0{}^{\mathrm{HT}}\beta^a{}_{\mu\nu} &= \epsilon^{\mathrm{HT}ab}{}_{\mu\nu\rho}\frac{\delta S}{\delta C^b{}_\rho},\\
\delta_0{}^{\mathrm{HT}}C^a{}_\mu &= -\frac{1}{2}\epsilon^{\mathrm{HT}ab}{}_{\nu\rho\mu}\frac{\delta S}{\delta\beta^b{}_{\nu\rho}},\\
\delta_0{}^{\mathrm{HT}}\gamma^A{}_{\mu\nu\rho} &= \epsilon^{\mathrm{HT}AB}{}_{\mu\nu\rho}\frac{\delta S}{\delta D^B},\\
\delta_0{}^{\mathrm{HT}}D^A &= -\frac{1}{3!}\epsilon^{\mathrm{HTAB}}{}_{\mu\nu\rho}\frac{\delta S}{\delta\gamma^B{}_{\mu\nu\rho}},
\end{aligned} \tag{125}$$

while the gauge parameters $\epsilon_{\mathfrak{g}}{}^\alpha$, $\epsilon_{\mathfrak{h}}{}^a{}_\mu$, $\epsilon_{\mathfrak{l}}{}^A{}_{\mu\nu}$, $\epsilon_{\mathrm{m}}{}^\alpha{}_\mu$, and $\epsilon_{\mathfrak{n}}^a$ are defined in theorems 1–5. Given these, there indeed exists a choice of these parameters, such that (123) is satisfied for all fields. Specifically, if one chooses the gauge parameters as

$$\begin{aligned}
\epsilon_{\mathfrak{g}}{}^\alpha &= -\xi^\lambda\alpha^\alpha{}_\lambda,\\
\epsilon_{\mathfrak{h}}{}^a{}_\mu &= \xi^\lambda\beta^a{}_{\mu\lambda},\\
\epsilon_{\mathfrak{l}}^A{}_{\mu\nu} &= \xi^\lambda\gamma^A{}_{\mu\nu\lambda},\\
\epsilon_{\mathrm{m}}{}^\alpha{}_\mu &= \xi^\lambda B^\alpha{}_{\mu\lambda},\\
\epsilon_{\mathfrak{n}}{}^a &= -\xi^\lambda C^a{}_\lambda,
\end{aligned} \tag{126}$$

and the HT parameters as

$$\begin{aligned}
\epsilon^{\mathrm{HT}\alpha\beta}{}_{\mu\nu\rho} &= \xi^\lambda g^{\alpha\beta}\epsilon_{\mu\nu\rho\lambda},\\
\epsilon^{\mathrm{HT}ab}{}_{\mu\nu\rho} &= \xi^\lambda g^{ab}\epsilon_{\lambda\mu\nu\rho},\\
\epsilon^{\mathrm{HT}AB}{}_{\mu\nu\rho} &= \xi^\lambda g^{AB}\epsilon_{\mu\nu\rho\lambda},
\end{aligned} \tag{127}$$

one can obtain, using (124), precisely the standard form variations corresponding to diffeomorphisms:

$$
\begin{aligned}
\delta_0{}^{\text{diff}}\alpha^{\alpha}{}_{\mu} &= -\partial_\mu\xi^\lambda\alpha^\alpha{}_\lambda - \xi^\lambda\partial_\lambda\alpha^\alpha{}_\mu,\\
\delta_0{}^{\text{diff}}\beta^{a}{}_{\mu\nu} &= -\partial_\mu\xi^\lambda\beta^a{}_{\lambda\nu} - \partial_\nu\xi^\lambda\beta^a{}_{\mu\lambda} - \xi^\lambda\partial_\lambda\beta^a{}_{\mu\nu},\\
\delta_0{}^{\text{diff}}\gamma^{A}{}_{\mu\nu\rho} &= -\partial_\mu\xi^\lambda\gamma^A{}_{\lambda\nu\rho} - \partial_\nu\xi^\lambda\gamma^A{}_{\mu\lambda\rho} - \partial_\rho\xi^\lambda\gamma^A{}_{\mu\nu\lambda} - \xi^\lambda\partial_\lambda\gamma^A{}_{\mu\nu\rho},\\
\delta_0{}^{\text{diff}}B^{\alpha}{}_{\mu\nu} &= -\partial_\mu\xi^\lambda B^\alpha{}_{\lambda\nu} - \partial_\nu\xi^\lambda B^\alpha{}_{\mu\lambda} - \xi^\lambda\partial_\lambda B^\alpha{}_{\mu\nu},\\
\delta_0{}^{\text{diff}}C^{a}{}_{\mu} &= -\partial_\mu\xi^\lambda C^a{}_\lambda - \xi^\lambda\partial_\lambda C^a{}_\mu,\\
\delta_0{}^{\text{diff}}D^{A} &= -\xi^\lambda\partial_\lambda D^A.
\end{aligned}
\tag{128}
$$

This establishes that diffeomorphisms are indeed contained in the full gauge symmetry group $\mathcal{G}_{3BF}$, up to the HT transformations, which are always a symmetry of the theory.

5.3. Future lines of investigation

Based on the results obtained in this work, one can imagine various additional topics for further research.

First, since we have obtained that the pure $3BF$ theory is a topological theory, it does not describe a realistic physical theory which ought to contain local propagating degrees of freedom. To build a realistic physical theory, one introduces the degrees of freedom by imposing the simplicity constraints on the topological action. In our previous work [13], we have formulated the classical actions that manifestly distinguish the topological sector from the simplicity constraints, for all the fields present in the standard model coupled to Einstein–Cartan gravity. Specifically, we have defined the constrained $2BF$ actions describing the Yang–Mills field and Einstein–Cartan gravity, and also the constrained $3BF$ actions describing the Klein–Gordon, Dirac, Weyl and Majorana fields coupled to gravity in the standard way. The natural continuation of this line of research would be the Hamiltonian analysis of all such constrained $3BF$ models of gravity coupled to various matter fields, and the study of their canonical quantization.

On the other hand, as an alternative to the canonical quantization, one may choose the spinfoam quantization approach, and define the path integral of the theory as the state sum for the Regge-discretized $3BF$ action. The topological nature of the $3BF$ action, together with the structure of the gauge three-group, should ensure that such a sum is a topological invariant, i.e. that it is triangulation independent. This construction was recently carried out in [14], where the $3BF$ state sum for a general two-crossed module and a closed and orientable four-dimensional manifold $\mathcal{M}_4$ is defined. Unfortunately, in order to rigorously define this state sum, one needs the higher category generalizations of the Peter–Weyl and Plancherel theorems, from ordinary groups to the cases of two-groups and three-groups. These theorems ought to determine the domains of various labels living on simplices of the triangulation, as a consequence of the representation theory of three-groups. Until these mathematical results are obtained, one can try to guess the appropriate structure of the irreducible representations of a three-group and construct the topological invariant Z for the $3BF$ topological action, in analogy with what was done in the case of $2BF$ theory, see [25, 27]. Once the topological state sum is obtained, one can proceed to impose the simplicity constraints, and thus construct the state sum corresponding to the tentative quantum theory of gravity with matter. The classical action for gravity and matter is formulated in [13] in a way that explicitly distinguishes between the topological sector and the simplicity constraints sector of the action, making the procedure of imposing the constraints straightforward.

Next, it would be useful to investigate in more depth the mathematical structure and properties of the simplicity constraints, in particular their role as the gauge fixing conditions for the symmetry group $\mathcal{G}_{3BF}$. The simplicity constraints should explicitly break the symmetry group $\mathcal{G}_{3BF}$ to the subgroup corresponding to the constrained $3BF$ theory, which may then be further spontaneously broken by the Higgs mechanism.

One of the results obtained in this work is a duality between the gauge symmetry group of the $3BF$ action, $\mathcal{G}_{3BF}$, and the underlining three-group, i.e. the two-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G, \triangleright, \{\_,\_\}_{\mathrm{pf}})$. This duality should be better understood. On one hand, the group $\mathcal{G}_{3BF}$ can provide further insight into the construction of the TQFT state sum, i.e. a topological invariant corresponding to the underlining three-group structure. On the other hand, this duality is interesting from the perspective of pure mathematics, since it can provide deeper insight in the structure of three-groups. In addition, one could expect that the $3BF$ theory would have a three-group of higher gauge symmetries, but it is not obvious if the five types of gauge transformations can form a three-group structure or not. This is an important topic for future research.

Finally, in [31] it was pointed out that it may be useful to make one more step in the categorical generalization, and consider a $4BF$ theory as a description of a quantum gravity model with matter fields. One could then calculate the gauge group of the $4BF$ action, and compare the results with the results obtained for the $3BF$ theory.

The list is not conclusive, and there may be many other interesting topics to study.

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Data availability statement

No new data were created or analysed in this study.

Appendix A. Two-crossed module

Definition (Differential two-crossed module). A differential two-crossed module is given by an exact sequence of Lie algebras:

$$\mathfrak{l} \xrightarrow{\delta} \mathfrak{h} \xrightarrow{\partial} \mathfrak{g},$$

together with left action $\triangleright$ of $\mathfrak{g}$ on $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$, by derivations, and on itself via adjoint representation, and a $\mathfrak{g}$-equivariant bilinear map called the **Peiffer lifting**:

$$\{\_,\_\}_{\mathrm{pf}} : \mathfrak{h} \times \mathfrak{h} \to \mathfrak{l}.$$

Fixing the basis in the algebras as $T_A \in \mathfrak{l}$, $t_a \in \mathfrak{h}$ and $\tau_\alpha \in \mathfrak{g}$:

$$[T_A, T_B] = f_{AB}{}^C\, T_C, \qquad [t_a, t_b] = f_{ab}{}^c\, t_c, \qquad [\tau_\alpha, \tau_\beta] = f_{\alpha\beta}{}^\gamma\, \tau_\gamma,$$

one defines the maps ∂ and δ as:

$$\partial(t_a) = \partial_a{}^\alpha\, \tau_\alpha, \qquad \delta(T_A) = \delta_A{}^a\, t_a,$$

and the action of $\mathfrak{g}$ on the generators of $\mathfrak{l}$, $\mathfrak{h}$, and $\mathfrak{g}$ is, respectively:

$$\tau_\alpha \triangleright T_A = \triangleright_{\alpha A}{}^B\, T_B, \qquad \tau_\alpha \triangleright t_a = \triangleright_{\alpha a}{}^b\, t_b, \qquad \tau_\alpha \triangleright \tau_\beta = \triangleright_{\alpha\beta}{}^\gamma\, \tau_\gamma.$$

The coefficients $X_{ab}{}^A$ are introduced as:

$$\{t_a,\, t_b\}_{\mathrm{pf}} = X_{ab}{}^A T_A.$$

The maps ∂ and δ satisfy the following identity:

$$\partial_a{}^\alpha\, \delta_A{}^a = 0. \tag{A.1}$$

Note that when η is a $\mathfrak{g}$-valued differential form and ω is $\mathfrak{l}$-, $\mathfrak{h}$-, or $\mathfrak{g}$-valued differential form, the previous action is defined as:

$$\eta \wedge^\triangleright \omega = \eta^\alpha \wedge \omega^A \triangleright_{\alpha A}{}^B\, T_B,$$
$$\eta \wedge^\triangleright \omega = \eta^\alpha \wedge \omega^a \triangleright_{\alpha a}{}^b\, t_b,$$
$$\eta \wedge^\triangleright \omega = \eta^\alpha \wedge \omega^\beta f_{\alpha\beta}{}^\gamma\, \tau_\gamma,$$

where the forms are multiplied via the wedge product $\wedge$, while the generators of G act on the generators of the three groups via the action $\triangleright$.

The following identities are satisfied:

(i) In the differential crossed module $(L \xrightarrow{\delta} H, \triangleright')$ the action $\triangleright'$ of $\mathfrak{h}$ on $\mathfrak{l}$ is defined for each $\underline{h} \in \mathfrak{h}$ and $\underline{l} \in \mathfrak{l}$ as:

$$\underline{h} \triangleright' \underline{l} = -\{\delta(\underline{l}),\, \underline{h}\}_{\mathrm{pf}},$$

or written in the basis where $t_a \triangleright' T_A = \triangleright'{}_{aA}{}^B T_B$ the previous identity becomes:

$$\triangleright'{}_{aA}{}^B = -\delta_A{}^b X_{ba}{}^B; \tag{A.2}$$

(ii) The action of $\mathfrak{g}$ on itself is via adjoint representation:

$$\triangleright_{\alpha\beta}{}^\gamma = f_{\alpha\beta}{}^\gamma; \tag{A.3}$$

(iii) The action of $\mathfrak{g}$ on $\mathfrak{h}$ and $\mathfrak{l}$ is equivariant, i.e. the following identities are satisfied:

$$\partial_a{}^\beta f_{\alpha\beta}{}^\gamma = \triangleright_{\alpha a}{}^b \partial_b{}^\gamma, \qquad \delta_A{}^a\, \triangleright_{\alpha a}{}^b = \triangleright_{\alpha A}{}^B \delta_B{}^b; \tag{A.4}$$

(iv) The Peiffer lifting is $\mathfrak{g}$-equivariant, i.e. for each $\underline{h}_1, \underline{h}_2 \in \mathfrak{h}$ and $\underline{g} \in \mathfrak{g}$:

$$\underline{g} \triangleright \{\underline{h}_1, \underline{h}_2\}_{\mathrm{pf}} = \{\underline{g} \triangleright \underline{h}_1, \underline{h}_2\}_{\mathrm{pf}} + \{\underline{h}_1,\, \underline{g} \triangleright \underline{h}_2\}_{\mathrm{pf}},$$

or written in the basis:

$$X_{ab}{}^{B} \rhd_{\alpha B}{}^{A} = \rhd_{\alpha a}{}^{c} X_{cb}{}^{A} + \rhd_{\alpha b}{}^{c} X_{ac}{}^{A}; \tag{A.5}$$

(v) $\delta(\{\underline{h}_1, \underline{h}_2\}_{\mathrm{pf}}) = \langle \underline{h}_1, \underline{h}_2 \rangle_{\mathrm{p}}, \ \forall\ \underline{h}_1, \underline{h}_2 \in \mathfrak{h}$.

The map $(\underline{h}_1, \underline{h}_2) \in \mathfrak{h} \times \mathfrak{h} \to \langle \underline{h}_1, \underline{h}_2 \rangle_{\mathrm{p}} \in \mathfrak{h}$ is bilinear $\mathfrak{g}$-equivariant map called the **Peiffer paring**, i.e. all $\underline{h}_1, \underline{h}_2 \in \mathfrak{h}$ and $\underline{g} \in \mathfrak{g}$ satisfy the following identity:

$$\underline{g} \rhd \langle \underline{h}_1, \underline{h}_2 \rangle_{\mathrm{p}} = \langle \underline{g} \rhd \underline{h}_1, \underline{h}_2 \rangle_{\mathrm{p}} + \langle \underline{h}_1, \underline{g} \rhd \underline{h}_2 \rangle_{\mathrm{p}}.$$

Fixing the basis the identity becomes:

$$X_{ab}{}^{A} \delta_{A}{}^{c} = f_{ab}{}^{c} - \partial_{a}{}^{\alpha} \rhd_{\alpha b}{}^{c}; \tag{A.6}$$

(vi) $[\underline{l}_1, \underline{l}_2] = \{\delta(\underline{l}_1), \delta(\underline{l}_2)\}_{\mathrm{pf}}, \ \forall\ \underline{l}_1, \underline{l}_2 \in \mathfrak{l}$, i.e.

$$f_{AB}{}^{C} = \delta_{A}{}^{a} \delta_{B}{}^{b} X_{ab}{}^{C}; \tag{A.7}$$

(vii) $\{[\underline{h}_1, \underline{h}_2], \underline{h}_3\}_{\mathrm{pf}} = \partial(\underline{h}_1) \rhd \{\underline{h}_2, \underline{h}_3\}_{\mathrm{pf}} + \{\underline{h}_1, [\underline{h}_2, \underline{h}_3]\}_{\mathrm{pf}} - \partial(\underline{h}_2) \rhd \{\underline{h}_1, \underline{h}_3\}_{\mathrm{pf}} - \{\underline{h}_2, [\underline{h}_1, \underline{h}_3]\}_{\mathrm{pf}}, \ \forall\ \underline{h}_1, \underline{h}_2, \underline{h}_3 \in \mathfrak{h}$, i.e.

$$\begin{aligned} \{[\underline{h}_1, \underline{h}_2], \underline{h}_3\}_{\mathrm{pf}} &= \{\partial(\underline{h}_1) \rhd \underline{h}_2, \underline{h}_3\}_{\mathrm{pf}} - \{\partial(\underline{h}_2) \rhd \underline{h}_1, \underline{h}_3\}_{\mathrm{pf}} \\ &\quad - \{\underline{h}_1, \delta\{\underline{h}_2, \underline{h}_3\}_{\mathrm{pf}}\}_{\mathrm{pf}} + \{\underline{h}_2, \delta\{\underline{h}_1, \underline{h}_3\}_{\mathrm{pf}}\}_{\mathrm{pf}}, \end{aligned} \tag{A.8}$$

$$f_{ab}{}^{d} X_{dc}{}^{B} = \partial_{a}{}^{\alpha} X_{bc}{}^{A} \rhd_{\alpha A}{}^{B} + X_{ad}{}^{B} f_{bc}{}^{d} - \partial_{b}{}^{\alpha} \rhd_{\alpha A}{}^{B} X_{ac}{}^{A} - X_{bd}{}^{B} f_{ac}{}^{d}; \tag{A.9}$$

(viii) $\{\underline{h}_1, [\underline{h}_2, \underline{h}_3]\}_{\mathrm{pf}} = \left\{\delta\{\underline{h}_1, \underline{h}_2\}_{\mathrm{pf}}, \underline{h}_3\right\}_{\mathrm{pf}} - \left\{\delta\{\underline{h}_1, \underline{h}_3\}_{\mathrm{pf}}, \underline{h}_2\right\}_{\mathrm{pf}}, \ \forall\ \underline{h}_1, \underline{h}_2, \underline{h}_3 \in \mathfrak{h}$, i.e.

$$X_{ad}{}^{A} f_{bc}{}^{d} = X_{ab}{}^{B} \delta_{B}{}^{d} X_{dc}{}^{A} - X_{ac}{}^{B} \delta_{B}{}^{d} X_{db}{}^{A}; \tag{A.10}$$

(ix) $\{\delta(\underline{l}), \underline{h}\}_{\mathrm{pf}} + \{\underline{h}, \delta(\underline{l})\}_{\mathrm{pf}} = -\partial(\underline{h}) \rhd \underline{l}, \ \forall\ \underline{l} \in \mathfrak{l}, \ \forall\ \underline{h} \in \mathfrak{h}$, i.e.

$$\delta_{A}{}^{a} X_{ab}{}^{B} + \delta_{A}{}^{a} X_{ba}{}^{B} = -\partial_{b}{}^{\alpha} \rhd_{\alpha A}{}^{B}. \tag{A.11}$$

A reader interested in more details about three-groups is referred to [21, 30].

The structure constants satisfy the Jacobi identities

$$\begin{aligned} f_{\alpha\gamma}{}^{\delta} f_{\beta\epsilon}{}^{\gamma} &= 2 f_{\alpha[\beta|}{}^{\gamma} f_{\gamma|\epsilon]}{}^{\delta}, \\ f_{ad}{}^{c} f_{be}{}^{d} &= 2 f_{a[b|}{}^{d} f_{d|e]}{}^{c}, \\ f_{AD}{}^{C} f_{BE}{}^{D} &= 2 f_{A[B|}{}^{D} f_{D|E]}{}^{C}. \end{aligned} \tag{A.12}$$

Also, the following relations are useful:

$$f_{\beta\gamma}{}^{\alpha} \rhd_{\alpha b}{}^{a} = 2 \rhd_{[\beta|c}{}^{a} \rhd_{|\gamma]b}{}^{c}, \qquad f_{\beta\gamma}{}^{\alpha} \rhd_{\alpha B}{}^{A} = 2 \rhd_{[\beta|C}{}^{A} \rhd_{|\gamma]B}{}^{C}. \tag{A.13}$$

Appendix B. Additional relations of the constraint algebra

In this appendix the useful technical results used in the subsection 3.2 are given. First, since the secondary constraints, given by the equation (30), must be preserved during the evolution of the system, the consistency conditions of secondary constraints must be enforced. However, no tertiary constraints arise from these conditions, since one obtains the following PB:

$$
\begin{aligned}
\{\mathcal{S}(\mathcal{F})^{\alpha i}, H_{\mathrm{T}}\} &= f_{\beta\gamma}{}^{\alpha}\mathcal{S}(\mathcal{F})^{\beta i}\alpha^{\gamma}{}_{0},\\
\{\mathcal{S}(\nabla B)_{\alpha}, H_{\mathrm{T}}\} &= f_{\beta\gamma\alpha}B^{\gamma}{}_{0k}\mathcal{S}(\mathcal{F})^{\beta k} + f_{\beta\alpha}{}^{\gamma}\alpha^{\beta}{}_{0}\mathcal{S}(\nabla B)_{\gamma} + C_{a0}\triangleright_{\alpha b}{}^{a}\mathcal{S}(\mathcal{G})^{b}\\
&\quad - \triangleright_{\alpha a}{}^{b}\beta^{a}{}_{0k}\mathcal{S}(\nabla C)_{b}{}^{k} + \frac{1}{2}\triangleright_{\alpha}{}^{B}{}_{A}\gamma^{A}{}_{0jk}\mathcal{S}(\nabla D)_{B}{}^{jk},\\
\{\mathcal{S}(\mathcal{G})^{a}, H_{\mathrm{T}}\} &= \triangleright_{\alpha b}{}^{a}\beta^{b}{}_{0k}\mathcal{S}(\mathcal{F})^{\alpha k} - \alpha^{\alpha}{}_{0}\triangleright_{\alpha b}{}^{a}\mathcal{S}(\mathcal{G})^{b},\\
\{\mathcal{S}(\nabla C)_{a}{}^{i}, H_{\mathrm{T}}\} &= C_{b0}\triangleright_{\alpha}{}^{b}{}_{a}\mathcal{S}(\mathcal{F})^{\alpha i} + \triangleright_{\alpha a}{}^{b}\alpha^{\alpha}{}_{0}\mathcal{S}(\nabla C)_{b}{}^{i} + 2X_{(ab)}{}^{A}\beta^{b}{}_{0j}\mathcal{S}(\nabla D)_{A}{}^{ij},\\
\{\mathcal{S}(\nabla D)_{A}{}^{ij}, H_{\mathrm{T}}\} &= \alpha^{\alpha}{}_{0}\triangleright_{\alpha A}{}^{B}\mathcal{S}(\nabla D)_{B}{}^{ij}.
\end{aligned}
\tag{B.1}
$$

The PB between the first-class constraints, given by the equation (34), and the second-class constraints, given by the equation (35), are given by:

$$
\begin{aligned}
\{\,\Phi(\mathcal{F})^{\alpha i}(\vec{x})\,,\,\chi(\alpha)_{\beta j}(\vec{y})\,\} &= -f_{\beta\gamma}{}^{\alpha}\,\chi(B)^{\gamma ij}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\mathcal{G})^{a}(\vec{x})\,,\,\chi(\alpha)_{\alpha}{}^{i}(\vec{y})\,\} &= \triangleright_{\alpha b}{}^{a}\,\chi(C)^{bi}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\mathcal{G})^{a}(\vec{x})\,,\,\chi(\beta)_{b}{}^{ij}(\vec{y})\,\} &= -\triangleright_{\alpha b}{}^{a}\,\chi(B)^{\alpha ij}(\vec{x})\,\delta^{(3)}(x-y),\\
\{\,\Phi(\nabla C)^{ai}(\vec{x})\,,\,\chi(\alpha)_{\alpha}{}^{j}(\vec{y})\,\} &= -\triangleright_{\alpha b}{}^{a}\,\chi(\beta)^{bij}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla C)^{ai}(\vec{x})\,,\,\chi(\beta)_{b}{}^{jk}(\vec{y})\,\} &= 2X^{(ac)A}g_{bc}\,\chi(\gamma)_{A}{}^{ijk}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla C)^{ai}(\vec{x})\,,\,\chi(C)_{b}{}^{j}(\vec{y})\,\} &= \triangleright_{\alpha b}{}^{a}\,\chi(B)^{\alpha ij}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla C)^{ai}(\vec{x})\,,\,\chi(D)_{A}(\vec{y})\,\} &= 2X^{(ab)}{}_{A}\,\chi(C)_{b}{}^{i}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla B)^{\alpha}(\vec{x})\,,\,\chi(\alpha)_{\beta}{}^{i}(\vec{y})\,\} &= f_{\beta\gamma}{}^{\alpha}\,\chi(\alpha)^{\gamma i}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla B)^{\alpha}(\vec{x})\,,\,\chi(\beta)_{a}{}^{ij}(\vec{y})\,\} &= g^{\alpha\beta}\triangleright_{\beta a}{}^{b}\,\chi(\beta)_{b}{}^{ij}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla B)^{\alpha}(\vec{x})\,,\,\chi(\gamma)_{A}{}^{ijk}(\vec{y})\,\} &= g^{\alpha\beta}\triangleright_{\beta A}{}^{B}\,\chi(\gamma)_{B}{}^{ijk}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla B)^{\alpha}(\vec{x})\,,\,\chi(B)_{\beta}{}^{ij}(\vec{y})\,\} &= f\beta\gamma^{\alpha}\,\chi(B)^{\gamma ij}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}).\\
\{\,\Phi(\nabla B)^{\alpha}(\vec{x})\,,\,\chi(C)_{a}{}^{i}(\vec{y})\,\} &= -\triangleright^{\alpha b}{}_{a}\,\chi(C)_{b}{}^{i}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}).\\
\{\,\Phi(\nabla B)^{\alpha}(\vec{x})\,,\,\chi(D)_{A}(\vec{y})\,\} &= g^{\alpha\beta}\triangleright_{\beta A}{}^{B}\,\chi(D)_{B}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla D)^{Aij}(\vec{x})\,,\,\chi(\alpha)_{\alpha}{}^{k}(\vec{y})\,\} &= \triangleright_{\alpha B}{}^{A}\chi(\gamma)^{Bijk}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}),\\
\{\,\Phi(\nabla D)^{Aij}(\vec{x})\,,\,\chi(D)_{B}(\vec{y})\,\} &= -\triangleright_{\alpha B}{}^{A}\chi(B)^{\alpha ij}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}).
\end{aligned}
\tag{B.2}
$$

Finally, it is useful to calculate PB between the first-class constraints, given by the equation (34), and the total Hamiltonian, given by the equation (33):

$$
\begin{aligned}
\{\Phi(\mathcal{F})^{\alpha i}, H_{\mathrm{T}}\} &= f_{\beta\gamma}{}^{\alpha}\Phi(\mathcal{F})^{\beta i}\alpha^{\gamma}{}_{0}, \\
\{\Phi(\nabla B)_{\alpha}, H_{\mathrm{T}}\} &= f_{\beta\gamma\alpha}B^{\gamma}{}_{0k}\Phi(\mathcal{F})^{\beta k} + f_{\beta\alpha}{}^{\gamma}\alpha^{\beta}{}_{0}\Phi(\nabla B)_{\gamma} + C_{a0}\rhd_{\alpha b}{}^{a}\Phi(\mathcal{G})^{b} \\
&\quad - \rhd_{\alpha a}{}^{b}\beta^{a}{}_{0k}\Phi(\nabla C)_{b}{}^{k} + \frac{1}{2}\rhd_{\alpha}{}^{B}{}_{A}\gamma^{A}{}_{0jk}\Phi(\nabla D)_{B}{}^{jk}, \\
\{\Phi(\mathcal{G})^{a}, H_{\mathrm{T}}\} &= \rhd_{\alpha b}{}^{a}\beta^{b}{}_{0k}\Phi(\mathcal{F})^{\alpha k} - \alpha^{\alpha}{}_{0}\rhd_{\alpha b}{}^{a}\Phi(\mathcal{G})^{b}, \\
\{\Phi(\nabla C)_{a}{}^{i}, H_{\mathrm{T}}\} &= C_{b0}\rhd_{\alpha}{}^{b}{}_{a}\Phi(\mathcal{F})^{\alpha i} + \rhd_{\alpha a}{}^{b}\alpha^{\alpha}{}_{0}\Phi(\nabla C)_{b}{}^{i} + 2X_{(ab)}{}^{A}\beta^{b}{}_{0j}\Phi(\nabla D)_{A}{}^{ij}, \\
\{\Phi(\nabla D)_{A}{}^{ij}, H_{\mathrm{T}}\} &= \alpha^{\alpha}{}_{0}\rhd_{\alpha A}{}^{B}\Phi(\nabla D)_{B}{}^{ij}.
\end{aligned}
\tag{B.3}
$$

The calculated PB brackets given by the equation (B.3) will be useful for calculation of the generator of gauge symmetries (55). With these results one can proceed to the construction of the gauge symmetry generator on one hypersurface Σ_3 given in the equation (55), and ultimately obtain the finite gauge symmetry of the whole spacetime.

The PB algebra of gauge symmetry generators $(\tilde{M}_0)_{\alpha}{}^{i}$, $(\tilde{M}_1)_{\alpha}{}^{i}$, $(\tilde{G}_0)_{\alpha}$, $(\tilde{G}_1)_{\alpha}$, $(\tilde{H}_0)_{a}{}^{i}$, $(\tilde{H}_1)_{a}{}^{i}$, $(\tilde{N}_0)_{a}$, $(\tilde{N}_1)_{a}$, $(\tilde{L}_0)_{A}{}^{ij}$, and $(\tilde{L}_1)_{A}{}^{ij}$, as defined in (56), is:

$$\{(\tilde{G}_0)_{\alpha}(\vec{x}), (\tilde{G}_0)_{\beta}(\vec{y})\} = f_{\alpha\beta}{}^{\gamma}(\tilde{G}_0)_{\gamma}\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.4}$$

$$\{(\tilde{H}_0)_{a}{}^{i}(\vec{x}), (\tilde{H}_0)_{b}{}^{j}(\vec{y})\} = 2X_{(ab)}{}^{A}(\tilde{L}_0)_{A}{}^{ij}\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.5}$$

$$\{(\tilde{H}_0)_{a}{}^{i}(\vec{x}), (\tilde{H}_1)_{b}{}^{j}(\vec{y})\} = 2X_{(ab)}{}^{A}(\tilde{L}_1)_{A}{}^{ij}\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.6}$$

$$\{(\tilde{H}_0)_{a}{}^{i}(\vec{x}), (\tilde{N}_0)^{b}(\vec{y})\} = \rhd_{\alpha a}{}^{b}(\tilde{M}_0)^{\alpha i}\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.7}$$

$$\{(\tilde{H}_1)_{a}{}^{i}(\vec{x}), (\tilde{N}_0)^{b}(\vec{y})\} = \rhd_{\alpha a}{}^{b}(\tilde{M}_1)^{\alpha i}\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.8}$$

$$\{(\tilde{H}_0)_{a}(\vec{x}), (\tilde{N}_1)^{bi}(\vec{y})\} = \rhd_{\alpha a}{}^{b}(\tilde{M}_1)^{\alpha i}\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.9}$$

$$\{(\tilde{G}_0)_{\alpha}(\vec{x}), (\tilde{M}_0)_{\beta}{}^{i}(\vec{y})\} = f_{\alpha\beta}{}^{\gamma}(\tilde{M}_0)_{\gamma}{}^{i}\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.10}$$

$$\{(\tilde{G}_0)_{\alpha}(\vec{x}), (\tilde{M}_1)_{\beta}{}^{i}(\vec{y})\} = f_{\alpha\beta}{}^{\gamma}(\tilde{M}_1)_{\gamma}{}^{i}\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.11}$$

$$\{(\tilde{G}_0)_{\alpha}(\vec{x}), (\tilde{H}_1)_{a}{}^{i}(\vec{y})\} = \rhd_{\alpha a}{}^{b}(\tilde{H}_1)_{b}{}^{i}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.12}$$

$$\{(\tilde{G}_0)_{\alpha}(\vec{x}), (\tilde{H}_0)_{a}{}^{i}(\vec{y})\} = \rhd_{\alpha a}{}^{b}(\tilde{H}_0)_{b}{}^{i}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.13}$$

$$\{(\tilde{G}_0)_{\alpha}(\vec{x}), (\tilde{N}_1)_{a}(\vec{y})\} = \rhd_{\alpha a}{}^{b}(\tilde{N}_1)_{b}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.14}$$

$$\{(\tilde{G}_0)_{\alpha}(\vec{x}), (\tilde{N}_0)_{a}(\vec{y})\} = \rhd_{\alpha a}{}^{b}(\tilde{N}_0)_{b}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}), \tag{B.15}$$

$$\{(\tilde{G}_0)_{\alpha}(\vec{x}), (\tilde{L}_0)_{A}{}^{ij}(\vec{y})\} = \rhd_{\alpha A}{}^{B}(\tilde{L}_0)_{B}{}^{ij}(\vec{x})\,\delta^{(3)}(\vec{x}-\vec{y}). \tag{B.16}$$

The gauge symmetry group has the following structure. First, the groups $\tilde{M}_1\times\tilde{M}_0$, $\tilde{N}_1\times\tilde{N}_0$ and $\tilde{L}_1\times\tilde{L}_0$ with the corresponding algebras $\mathfrak{a}_1$, $\mathfrak{a}_2$ and $\mathfrak{a}_3$, respectively, where:

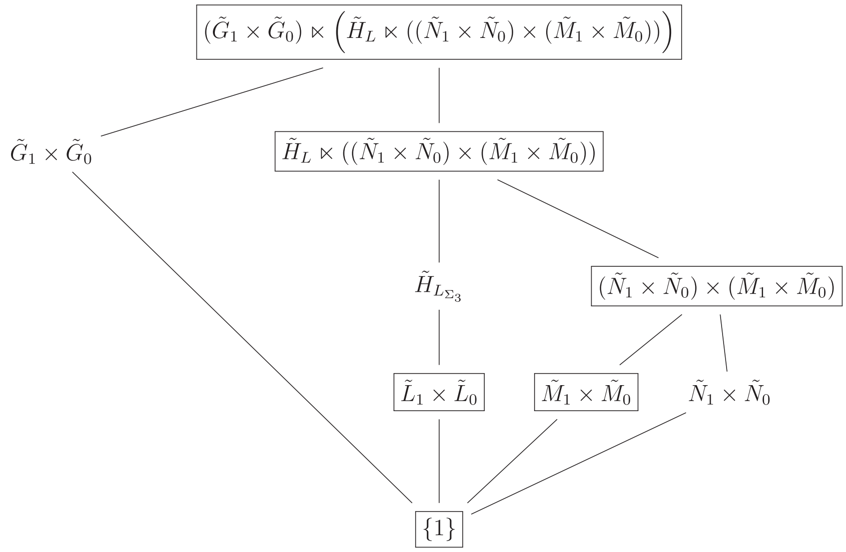

Figure B1. The symmetry group $\mathcal{G}_{\Sigma_3}$ of the Poisson bracket algebra in the phase space. The invariant subgroups are boxed.

$$
\begin{aligned}
\mathfrak{a}_1 &= \text{span}\{(\tilde{M}_1)_\alpha{}^i\} \oplus \text{span}\{(\tilde{M}_0)_\alpha{}^i\}, \\
\mathfrak{a}_2 &= \text{span}\{(\tilde{N}_1)_a\} \oplus \text{span}\{(\tilde{N}_0)_a\}, \\
\mathfrak{a}_3 &= \text{span}\{(\tilde{L}_1)_A{}^{ij}\} \oplus \text{span}\{(\tilde{L}_0)_A{}^{ij}\},
\end{aligned}
\tag{B.17}
$$

are the subgroups of the full symmetry group $\tilde{\mathcal{G}}_{\Sigma_3}$. Besides, the subgroups $\tilde{L}_1 \times \tilde{L}_0$ and $\tilde{M}_1 \times \tilde{M}_0$ are the invariant subgroups. The group $\tilde{N}_1 \times \tilde{N}_0$ is not an invariant subgroup of the whole symmetry group, since the Poisson brackets $\{(\tilde{H}_0)_a{}^i(\vec{x}), (\tilde{N}_0)^b(\vec{y})\}$ and $\{(\tilde{H}_1)_a{}^i(\vec{x}), (\tilde{N}_0)^b(\vec{y})\}$ are equal to some linear combinations of the generators of $\tilde{M}_1 \times \tilde{M}_0$. Nevertheless, one can form a direct product $(\tilde{N}_1 \times \tilde{N}_0) \times (\tilde{M}_1 \times \tilde{M}_0)$, since the generators of these groups are mutually commuting, giving a group which is an invariant subgroup of the complete symmetry group.

Next, consider a subgroup $\tilde{H}_{L_{\Sigma_3}}$ determined by the algebra spanned by the generators $(\tilde{L}_1)_A{}^{ij}$, $(\tilde{L}_0)_A{}^{ij}$, $(\tilde{H}_1)_a{}^i$, and $(\tilde{H}_0)_a{}^i$. This group is not invariant subgroup of the whole symmetry group, because of the PB $\{(\tilde{H}_0)_a{}^i(\vec{x}), (\tilde{N}_0)^b(\vec{y})\}$ and $\{(\tilde{H}_1)_a{}^i(\vec{x}), (\tilde{N}_0)^b(\vec{y})\}$, due to the same argument as before. Now, one can join these two subgroups, of which one is invariant and one is not, using a semidirect product into an invariant subgroup $H_L \ltimes ((N_1 \times N_0) \times (M_1 \times M_0))$, determined by the algebra $\mathfrak{a}_4$:

$$
\mathfrak{a}_4 = \text{span}\{(\tilde{M}_0)_\alpha{}^i, (\tilde{M}_1)_\alpha{}^i, (\tilde{H}_0)_a{}^i, (\tilde{H}_1)_a{}^i, (\tilde{N}_0)_a, (\tilde{N}_1)_a, (\tilde{L}_0)_A{}^{ij}, (\tilde{L}_1)_A{}^{ij}\}.
$$

Finally, following the same line of reasoning, one adds the group $\tilde{G}_1 \times \tilde{G}_0$ and obtains the full gauge symmetry group $\tilde{\mathcal{G}}_{\Sigma_3}$ to be equal to:

$$\tilde{\mathcal{G}}_{\Sigma_3} = (\tilde{G}_1 \times \tilde{G}_0) \ltimes \left(\tilde{H}_L \ltimes ((\tilde{N}_1 \times \tilde{N}_0) \times (\tilde{M}_1 \times \tilde{M}_0))\right).$$

The complete symmetry group structure is shown in the figure B1 appendix B. Here, the invariant subgroups of the whole symmetry group are boxed.

Appendix C. Construction of the symmetry generator

When one substitutes the generators (56) into the equation (55), one obtains the gauge generator of the 3BF theory in the following form

$$\begin{aligned} G = &-\int_{\Sigma_3} d^3\vec{x} \Bigg((\nabla_0 \epsilon_{\mathfrak{m}}{}^{\alpha}{}_i)\Phi(B)_\alpha{}^i - \epsilon_{\mathfrak{m}}{}^{\alpha}{}_i \Phi(\mathcal{F})_\alpha{}^i + (\nabla_0 \epsilon_{\mathfrak{g}}{}^{\alpha})\Phi(\alpha)_\alpha \\ &+ \epsilon_{\mathfrak{g}}{}^{\alpha} \left(f_{\alpha\gamma}{}^{\beta} B_{\beta 0i} \Phi(B)^{\gamma i} + C_{a0} \rhd_{\alpha b}{}^a \Phi(C)^{b0} + \beta_{a0i} \rhd_{\alpha b}{}^a \Phi(\beta)^{b0i} \right. \\ &\left. - \frac{1}{2}\gamma^A{}_{0ij} \rhd_{\alpha A}{}^B \Phi(\gamma)_B{}^{ij} - \Phi(\nabla B)_\alpha \right) + (\nabla_0 \epsilon_{\mathfrak{n}}{}^a)\Phi(C)_a \\ &- \epsilon_{\mathfrak{n}}{}^a \left(\beta_{b0i} \rhd_{\alpha a}{}^b \Phi(B)^{\alpha i} + \Phi(\mathcal{G})_a + (\nabla_0 \epsilon_{\mathfrak{h}}{}^a{}_i)\Phi(\beta)_a{}^i \right) \\ &- \epsilon_{\mathfrak{h}}{}^a{}_i \left(C_{b0} \rhd_{\alpha a}{}^b \Phi(B)^{\alpha i} - 2\beta^b{}_{0j} X_{(ab)}{}^A \Phi(\gamma)_A{}^{ij} + \Phi(\nabla C)_a{}^i \right) \\ &- \frac{1}{2}(\nabla_0 \epsilon_{\mathfrak{l}}^A{}_{ij})\Phi(\gamma)_A{}^{ij} + \frac{1}{2}\epsilon_{\mathfrak{l}}^A{}_{ij} \Phi(\nabla D)_A{}^{ij} \Bigg), \end{aligned} \tag{C.1}$$

where $\epsilon_{\mathfrak{g}}{}^{\alpha}$, $\epsilon_{\mathfrak{h}i}^{a}$, $\epsilon_{\mathfrak{l}ij}^{A}$, $\epsilon_{\mathfrak{m}i}^{\alpha}$, and $\epsilon_{\mathfrak{n}}{}^a$ are the independent parameters of the gauge transformations.

The generator of gauge transformations (C.1) in 3BF theory given by the action (15), is obtained by the Castellani's procedure, requiring the following requirements to be met

$$G_1 = C_{\text{PFC}}, \tag{C.2}$$

$$G_0 + \{G_1, H_{\text{T}}\} = C_{\text{PFC}}, \tag{C.3}$$

$$\{G_0, H_{\text{T}}\} = C_{\text{PFC}}, \tag{C.4}$$

where C_{PFC} denotes some first-class constraints, and assuming that the generator has the following structure:

$$\begin{aligned} G = \int_{\Sigma_3} d^3\vec{x} \Bigg(&\dot{\epsilon}_{\mathfrak{m}}{}^{\alpha}{}_i (G_1)_{\mathfrak{m}\alpha}{}^i + \epsilon_{\mathfrak{m}}{}^{\alpha}{}_i (G_0)_{\mathfrak{m}\alpha}{}^i + \dot{\epsilon}_{\mathfrak{g}}{}^{\alpha}(G_1)_{\mathfrak{g}\alpha} + \epsilon_{\mathfrak{g}}{}^{\alpha}(G_0)_{\mathfrak{g}\alpha} \\ &+ \dot{\epsilon}_{\mathfrak{h}}{}^a{}_i (G_1)_{\mathfrak{h}a}{}^i + \epsilon_{\mathfrak{h}}{}^a{}_i (G_0)_{\mathfrak{h}a}{}^i + \dot{\epsilon}_{\mathfrak{n}}{}^a (G_1)_{\mathfrak{n}a} + \epsilon_{\mathfrak{n}}{}^a (G_0)_{\mathfrak{n}a} \\ &+ \frac{1}{2}\dot{\epsilon}_{\mathfrak{l}}^A{}_{ij}(G_1)_{\mathfrak{l}A}{}^{ij} + \frac{1}{2}\epsilon_{\mathfrak{l}}^A{}_{ij}(G_0)_{\mathfrak{l}A}{}^{ij} \Bigg). \end{aligned} \tag{C.5}$$

The first step of Castellani's procedure, imposing the set of conditions

$$
\begin{aligned}
(G_1)_{\mathfrak{m}\alpha}{}^{i} &= C_{\text{PFC}}, \\
(G_1)_{\mathfrak{g}\alpha} &= C_{\text{PFC}}, \\
(G_1)_{\mathfrak{h}a}{}^{i} &= C_{\text{PFC}}, \\
(G_1)_{\mathfrak{n}a} &= C_{\text{PFC}}, \\
(G_1)_{\mathfrak{l}A}{}^{ij} &= C_{\text{PFC}},
\end{aligned}
\tag{C.6}
$$

is satisfied with a natural choice:

$$
\begin{aligned}
(G_1)_{\mathfrak{m}\alpha}{}^{i} &= -\Phi(B)_{\alpha}{}^{i}, \\
(G_1)_{\mathfrak{g}\alpha} &= -\Phi(\alpha)_{\alpha}, \\
(G_1)_{\mathfrak{h}a}{}^{i} &= -\Phi(C)_{\alpha}{}^{i}, \\
(G_1)_{\mathfrak{n}a} &= -\Phi(\beta)_{a}, \\
(G_1)_{\mathfrak{l}A}{}^{ij} &= \Phi(\gamma)_{A}{}^{ij}.
\end{aligned}
\tag{C.7}
$$

It remains to determine the five generators G_0.

The Castellani's second condition for the generator $(G_0)_{\mathfrak{m}\alpha}{}^{i}$ gives:

$$
\begin{aligned}
(G_0)_{\mathfrak{m}\alpha}{}^{i} - \{\Phi(B)_{\alpha}{}^{i}, H_{\text{T}}\} &= (C_{\text{PFC}})_{\alpha}{}^{i}, \\
(G_0)_{\mathfrak{m}\alpha}{}^{i} - \Phi(\mathcal{F})_{\alpha}{}^{i} &= (C_{\text{PFC}})_{\alpha}{}^{i},
\end{aligned}
\tag{C.8}
$$

that is $(G_0)_{\mathfrak{m}\alpha}{}^{i} = (C_{\text{PFC}})_{\alpha}{}^{i} + \Phi(\mathcal{F})_{\alpha}{}^{i}$. Subsequently, from the Castellani's third condition it follows

$$
\begin{aligned}
&\{(G_0)_{\mathfrak{m}\alpha}{}^{i}, H_{\text{T}}\} = (C_{\text{PFC1}})_{\alpha}{}^{i}, \\
&\{(C_{\text{PFC}})_{\alpha}{}^{i} + \Phi(\mathcal{F})_{\alpha}{}^{i}, H_{\text{T}}\} = (C_{\text{PFC1}})_{\alpha}{}^{i}, \\
&\{(C_{\text{PFC}})_{\alpha}{}^{i}, H_{\text{T}}\} - f_{\beta\gamma\alpha}\alpha^{\beta}{}_{0}\Phi(\mathcal{F})^{\gamma i} = (C_{\text{PFC1}})_{\alpha}{}^{i},
\end{aligned}
\tag{C.9}
$$

which gives

$$
(C_{\text{PFC}})_{\alpha}{}^{i} = f_{\beta\gamma\alpha}\alpha^{\beta}{}_{0}\Phi(B)^{\gamma i}.
$$

It follows that the generator is:

$$
(G_0)_{\mathfrak{m}\alpha}{}^{i} = f_{\beta\gamma\alpha}\alpha^{\beta}{}_{0}\Phi(B)^{\gamma i} + \Phi(\mathcal{F})_{\alpha}{}^{i}.
\tag{C.10}
$$

The Castellani's second condition for the generator $(G_0)_{\mathfrak{g}\alpha}$ gives:

$$
\begin{aligned}
(G_0)_{\mathfrak{g}\alpha} - \{\Phi(\alpha)_{\alpha}, H_{\text{T}}\} &= (C_{\text{PFC}})_{\alpha}, \\
(G_0)_{\mathfrak{g}\alpha} - \Phi(\nabla B)_{\alpha} &= (C_{\text{PFC}})_{\alpha},
\end{aligned}
\tag{C.11}
$$

that is $(G_0)_{\mathfrak{g}\alpha} = (C_{\text{PFC}})_\alpha + \Phi(\nabla B)_\alpha$. Subsequently, from the Castellani's third condition it follows

$$\begin{aligned}
&\left\{(G_0)_{\mathfrak{g}\alpha}, H_{\text{T}}\right\} = (C_{\text{PFC1}})_\alpha,\\
&\left\{(C_{\text{PFC}})_\alpha + \Phi(\nabla B)_\alpha, H_{\text{T}}\right\} = (C_{\text{PFC1}})_\alpha,\\
&\left\{(C_{\text{PFC}})_\alpha, H_{\text{T}}\right\} + B_{\beta 0i} f_{\alpha\gamma}{}^{\beta}\Phi(\mathcal{F})^{\gamma i} - \alpha^{\beta}{}_0 f_{\alpha\beta}{}^{\gamma}\Phi(\nabla B)_\gamma + C_{a0}\triangleright_{\alpha b}{}^{a}\Phi(\mathcal{G})^{b}\\
&\qquad + \beta_{a0i}\triangleright_{\alpha b}{}^{a}\Phi(\nabla C)^{bi} - \frac{1}{2}\gamma^{A}{}_{0ij}\triangleright_{\alpha A}{}^{B}\Phi(\nabla D)_B{}^{ij} = (C_{\text{PFC1}})_\alpha,
\end{aligned} \tag{C.12}$$

which gives

$$\begin{aligned}
(C_{\text{PFC}})_\alpha = {}& -B_{\beta 0i} f_{\alpha\gamma}{}^{\beta}\Phi(B)^{\gamma i} + \alpha^{\beta}{}_0 f_{\alpha\beta}{}^{\gamma}\Phi(\alpha)_\gamma - C_{a0}\triangleright_{\alpha b}{}^{a}\Phi(C)^{b}\\
& - \beta_{a0i}\triangleright_{\alpha b}{}^{a}\Phi(\beta)^{bi} + \frac{1}{2}\gamma^{A}{}_{0ij}\triangleright_{\alpha A}{}^{B}\Phi(\gamma)_B{}^{ij}.
\end{aligned}$$

It follows that the generator is:

$$\begin{aligned}
(G_0)_{\mathfrak{g}\alpha} = {}& -B_{\beta 0i} f_{\alpha\gamma}{}^{\beta}\Phi(B)^{\gamma i} + \alpha^{\beta}{}_0 f_{\alpha\beta}{}^{\gamma}\Phi(\alpha)_\gamma - C_{a0}\triangleright_{\alpha b}{}^{a}\Phi(C)^{b}\\
& - \beta_{a0i}\triangleright_{\alpha b}{}^{a}\Phi(\beta)^{bi} + \frac{1}{2}\gamma^{A}{}_{0ij}\triangleright_{\alpha A}{}^{B}\Phi(\gamma)_B{}^{ij} + \Phi(\nabla B)_\alpha.
\end{aligned} \tag{C.13}$$

The Castellani's second condition for the generator $(G_0)_{\mathfrak{n}a}$ gives

$$\begin{aligned}
&(G_0)_{\mathfrak{n}a} - \left\{\Phi(C)_a, H_{\text{T}}\right\} = (C_{\text{PFC}})_a,\\
&\qquad (G_0)_{\mathfrak{n}a} - \Phi(\mathcal{G})_a = (C_{\text{PFC}})_a,
\end{aligned} \tag{C.14}$$

that is $(G_0)_{\mathfrak{n}a} = (C_{\text{PFC}})_a + \Phi(\mathcal{G})_a$. Subsequently, from the Castellani's third condition it follows

$$\begin{aligned}
&\left\{(G_0)_{\mathfrak{n}a}, H_{\text{T}}\right\} = (C_{\text{PFC1}})_a,\\
&\left\{(C_{\text{PFC}})_a + \Phi(\mathcal{G})_a, H_{\text{T}}\right\} = (C_{\text{PFC1}})_a,\\
&\left\{(C_{\text{PFC}})_a, H_{\text{T}}\right\} + \alpha^{\alpha}{}_0\triangleright_{\alpha a}{}^{b}\Phi(\mathcal{G})_b - \beta_{b0i}\triangleright_{\alpha a}{}^{b}\Phi(\mathcal{F})^{\alpha i} = (C_{\text{PFC1}})_a,
\end{aligned} \tag{C.15}$$

which gives

$$(C_{\text{PFC}})_a = -\alpha^{\alpha}{}_0\triangleright_{\alpha a}{}^{b}\Phi(C)_b + \beta_{b0i}\triangleright_{\alpha a}{}^{b}\Phi(B)^{\alpha i}.$$

It follows that the generator is:

$$(G_0)_{\mathfrak{n}a} = -\alpha^{\alpha}{}_0\triangleright_{\alpha a}{}^{b}\Phi(C)_b + \beta_{b0i}\triangleright_{\alpha a}{}^{b}\Phi(B)^{\alpha i} + \Phi(\mathcal{G})_a.$$

The Castellani's second condition for the generator $(G_0)_{\mathfrak{h}a}{}^{i}$ gives:

$$\begin{aligned}
&(G_0)_{\mathfrak{h}a}{}^{i} - \left\{\Phi(\beta)_a{}^{i}, H_{\text{T}}\right\} = (C_{\text{PFC}})_a{}^{i},\\
&(G_0)_{\mathfrak{h}a}{}^{i} - \Phi(\nabla C)_a{}^{i} = (C_{\text{PFC}})_a{}^{i},
\end{aligned} \tag{C.16}$$

that is $(G_0)_{\mathfrak{h}a}{}^i = (C_{\text{PFC}})_a{}^i + \Phi(\nabla C)_a{}^i$. Subsequently, from the Castellani's third condition it follows

$$\begin{aligned}
&\{(G_0)_{\mathfrak{h}a}{}^i, H_{\text{T}}\} = (C_{\text{PFC1}})_a{}^i,\\
&\{(C_{\text{PFC}})_a{}^i + \Phi(\nabla C)_a{}^i, H_{\text{T}}\} = (C_{\text{PFC1}})_a{}^i,\\
&\{(C_{\text{PFC}})_a{}^i, H_{\text{T}}\} + \alpha^{\alpha}{}_0 \rhd_{\alpha a}{}^b \Phi(\nabla C)_b{}^i - C_{b0} \rhd_{\alpha a}{}^b \Phi(\mathcal{F})^{\alpha i} + 2\beta^b{}_{0j} X_{(ab)}{}^A \Phi(\nabla D)_A{}^{ij} = (C_{\text{PFC1}})_a{}^i,
\end{aligned}$$

which gives

$$(C_{\text{PFC}})_a{}^i = -\alpha^{\alpha}{}_0 \rhd_{\alpha a}{}^b \Phi(\beta)_b{}^i + C_{b0} \rhd_{\alpha a}{}^b \Phi(B)^{\alpha i} - 2\beta^b{}_{0j} X_{(ab)}{}^A \Phi(\gamma)_A{}^{ij}.$$

It follows that the generator is:

$$(G_0)_{\mathfrak{h}a}{}^i = -\alpha^{\alpha}{}_0 \rhd_{\alpha a}{}^b \Phi(\beta)_b{}^i + C_{b0} \rhd_{\alpha a}{}^b \Phi(B)^{\alpha i} - 2\beta^b{}_{0j} X_{(ab)}{}^A \Phi(\gamma)_A{}^{ij} + \Phi(\nabla C)_a{}^i.$$

The Castellani's second condition for the generator $(G_0)_{\mathfrak{l}A}{}^{ij}$ gives:

$$\begin{aligned}
&(G_0)_{\mathfrak{l}A}{}^{ij} + \{\Phi(\gamma)_A{}^{ij}, H_{\text{T}}\} = (C_{\text{PFC}})_A{}^{ij},\\
&(G_0)_{\mathfrak{l}A}{}^{ij} + \Phi(\nabla D)_A{}^{ij} = (C_{\text{PFC}})_A{}^{ij},
\end{aligned} \tag{C.17}$$

that is $(G_0)_{\mathfrak{l}A}{}^{ij} = (C_{\text{PFC}})_A{}^{ij} - \Phi(\nabla D)_A{}^{ij}$. Subsequently, from the Castellani's third condition it follows:

$$\begin{aligned}
&\{(G_0)_{\mathfrak{l}A}{}^{ij}, H_{\text{T}}\} = (C_{\text{PFC1}})_A{}^{ij},\\
&\{(C_{\text{PFC}})_A{}^{ij} - \Phi(\nabla D)_A{}^{ij}, H_{\text{T}}\} = (C_{\text{PFC1}})_A{}^{ij},\\
&\{(C_{\text{PFC}})_A{}^{ij}, H_{\text{T}}\} - \alpha^{\alpha}{}_0 \rhd_{\alpha A}{}^B \Phi(\nabla D)_B{}^{ij} = (C_{\text{PFC1}})_A{}^{ij},
\end{aligned} \tag{C.18}$$

which gives

$$(C_{\text{PFC}})_A{}^{ij} = \alpha^{\alpha}{}_0 \rhd_{\alpha A}{}^B \Phi(\gamma)_B{}^{ij}.$$

It follows that the generator is:

$$(G_0)_{\mathfrak{l}A}{}^{ij} = \alpha^{\alpha}{}_0 \rhd_{\alpha A}{}^B \Phi(\gamma)_B{}^{ij} - \Phi(\nabla D)_A{}^{ij}. \tag{C.19}$$

At this point, it is useful to summarize the results, and introduce the new notation:

$$\begin{aligned}
\dot{\epsilon}_{\mathfrak{m}}{}^{\alpha}{}_i (G_1)_{\mathfrak{m}\alpha}{}^i + \epsilon_{\mathfrak{m}}{}^{\alpha}{}_i (G_0)_{\mathfrak{m}\alpha}{}^i &= -\nabla_0 \epsilon_{\mathfrak{m}}{}^{\alpha}{}_i \Phi(B)_{\alpha}{}^i + \epsilon_{\mathfrak{m}}{}^{\alpha}{}_i \Phi(\mathcal{F})_{\alpha}{}^i\\
&= \nabla_0 \epsilon_{\mathfrak{m}}{}^{\alpha}{}_i (\tilde{M}_1)_{\alpha}{}^i + \epsilon_{\mathfrak{m}}{}^{\alpha}{}_i (\tilde{M}_0)_{\alpha}{}^i.
\end{aligned} \tag{C.20}$$

Note that the time derivative of the parameter combines with some of the other terms into a covariant derivative in the time directions.

For the second part of the total generator one obtains:

$$
\begin{aligned}
&{}^{\alpha}\dot{\epsilon}_{\mathfrak{g}}(G_1)_{\mathfrak{g}\alpha} + \epsilon_{\mathfrak{g}}{}^{\alpha}(G_0)_{\mathfrak{g}\alpha} \\
&= -{}^{\alpha}\dot{\epsilon}_{\mathfrak{g}}\Phi(\alpha)_{\alpha} - \epsilon_{\mathfrak{g}}{}^{\alpha}\Bigg(B_{\beta 0i}f_{\alpha\gamma}{}^{\beta}\Phi(B)^{\gamma i} - \alpha^{\beta}{}_0 f_{\alpha\beta}{}^{\gamma}\Phi(\alpha)_{\gamma} + C_{a0}\rhd_{\alpha b}{}^{a}\Phi(C)^{b} \\
&+ \beta_{a0i}\rhd_{\alpha b}{}^{a}\Phi(\beta)_{b}{}^{i} - \frac{1}{2}\gamma^{A}{}_{0ij}\rhd_{\alpha A}{}^{B}\Phi(\gamma)_{B}{}^{ij} - \Phi(\nabla B)_{\alpha}\Bigg) \\
&= -\nabla_0\epsilon_{\mathfrak{g}}{}^{\alpha}\Phi(\alpha)_{\alpha} - \epsilon_{\mathfrak{g}}{}^{\alpha}\Bigg(B_{\beta 0i}f_{\alpha\gamma}{}^{\beta}\Phi(B)^{\gamma i} + C_{a0}\rhd_{\alpha b}{}^{a}\Phi(C)^{b} \\
&+ \beta_{a0i}\rhd_{\alpha b}{}^{a}\Phi(\beta)_{b}{}^{i} - \frac{1}{2}\gamma^{A}{}_{0ij}\rhd_{\alpha A}{}^{B}\Phi(\gamma)_{B}{}^{ij} - \Phi(\nabla B)_{\alpha}\Bigg) \\
&= \nabla_0\epsilon_{\mathfrak{g}}{}^{\alpha}(\tilde{G}_1)_{\alpha} + \epsilon_{\mathfrak{g}}{}^{\alpha}(\tilde{G}_0)_{\alpha}.
\end{aligned}
\tag{C.21}
$$

Furthermore, it follows:

$$
\begin{aligned}
\dot{\epsilon}_{\mathfrak{h}i}^{a}(G_1)_{\mathfrak{h}a}{}^{i} + \epsilon_{\mathfrak{h}}{}^{a}{}_{i}(G_0)_{\mathfrak{h}a}{}^{i} &= -\nabla_0\epsilon_{\mathfrak{h}}{}^{a}{}_{i}\Phi(\beta)_{\alpha}{}^{i} + \epsilon_{\mathfrak{h}}{}^{a}{}_{i}\big(C_{b0}\rhd_{\alpha a}{}^{b}\Phi(B)^{\alpha i} \\
&\quad - 2\beta^{b}{}_{0j}X_{(ab)}{}^{A}\Phi(\gamma)_{A}{}^{ij} + \Phi(\nabla C)_{a}{}^{i}\big) \\
&= \nabla_0\epsilon_{\mathfrak{h}}{}^{a}{}_{i}(\tilde{H}_1)_{a}{}^{i} + \epsilon_{\mathfrak{h}}{}^{a}{}_{i}(\tilde{H}_0)_{a}{}^{i},
\end{aligned}
\tag{C.22}
$$

$$
\begin{aligned}
\dot{\epsilon}_{\mathfrak{n}}{}^{a}(G_1)_{\mathfrak{n}a} + \epsilon_{\mathfrak{n}}{}^{a}(G_0)_{\mathfrak{n}a} &= -\nabla_0\epsilon_{\mathfrak{n}}{}^{a}\Phi(C)_{a} + \epsilon_{\mathfrak{n}}{}^{a}(\beta_{b0i}\rhd_{\alpha a}{}^{b}\Phi(B)^{\alpha i} + \Phi(\mathcal{G})_{a}) \\
&= \nabla_0\epsilon_{\mathfrak{n}}{}^{a}(\tilde{N}_1)_{a} + \epsilon_{\mathfrak{n}}{}^{a}(\tilde{N}_0)_{a}.
\end{aligned}
\tag{C.23}
$$

Finally, one gets:

$$
\begin{aligned}
\frac{1}{2}\dot{\epsilon}_{\mathfrak{l}ij}^{A}(G_1)_{\mathfrak{l}A}{}^{ij} + \frac{1}{2}\epsilon_{\mathfrak{l}}^{A}{}_{ij}(G_0)_{\mathfrak{l}A}{}^{ij} &= \frac{1}{2}\dot{\epsilon}_{\mathfrak{l}ij}^{A}\Phi(\gamma)_{A}{}^{ij} + \frac{1}{2}\epsilon_{\mathfrak{l}}^{A}{}_{ij}\alpha^{\alpha}{}_{0}\rhd_{\alpha A}{}^{B}\Phi(\gamma)_{B}{}^{ij} \\
&\quad - \frac{1}{2}\epsilon_{\mathfrak{l}}^{A}{}_{ij}\Phi(\nabla D)_{A}{}^{ij} \\
&= \frac{1}{2}\nabla_0\epsilon_{\mathfrak{l}}^{A}{}_{ij}\Phi(\gamma)_{A}{}^{ij} - \frac{1}{2}\epsilon_{\mathfrak{l}}^{A}{}_{ij}\Phi(\nabla D)_{A}{}^{ij} \\
&= \frac{1}{2}\nabla_0\epsilon_{\mathfrak{l}}^{A}{}_{ij}(\tilde{L}_1)_{A}{}^{ij} + \frac{1}{2}\epsilon_{\mathfrak{l}}^{A}{}_{ij}(\tilde{L}_0)_{A}{}^{ij}.
\end{aligned}
\tag{C.24}
$$

Appendix D. Definitions of maps $\mathcal{T}$, $\mathcal{S}$, $\mathcal{D}$, $\mathcal{X}_1$, and $\mathcal{X}_2$

Given G-invariant symmetric non-degenerate bilinear forms in $\mathfrak{g}$ and $\mathfrak{h}$, one can define a bilinear antisymmetric map $\mathcal{T} : \mathfrak{h} \times \mathfrak{h} \to \mathfrak{g}$ by the rule:

$$
\langle \mathcal{T}(\underline{h}_1, \underline{h}_2), \underline{g}\rangle_{\mathfrak{g}} = -\langle \underline{h}_1, \underline{g} \rhd \underline{h}_2\rangle_{\mathfrak{h}}, \quad \forall\ \underline{h}_1, \underline{h}_2 \in \mathfrak{h},\ \forall\ \underline{g} \in \mathfrak{g}.
$$

Written in basis:

$$\mathcal{T}(t_a, t_b) = \mathcal{T}_{ab}{}^{\alpha} \tau_{\alpha},$$

where the components of the map $\mathcal{T}$ are:

$$\mathcal{T}_{ab}{}^{\alpha} = -g_{ac} \triangleright_{\beta b}{}^{c} g^{\alpha\beta}.$$

See [26] for more properties and the construction of $2BF$ invariant topological action using this map.

The transformations of the Lagrange multipliers and the $3BF$ invariant topological action is defined via maps

$$\mathcal{S} : \mathfrak{l} \times \mathfrak{l} \to \mathfrak{g}, \qquad \mathcal{X}_1 : \mathfrak{l} \times \mathfrak{h} \to \mathfrak{h}, \qquad \mathcal{X}_2 : \mathfrak{l} \times \mathfrak{h} \to \mathfrak{h}, \quad \mathcal{D} : \mathfrak{h} \times \mathfrak{h} \times \mathfrak{l} \to \mathfrak{g},$$

as it is defined in [13]. The map $\mathcal{S} : \mathfrak{l} \times \mathfrak{l} \to \mathfrak{g}$ is defined by the rule:

$$\langle \mathcal{S}(\underline{l}_1, \underline{l}_2), \underline{g} \rangle_{\mathfrak{g}} = -\langle \underline{l}_1, \underline{g} \triangleright \underline{l}_2 \rangle_{\mathfrak{l}}, \quad \forall\, \underline{l}_1, \forall\, \underline{l}_2 \in \mathfrak{l}, \ \forall\, \underline{g} \in \mathfrak{g}.$$

Written in the basis:

$$\mathcal{S}(T_A, T_B) = \mathcal{S}_{AB}{}^{\alpha} \tau_{\alpha},$$

the defining relation for $\mathcal{S}$ becomes:

$$\mathcal{S}_{AB}{}^{\alpha} = -\triangleright_{\beta [B}{}^{C} \ g_{A]C} g^{\alpha\beta}.$$

Given two $\mathfrak{l}$-valued forms η and ω, one can define a $\mathfrak{g}$-valued form:

$$\omega \wedge^{\mathcal{S}} \eta = \omega^A \wedge \eta^B \mathcal{S}_{AB}{}^{\alpha} \tau_{\alpha}.$$

Using this map, the transformations of the Lagrange multipliers under L-gauge are defined in [13].

Further, to define the transformations of the Lagrange multipliers under H-gauge transformations the bilinear map $\mathcal{X}_1 : \mathfrak{l} \times \mathfrak{h} \to \mathfrak{h}$ is defined:

$$\langle \mathcal{X}_1(\underline{l}, \underline{h}_1), \underline{h}_2 \rangle_{\mathfrak{h}} = -\langle \underline{l}, \{\underline{h}_1, \underline{h}_2\} \rangle_{\mathfrak{l}}, \quad \forall\, \underline{h}_1, \underline{h}_2 \in \mathfrak{h}, \ \forall\, \underline{l} \in \mathfrak{l},$$

and bilinear map $\mathcal{X}_2 : \mathfrak{l} \times \mathfrak{h} \to \mathfrak{h}$ by the rule:

$$\langle \mathcal{X}_2(\underline{l}, \underline{h}_2), \underline{h}_1 \rangle_{\mathfrak{h}} = -\langle \underline{l}, \{\underline{h}_1, \underline{h}_2\} \rangle_{\mathfrak{l}}, \quad \forall\, \underline{h}_1, \underline{h}_2 \in \mathfrak{h}, \ \forall\, \underline{l} \in \mathfrak{l}.$$

As far as the bilinear maps $\mathcal{X}_1$ and $\mathcal{X}_2$ one can define the coefficients in the basis as:

$$\mathcal{X}_1(T_A, t_a) = \mathcal{X}_{1\ Aa}{}^b\, t_b, \qquad \mathcal{X}_2(T_A, t_a) = \mathcal{X}_{2\ Aa}{}^b\, t_b.$$

When written in the basis the defining relations for the maps $\mathcal{X}_1$ and $\mathcal{X}_2$ become:

$$\mathcal{X}_{1Ab}{}^c = -X_{ba}{}^B g_{AB} g^{ac}, \qquad \mathcal{X}_{2Ab}{}^c = -X_{ab}{}^B g_{AB} g^{ac}.$$

Given $\mathfrak{l}$-valued differential form ω and $\mathfrak{h}$-valued differential form η, one defines a $\mathfrak{h}$-valued form as:

$$\omega \wedge^{\mathcal{X}_1} \eta = \omega^A \wedge \eta^a \mathcal{X}_{1Aa}{}^b t_b, \qquad \omega \wedge^{\mathcal{X}_2} \eta = \omega^A \wedge \eta^a \mathcal{X}_{2Aa}{}^b t_b.$$

Finally, a trilinear map $\mathcal{D} : \mathfrak{h} \times \mathfrak{h} \times \mathfrak{l} \to \mathfrak{g}$ is needed:

$$\langle \mathcal{D}(\underline{h}_1, \underline{h}_2, \underline{l}), \underline{g} \rangle_{\mathfrak{g}} = -\langle \underline{l}, \{\underline{g} \triangleright \underline{h}_1, \underline{h}_2\} \rangle_{\mathfrak{l}}, \quad \forall\, \underline{h}_1, \underline{h}_2 \in \mathfrak{h},\ \forall\, \underline{l} \in \mathfrak{l},\ \forall\, \underline{g} \in \mathfrak{g},$$

One can define the coefficients of the trilinear map as:

$$\mathcal{D}(t_a, t_b, T_A) = \mathcal{D}_{abA}{}^\alpha \tau_\alpha,$$

and the defining relation for the map $\mathcal{D}$ expressed in terms of coefficients becomes:

$$\mathcal{D}_{abA}{}^\beta = -\triangleright_{\alpha a}{}^c X_{cb}{}^B g_{AB} g^{\alpha\beta}.$$

Given two $\mathfrak{h}$-valued forms ω and η, and $\mathfrak{l}$-valued form ξ, the g-valued form is given by the formula:

$$\omega \wedge^{\mathcal{D}} \eta \wedge^{\mathcal{D}} \xi = \omega^a \wedge \eta^b \wedge \xi^A \mathcal{D}_{abA}{}^\beta \tau_\beta.$$

With these maps in hand, the transformations of the Lagrange multipliers under H-gauge transformations are defined, see [13].

Appendix E. Form-variations of all fields and momenta

The obtained gauge generator (55) is employed to calculate the form variations of variables and their corresponding canonical momenta, denoted as $A(t, \vec{x})$, using the following equation,

$$\delta_0 A(t, \vec{x}) = \{A(t, \vec{x}), G\}. \tag{E.1}$$

The computed form variations are given as follows:

$$\delta_0 B^{\alpha}{}_{0i} = -\nabla_0 \epsilon_{\mathfrak{m}i}{}^{\alpha} + f_{\beta\gamma}{}^{\alpha}\epsilon_{\mathfrak{g}}{}^{\beta}B^{\gamma}{}_{0i} + \epsilon_{\mathfrak{n}}{}^{a}\triangleright_{\alpha a}{}^{b}\beta_{b0i} + \epsilon_{\mathfrak{h}i}{}^{a}\triangleright_{\alpha a}{}^{b}C_{b0}, \qquad \delta_0\pi(B)_{\alpha}^{0i} = f_{\alpha\beta}{}^{\gamma}\epsilon_{\mathfrak{g}}{}^{\beta}\pi(B)_{\gamma}{}^{0i},$$

$$\delta_0 B^{\alpha}{}_{ij} = -2\nabla_{[i|}\epsilon_{\mathfrak{m}|j]}{}^{\alpha} + f_{\beta\gamma}{}^{\alpha}\epsilon_{\mathfrak{g}}{}^{\beta}B^{\gamma}{}_{ij} - \epsilon_{\mathfrak{l}ij}{}^{A}\triangleright_{\alpha A}{}^{B}D_B + \epsilon_{\mathfrak{n}}{}^{a}\triangleright_{\alpha a}{}^{b}\beta_{bij} + 2\epsilon_{\mathfrak{h}}{}^{a}{}_{[j|}\triangleright_{\alpha a}{}^{b}C_{b|i]}, \qquad \delta_0\pi(B)_{\alpha}{}^{ij} = f_{\alpha\beta}{}^{\gamma}\epsilon_{\mathfrak{g}}{}^{\beta}\pi(B)_{\gamma}{}^{ij},$$

$$\delta_0\alpha^{\alpha}{}_0 = -\nabla_0\epsilon_{\mathfrak{g}}{}^{\alpha}, \qquad \delta_0\pi(\alpha)_{\alpha}^{0} = f_{\alpha\beta}{}^{\gamma}\epsilon_{\mathfrak{m}}{}^{\beta}{}_{i}\pi(B)_{\gamma}{}^{0i} + f_{\alpha\beta}{}^{\gamma}\epsilon_{\mathfrak{g}}{}^{\beta}\pi(\alpha)_{\gamma}{}^{0} + \triangleright_{\alpha b}{}^{a}\epsilon_{\mathfrak{n}}{}^{b}\pi(C)_a^0 + \triangleright_{\alpha b}{}^{a}\epsilon_{\mathfrak{h}}{}^{b}{}_{i}\pi(\beta)_a^i - \frac{1}{2}\triangleright_{\alpha B}{}^{A}\epsilon_{\mathfrak{l}}{}^{B}{}_{ij}\pi(\gamma)_A{}^{0ij},$$

$$\delta_0\alpha^{\alpha}{}_i = -\nabla_i\epsilon_{\mathfrak{g}}{}^{\alpha} - \partial_a{}^{\alpha}\epsilon_{\mathfrak{h}i}{}^{a}, \qquad \delta_0\pi(\alpha)_{\alpha}^{i} = f_{\alpha\beta}{}^{\gamma}\epsilon_{\mathfrak{m}}{}^{\beta}{}_{j}\pi(B)_{\gamma}{}^{ij} + f_{\alpha\beta}{}^{\gamma}\epsilon_{\mathfrak{g}}{}^{\beta}\pi(\alpha)_{\gamma}{}^{i} + \triangleright_{\alpha b}{}^{\alpha}\epsilon_{\mathfrak{n}}{}^{b}\pi(C)_a^i + \triangleright_{\alpha b}{}^{\alpha}\epsilon_{\mathfrak{h}j}{}^{b}\pi(\beta)_a^{ij} - \frac{1}{2}\triangleright_{\alpha B}{}^{A}\epsilon_{\mathfrak{l}jk}{}^{B}\pi(\gamma)_A^{ijk} - \epsilon^{0ijk}\nabla_j\epsilon_{\mathfrak{m}\alpha k}, - \frac{1}{2}\epsilon^{0ijk}\epsilon_{\mathfrak{n}}{}^{a}\triangleright_{\alpha b}{}^{a}\beta^{b}{}_{jk},$$

$$\delta_0 C^{a}{}_0 = -\nabla_0\epsilon_{\mathfrak{n}}{}^{a} + \epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha b}{}^{a}C^{b}{}_0, \qquad \delta_0\pi(C)_a^0 = -\epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha a}{}^{b}\pi(C)_b^0 + \epsilon_{\mathfrak{h}bi}\triangleright_{\alpha a}{}^{b}\pi(B)^{\alpha 0i},$$

$$\delta_0 C^{a}{}_i = -\nabla_i\epsilon_{\mathfrak{n}}{}^{a} + \epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha b}{}^{a}C^{b}{}_i - \epsilon_{\mathfrak{m}i}{}^{\alpha}\partial^{a}{}_{\alpha} + 2\epsilon_{\mathfrak{h}}{}^{b}{}_{i}D_A X_{(bc)}{}^{A}g^{ac}, \qquad \delta_0\pi(C)_a^i = -\epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha a}{}^{b}\pi(C)_b^i + \epsilon_{\mathfrak{h}bj}\triangleright_{\alpha a}{}^{b}\pi(B)^{\alpha ij},$$

$$\delta_0\beta^{a}{}_{0i} = -\nabla_0\epsilon_{\mathfrak{h}i}{}^{a} + \epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha b}{}^{a}\beta_{b0i}, \qquad \delta_0\pi(\beta)_a{}^{0i} = -\epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha a}{}^{b}\pi(\beta)_b{}^{0i} + \epsilon_{\mathfrak{n}b}\triangleright_{\alpha a}{}^{b}\pi(B)^{\alpha 0i} - 2\epsilon_{\mathfrak{h}j}{}^{b}X_{(ab)}{}^{A}\pi(\gamma)_A^{0ij},$$

$$\delta_0\beta^{a}{}_{ij} = -2\nabla_{[i|}\epsilon_{\mathfrak{h}|j]}{}^{a} + \epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha b}{}^{a}\beta^{b}{}_{ij} + \epsilon_{\mathfrak{l}ij}{}^{A}\delta_A{}^{a}, \qquad \delta_0\pi(\beta)_a{}^{ij} = -\epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha a}{}^{b}\pi(\beta)_b{}^{ij} + \epsilon_{\mathfrak{n}b}\triangleright_{\alpha a}{}^{b}\pi(B)^{\alpha ij} - 2\epsilon_{\mathfrak{h}k}{}^{b}X_{(ab)}{}^{A}\pi(\gamma)_A{}^{ijk} + \epsilon^{0ijk}\nabla_k\epsilon_{\mathfrak{n}a} + \epsilon^{0ijk}\epsilon_{\mathfrak{h}k}{}^{a}\partial_{a\alpha},$$

$$\delta_0\gamma^{A}{}_{0ij} = \epsilon_{\mathfrak{g}}{}^{\alpha}\gamma^{B}{}_{0ij}\triangleright_{\alpha B}{}^{A} + \nabla_0\epsilon_{\mathfrak{l}ij}{}^{A} - 4\epsilon_{\mathfrak{h}}{}^{a}{}_{[i|}\beta^{b}{}_{0|j]}X_{(ab)}{}^{A}, \qquad \delta_0\pi(\gamma)_A{}^{0ij} = -\epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha A}{}^{B}\pi(\gamma)_B{}^{0ij},$$

$$\delta_0\gamma^{A}{}_{ijk} = \epsilon_{\mathfrak{g}}{}^{\alpha}\gamma^{B}{}_{ijk}\triangleright_{\alpha B}{}^{A} + \nabla_i\epsilon_{\mathfrak{l}jk}{}^{A} - \nabla_j\epsilon_{\mathfrak{l}ik}{}^{A} + \nabla_k\epsilon_{\mathfrak{l}ij}{}^{A} + 3!\epsilon_{\mathfrak{h}[i}{}^{a}\beta^{b}{}_{jk]}X_{(ab)}{}^{A}, \qquad \delta_0\pi(\gamma)_A{}^{ijk} = -\epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha A}{}^{B}\pi(\gamma)_B{}^{ijk} + \epsilon^{oijk}\delta_{aA}\epsilon_{\mathfrak{n}}{}^{a},$$

$$\delta_0 D^{A} = \epsilon_{\mathfrak{n}}{}^{a}\delta_a{}^{A} + \epsilon_{\mathfrak{g}}{}^{\alpha}D^{B}\triangleright_{\alpha B}{}^{A}, \qquad \delta_0\pi(D)_A = -2\epsilon_{\mathfrak{h}i}{}^{a}X_{(ab)A}\pi(C)^{bi} - \frac{1}{2}\epsilon_{\mathfrak{l}B}{}^{ij}\triangleright_{\alpha A}{}^{B}\pi(B)_{0ij}^{\alpha} - \epsilon_{\mathfrak{g}}{}^{\alpha}\triangleright_{\alpha A}{}^{B}\pi(D)_B \tag{E.2}$$

Appendix F. Symmetry algebra calculations

To obtain the structure of the symmetry group of the 3*BF* action, as presented in the subsection 4.4, one has to calculate the commutators between the generators of all the symmetries, i.e. the *G*-, *H*-, *L*-, *M*-, and *N*-gauge symmetries. This process is described in the subsections 4.1–4.3, while details of the calculation which are not straightforward will be given in the following.

F.1. Commutator [H, H]

Let us derive the commutator of the generators of the *H*-gauge transformations, i.e. the equation (76). After transforming the variables under *H*-gauge transformations for the parameter $\epsilon_{\mathfrak{h}1}$ one obtains the following

$$\alpha' = \alpha - \partial\epsilon_{\mathfrak{h}1}, \tag{F.1}$$

$$\beta' = \beta - \overset{\alpha-\partial\epsilon_{\mathfrak{h}1}}{\nabla}\epsilon_{\mathfrak{h}1} - \epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}1}, \tag{F.2}$$

$$\gamma' = \gamma + \{\beta - \overset{\alpha-\partial\epsilon_{\mathfrak{h}1}}{\nabla}\epsilon_{\mathfrak{h}1} - \epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}1}, \epsilon_{\mathfrak{h}1}\}_{\text{pf}} + \{\epsilon_{\mathfrak{h}1}, \beta\}_{\text{pf}}, \tag{F.3}$$

$$B' = B - (C - D\wedge^{\mathcal{X}_1}\epsilon_{\mathfrak{h}1} - D\wedge^{\mathcal{X}_2}\epsilon_{\mathfrak{h}1})\wedge^{\mathcal{T}}\epsilon_{\mathfrak{h}1} - \epsilon_{\mathfrak{h}1}\wedge^{\mathcal{D}}\epsilon_{\mathfrak{h}1}\wedge^{\mathcal{D}}D, \tag{F.4}$$

$$C' = C - D\wedge^{\mathcal{X}_1}\epsilon_{\mathfrak{h}1} - D\wedge^{\mathcal{X}_2}\epsilon_{\mathfrak{h}1}, \tag{F.5}$$

$$D' = D, \tag{F.6}$$

and transforming the variables once more for the parameter $\epsilon_{\mathfrak{h}2}$ one obtains:

$$\begin{aligned}
\alpha'' &= \alpha - \partial\epsilon_{\mathfrak{h}1} - \partial\epsilon_{\mathfrak{h}2},\\
\beta'' &= \beta - \overset{\alpha-\partial\epsilon_{\mathfrak{h}1}}{\nabla}\epsilon_{\mathfrak{h}1} - \epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}1} - \overset{\alpha-\partial\epsilon_{\mathfrak{h}1}-\partial\epsilon_{\mathfrak{h}2}}{\nabla}\epsilon_{\mathfrak{h}2} - \epsilon_{\mathfrak{h}2}\wedge\epsilon_{\mathfrak{h}2},\\
\gamma'' &= \gamma + \{\beta - \overset{\alpha-\partial\epsilon_{\mathfrak{h}1}}{\nabla}\epsilon_{\mathfrak{h}1} - \epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}1}, \epsilon_{\mathfrak{h}1}\}_{\text{pf}} + \{\epsilon_{\mathfrak{h}1}, \beta\}_{\text{pf}}\\
&\quad + \{\beta - \overset{\alpha-\partial\epsilon_{\mathfrak{h}1}}{\nabla}\epsilon_{\mathfrak{h}1} - \epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}1} - \overset{\alpha-\partial\epsilon_{\mathfrak{h}1}-\partial\epsilon_{\mathfrak{h}2}}{\nabla}\epsilon_{\mathfrak{h}2} - \epsilon_{\mathfrak{h}2}\wedge\epsilon_{\mathfrak{h}2}, \epsilon_{\mathfrak{h}2}\}_{\text{pf}}\\
&\quad + \{\epsilon_{\mathfrak{h}2}, \beta - \overset{\alpha-\partial\epsilon_{\mathfrak{h}1}}{\nabla}\epsilon_{\mathfrak{h}1} - \epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}1}\}_{\text{pf}},\\
B'' &= B - (C - D\wedge^{\mathcal{X}_1}\epsilon_{\mathfrak{h}1} - D\wedge^{\mathcal{X}_2}\epsilon_{\mathfrak{h}1})\wedge^{\mathcal{T}}\epsilon_{\mathfrak{h}1} - \epsilon_{\mathfrak{h}1}\wedge^{\mathcal{D}}\epsilon_{\mathfrak{h}1}\wedge^{\mathcal{D}}D\\
&\quad - (C - D\wedge^{\mathcal{X}_1}\epsilon_{\mathfrak{h}1} - D\wedge^{\mathcal{X}_2}\epsilon_{\mathfrak{h}1} - D\wedge^{\mathcal{X}_1}\epsilon_{\mathfrak{h}2} - D\wedge^{\mathcal{X}_2}\epsilon_{\mathfrak{h}2})\wedge^{\mathcal{T}}\epsilon_{\mathfrak{h}2}\\
&\quad - \epsilon_{\mathfrak{h}2}\wedge^{\mathcal{D}}\epsilon_{\mathfrak{h}2}\wedge^{\mathcal{D}}D,\\
C'' &= C - D\wedge^{\mathcal{X}_1}\epsilon_{\mathfrak{h}1} - D\wedge^{\mathcal{X}_2}\epsilon_{\mathfrak{h}1} - D\wedge^{\mathcal{X}_1}\epsilon_{\mathfrak{h}2} - D\wedge^{\mathcal{X}_2}\epsilon_{\mathfrak{h}2},\\
D'' &= D.
\end{aligned} \tag{F.7}$$

It is easy to see that for variables $\alpha^\alpha{}_\mu$, $C^a{}_\mu$ and D^A the following is obtained:

$$\begin{aligned} e^{\epsilon_{\mathfrak{h}1}\cdot H}e^{\epsilon_{\mathfrak{h}2}\cdot H}\alpha^\alpha{}_\mu &= e^{\epsilon_{\mathfrak{h}2}\cdot H}e^{\epsilon_{\mathfrak{h}1}\cdot H}\alpha^\alpha{}_\mu, \\ e^{\epsilon_{\mathfrak{h}1}\cdot H}e^{\epsilon_{\mathfrak{h}2}\cdot H}C^a{}_\mu &= e^{\epsilon_{\mathfrak{h}2}\cdot H}e^{\epsilon_{\mathfrak{h}1}\cdot H}C^a{}_\mu, \\ e^{\epsilon_{\mathfrak{h}1}\cdot H}e^{\epsilon_{\mathfrak{h}2}\cdot H}D^A &= e^{\epsilon_{\mathfrak{h}2}\cdot H}e^{\epsilon_{\mathfrak{h}1}\cdot H}D^A. \end{aligned} \tag{F.8}$$

For the remaining variables, $\beta^a{}_{\mu\nu}$, $\gamma^A{}_{\mu\nu\rho}$ and $B^\alpha{}_{\mu\nu}$, after subtracting (appendix F.1) and the corresponding equation where $\epsilon_{\mathfrak{h}1} \leftrightarrow \epsilon_{\mathfrak{h}2}$, one obtains:

$$\begin{aligned} \left(e^{\epsilon_{\mathfrak{h}1}\cdot H}e^{\epsilon_{\mathfrak{h}2}\cdot H} - e^{\epsilon_{\mathfrak{h}2}\cdot H}e^{\epsilon_{\mathfrak{h}1}\cdot H}\right)\frac{1}{2}\beta^a{}_{\mu\nu} &= \partial_b{}^\alpha \epsilon_{\mathfrak{h}2}{}^b{}_{[\mu|}\epsilon_{\mathfrak{h}1}{}^c{}_{|\nu]}\triangleright_{\alpha c}{}^a - \partial_b{}^\alpha \epsilon_{\mathfrak{h}1}{}^b{}_{[\mu|}\epsilon_{\mathfrak{h}2}{}^c{}_{|\nu]}\triangleright_{\alpha c}{}^a \\ &= 2\delta_A{}^a X_{(bc)}{}^A \epsilon_{\mathfrak{h}1}{}^b{}_{[\mu|}\epsilon_{\mathfrak{h}2}{}^c{}_{|\nu]} \\ &= \delta_A{}^a(\{\epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}2}\}_{\mathrm{pf}} - \{\epsilon_{\mathfrak{h}2}\wedge\epsilon_{\mathfrak{h}1}\}_{\mathrm{pf}})^A_{\mu\nu}, \\ \left(e^{\epsilon_{\mathfrak{h}1}\cdot H}e^{\epsilon_{\mathfrak{h}2}\cdot H} - e^{\epsilon_{\mathfrak{h}2}\cdot H}e^{\epsilon_{\mathfrak{h}1}\cdot H}\right)\frac{1}{3!}\gamma^A{}_{\mu\nu\rho} &= 2(\partial_{[\mu}\epsilon_{\mathfrak{h}1}{}^a_\nu)\epsilon_{\mathfrak{h}2}{}^b_{\rho]}X_{(ab)}{}^A + 2\epsilon_{\mathfrak{h}1}{}^a_{[\nu}(\partial_\mu\epsilon_{\mathfrak{h}2}{}^b_{\rho]})X_{(ab)}{}^A \\ &\quad + 2\alpha^\alpha{}_{[\mu}\epsilon_{\mathfrak{h}1}{}^a_\nu\epsilon_{\mathfrak{h}2}{}^b_{\rho]}X_{(ab)}{}^B\triangleright_{\alpha B}{}^A \\ &= \nabla_{[\mu}(\{\epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}2}\}_{\mathrm{pf}} - \{\epsilon_{\mathfrak{h}2}\wedge\epsilon_{\mathfrak{h}1}\}_{\mathrm{pf}})^A{}_{\nu\rho]}, \\ \left(e^{\epsilon_{\mathfrak{h}1}\cdot H}e^{\epsilon_{\mathfrak{h}2}\cdot H} - e^{\epsilon_{\mathfrak{h}2}\cdot H}e^{\epsilon_{\mathfrak{h}1}\cdot H}\right)\frac{1}{2}B^\alpha{}_{\mu\nu} &= D^A\epsilon_{\mathfrak{h}2}{}^a_{[\mu|}\epsilon_{\mathfrak{h}1}{}^b_{|\nu]}(X_{1Aa}{}^c + X_{2Aa}{}^c)\mathcal{T}_{cb}{}^\alpha \\ &\quad - D^A\epsilon_{\mathfrak{h}1}{}^b_{[\mu|}\epsilon_{\mathfrak{h}2}{}^a_{|\nu]}(X_{1Ab}{}^c + X_{2Ab}{}^c)\mathcal{T}_{ca}{}^\alpha \\ &= -2D_A\epsilon_{\mathfrak{h}1}{}^a_{[\mu|}\epsilon_{\mathfrak{h}2}{}^b_{|\nu]}\,(X_{(ac)}{}^A\triangleright_{\alpha b}{}^c + X_{(bc)}{}^A\triangleright_{\alpha a}{}^c) \\ &= -2D_A\epsilon_{\mathfrak{h}1}{}^a_{[\mu|}\epsilon_{\mathfrak{h}2}{}^b_{|\nu]}X_{(ab)}{}^B\triangleright_{\alpha B}{}^A \\ &= \left(D\wedge^{\mathcal{S}}(\{\epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}2}\}_{\mathrm{pf}} - \{\epsilon_{\mathfrak{h}2}\wedge\epsilon_{\mathfrak{h}1}\}_{\mathrm{pf}}\right)^\alpha_{\mu\nu}. \end{aligned} \tag{F.9}$$

Comparing (F.8) and (F.9) with (72), one concludes that the commutator of two H-gauge transformations is the L-gauge transformation with the parameter $\epsilon_{\mathfrak{l}}^A{}_{\mu\nu} = 4\epsilon_{\mathfrak{h}1}{}^a{}_{[\mu|}\epsilon_{\mathfrak{h}2}{}^b{}_{|\nu]}X_{(ac)}{}^A$:

$$e^{\epsilon_{\mathfrak{h}1}\cdot H}e^{\epsilon_{\mathfrak{h}2}\cdot H} - e^{\epsilon_{\mathfrak{h}2}\cdot H}e^{\epsilon_{\mathfrak{h}1}\cdot H} = 2\left(\{\epsilon_{\mathfrak{h}1}\wedge\epsilon_{\mathfrak{h}2}\}_{\mathrm{pf}} - \{\epsilon_{\mathfrak{h}2}\wedge\epsilon_{\mathfrak{h}1}\}_{\mathrm{pf}}\right)\cdot\hat{L}. \tag{F.10}$$

F.2. Commutator [H, N]

Let us calculate the commutator between the generators of H-gauge transformation and N-gauge transformation, i.e. derive the equation (109). This is done by calculating the expressions

$$\left(e^{\epsilon_{\mathfrak{h}}\cdot H}e^{\epsilon_{\mathfrak{n}}\cdot N} - e^{\epsilon_{\mathfrak{n}}\cdot N}e^{\epsilon_{\mathfrak{h}}\cdot H}\right)A, \tag{F.11}$$

for all variables A present in the theory. It is easy to see that for variables $\alpha^\alpha{}_\mu$, $\beta^a{}_{\mu\nu}$, $\gamma^A{}_{\mu\nu\rho}$, and D^A the following is obtained:

$$
\begin{aligned}
e^{\epsilon_{\mathfrak{h}}\cdot H} e^{\epsilon_{\mathfrak{n}}\cdot N} \alpha^{\alpha}{}_{\mu} &= e^{\epsilon_{\mathfrak{n}}\cdot N} e^{\epsilon_{\mathfrak{h}}\cdot H} \alpha^{\alpha}{}_{\mu}, \\
e^{\epsilon_{\mathfrak{h}}\cdot H} e^{\epsilon_{\mathfrak{n}}\cdot N} \beta^{a}{}_{\mu\nu} &= e^{\epsilon_{\mathfrak{n}}\cdot N} e^{\epsilon_{\mathfrak{h}}\cdot H} \beta^{a}{}_{\mu\nu}, \\
e^{\epsilon_{\mathfrak{h}}\cdot H} e^{\epsilon_{\mathfrak{n}}\cdot N} \gamma^{A}{}_{\mu\nu\rho} &= e^{\epsilon_{\mathfrak{n}}\cdot N} e^{\epsilon_{\mathfrak{h}}\cdot H} \gamma^{A}{}_{\mu\nu\rho}, \\
e^{\epsilon_{\mathfrak{h}}\cdot H} e^{\epsilon_{\mathfrak{n}}\cdot N} D^{A} &= e^{\epsilon_{\mathfrak{n}}\cdot N} e^{\epsilon_{\mathfrak{h}}\cdot H} D^{A}.
\end{aligned}
\tag{F.12}
$$

For the remaining variables, $B^{\alpha}{}_{\mu\nu}$ and $C^{a}{}_{\mu}$, after the H-gauge transformation one obtains the following:

$$
B' = B - (C - D\wedge^{\chi_1}\epsilon_{\mathfrak{h}} - D\wedge^{\chi_2}\epsilon_{\mathfrak{h}})\wedge^{\tau}\epsilon_{\mathfrak{h}} - \epsilon_{\mathfrak{h}}\wedge^{\mathcal{D}}\epsilon_{\mathfrak{h}}\wedge^{\mathcal{D}}D, \tag{F.13}
$$

$$
C' = C - D\wedge^{\chi_1}\epsilon_{\mathfrak{h}} - D\wedge^{\chi_2}\epsilon_{\mathfrak{h}}. \tag{F.14}
$$

Next, transforming those variables with N-gauge transformation one obtains:

$$
\begin{aligned}
B'' &= B' - \beta'\wedge^{\mathcal{T}}\epsilon_{\mathfrak{n}} \\
&= B - (C - D\wedge^{\chi_1}\epsilon_{\mathfrak{h}} - D\wedge^{\chi_2}\epsilon_{\mathfrak{h}})\wedge^{\tau}\epsilon_{\mathfrak{h}} - \epsilon_{\mathfrak{h}}\wedge^{\mathcal{D}}\epsilon_{\mathfrak{h}}\wedge^{\mathcal{D}}D \\
&\quad - (\beta - \overset{\{\alpha^{\alpha}-\partial_a{}^{\alpha}\epsilon_{\mathfrak{h}}^{a}\}}{\nabla}\epsilon_{\mathfrak{h}} - \epsilon_{\mathfrak{h}}\wedge\epsilon_{\mathfrak{h}})\wedge^{\mathcal{T}}\epsilon_{\mathfrak{n}}, \\
C'' &= C' - \overset{\{\alpha^{\alpha}-\partial_a{}^{\alpha}\epsilon_{\mathfrak{h}}^{a}\}}{\nabla}\epsilon_{\mathfrak{n}} \\
&= C - D\wedge^{\chi_1}\epsilon_{\mathfrak{h}} - D\wedge^{\chi_2}\epsilon_{\mathfrak{h}} - \overset{\{\alpha^{\alpha}-\partial_a{}^{\alpha}\epsilon_{\mathfrak{h}}^{a}\}}{\nabla}\epsilon_{\mathfrak{n}}.
\end{aligned}
\tag{F.15}
$$

Let us now exchange the order of transformations, and first transform the variables with N-gauge transformation,

$$
B^{\cdot} = B - \beta\wedge^{\mathcal{T}}\epsilon_{\mathfrak{n}}, \tag{F.16}
$$

$$
C^{\cdot} = C - \nabla\epsilon_{\mathfrak{n}}, \tag{F.17}
$$

and then with H-gauge transformation:

$$
\begin{aligned}
B^{\cdot\cdot} &= B^{\cdot} - (C^{\cdot} - D^{\cdot}\wedge^{\chi_1}\epsilon_{\mathfrak{h}} - D^{\cdot}\wedge^{\chi_2}\epsilon_{\mathfrak{h}})\wedge^{\tau}\epsilon_{\mathfrak{h}} - \epsilon_{\mathfrak{h}}\wedge^{\mathcal{D}}\epsilon_{\mathfrak{h}}\wedge^{\mathcal{D}}D^{\cdot} \\
&= B - \beta\wedge^{\mathcal{T}}\epsilon_{\mathfrak{n}} - \big(C - \nabla\epsilon_{\mathfrak{n}} - (D+\delta\epsilon_{\mathfrak{n}})\wedge^{\chi_1}\epsilon_{\mathfrak{h}} \\
&\quad - (D+\delta\epsilon_{\mathfrak{n}})\wedge^{\chi_2}\epsilon_{\mathfrak{h}}\big)\wedge^{\tau}\epsilon_{\mathfrak{h}} - \epsilon_{\mathfrak{h}}\wedge^{\mathcal{D}}\epsilon_{\mathfrak{h}}\wedge^{\mathcal{D}}(D+\delta\epsilon_{\mathfrak{n}}), \\
C^{\cdot\cdot} &= C^{\cdot} - D^{\cdot}\wedge^{\chi_1}\epsilon_{\mathfrak{h}} - D^{\cdot}\wedge^{\chi_2}\epsilon_{\mathfrak{h}} \\
&= C - \nabla\epsilon_{\mathfrak{n}} - (D+\delta\epsilon_{\mathfrak{n}})\wedge^{\chi_1}\epsilon_{\mathfrak{h}} - (D+\delta\epsilon_{\mathfrak{n}})\wedge^{\chi_2}\epsilon_{\mathfrak{h}}.
\end{aligned}
\tag{F.18}
$$

After subtracting (F.15) and (F.18) one obtains:

$$
\begin{aligned}
\left(\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N} - \mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N}\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\right) B^{\alpha} &= \nabla\epsilon_{\mathfrak{n}}^{a} \wedge \epsilon_{\mathfrak{h}}{}^{b}\mathcal{T}_{ab}{}^{\alpha} + \delta^{A}{}_{a}\epsilon_{\mathfrak{n}}^{a}\epsilon_{\mathfrak{h}}{}^{b} \wedge \epsilon_{\mathfrak{h}}{}^{d}X_{1Ab}{}^{c}\mathcal{T}_{cd}{}^{\alpha} \\
&\quad + \delta^{A}{}_{a}\epsilon_{\mathfrak{n}}^{a}\epsilon_{\mathfrak{h}}{}^{b} \wedge \epsilon_{\mathfrak{h}}{}^{d}X_{2Ab}{}^{c}\mathcal{T}_{cd}{}^{\alpha} - \epsilon_{\mathfrak{h}}{}^{a} \wedge \epsilon_{\mathfrak{h}}{}^{b}\delta_{A}{}^{c}\epsilon_{\mathfrak{n}}{}^{c}D_{Aab}{}^{\alpha}, \\
&\quad - \nabla\epsilon_{\mathfrak{h}}^{a} \wedge \epsilon_{\mathfrak{n}}^{b}\mathcal{T}_{ab}{}^{\alpha} + \partial_{a}{}^{\beta}\epsilon_{\mathfrak{h}}^{a} \rhd_{\beta c}{}^{b}\epsilon_{\mathfrak{h}}^{c}\epsilon_{\mathfrak{n}}^{d}\mathcal{T}_{bd}{}^{\alpha} - \epsilon_{\mathfrak{h}}^{a} \wedge \epsilon_{\mathfrak{h}}^{b}f_{ab}{}^{c}\epsilon_{\mathfrak{n}}^{d}\mathcal{T}_{cd}{}^{\alpha}, \\
\left(\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N} - \mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N}\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\right) C^{c} &= -(\delta^{A}{}_{a}\epsilon_{\mathfrak{n}}^{a}) \wedge \epsilon_{\mathfrak{h}}^{b}X_{1Ab}{}^{c} - (\delta^{A}{}_{a}\epsilon_{\mathfrak{n}}^{a}) \wedge \epsilon_{\mathfrak{h}}^{b}X_{2Ab}{}^{c} - \partial_{a}{}^{\beta}\epsilon_{\mathfrak{h}}^{a} \rhd_{\beta b}{}^{c}\epsilon_{\mathfrak{n}}^{b},
\end{aligned}
\tag{F.19}
$$

where after using the definitions of the maps $\mathcal{T}$, $\mathcal{D}$, χ_1, and χ_2 one obtains the result

$$
\begin{aligned}
\left(\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N} - \mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N}\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\right) B^{\alpha} &= \nabla\epsilon_{\mathfrak{n}}^{a} \wedge \epsilon_{\mathfrak{h}}{}^{b}\mathcal{T}_{ab}{}^{\alpha} - \nabla\epsilon_{\mathfrak{h}}^{a} \wedge \epsilon_{\mathfrak{n}}^{b}\mathcal{T}_{ab}{}^{\alpha} \\
&= \nabla(\epsilon_{\mathfrak{n}} \wedge^{\mathcal{T}} \epsilon_{\mathfrak{h}})^{\alpha}, \\
\left(\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N} - \mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N}\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\right) C^{c} &= \partial^{c}{}_{\alpha}(\epsilon_{\mathfrak{n}} \wedge^{\mathcal{T}} \epsilon_{\mathfrak{h}})^{\alpha},
\end{aligned}
\tag{F.20}
$$

Comparing (F.12) and (F.20) with (85), one obtains that:

$$
\left(\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N} - \mathrm{e}^{\epsilon_{\mathfrak{n}}\cdot N}\mathrm{e}^{\epsilon_{\mathfrak{h}}\cdot H}\right) = -(\epsilon_{\mathfrak{n}} \wedge^{\mathcal{T}} \epsilon_{\mathfrak{h}}) \cdot M. \tag{F.21}
$$

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Higher gauge theories based on 3-groups

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Abstract: We study the categorical generalizations of a BF theory to $2BF$ and $3BF$ theories, corresponding to 2-groups and 3-groups, in the framework of higher gauge theory. In particular, we construct the constrained $3BF$ actions describing the correct dynamics of Yang-Mills, Klein-Gordon, Dirac, Weyl, and Majorana fields coupled to Einstein-Cartan gravity. The action is naturally split into a topological sector and a sector with simplicity constraints, adapted to the spinfoam quantization programme. In addition, the structure of the 3-group gives rise to a novel gauge group which specifies the spectrum of matter fields present in the theory, just like the ordinary gauge group specifies the spectrum of gauge bosons in the Yang-Mills theory. This allows us to rewrite the whole Standard Model coupled to gravity as a constrained $3BF$ action, facilitating the nonperturbative quantization of both gravity and matter fields. Moreover, the presence and the properties of this new gauge group open up a possibility of a nontrivial unification of all fields and a possible explanation of fermion families and all other structure in the matter spectrum of the theory.

Keywords: Models of Quantum Gravity, Topological Field Theories, Gauge Symmetry, Beyond Standard Model

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1 Introduction

The quantization of the gravitational field is one of the most prominent open problems in modern theoretical physics. Within the Loop Quantum Gravity framework, one can study the nonperturbative quantization of gravity, both canonically and covariantly, see [1–3] for an overview and a comprehensive introduction. The covariant approach focuses on the definition of the path integral for the gravitational field,

$$Z = \int \mathcal{D}g \, e^{iS[g]} \,, \tag{1.1}$$

by considering a triangulation of a spacetime manifold, and defining the path integral as a discrete state sum of the gravitational field configurations living on the simplices in the triangulation. This quantization technique is known as the *spinfoam* quantization method, and roughly goes along the following lines:

1. first, one writes the classical action $S[g]$ as a topological BF action plus a simplicity constraint,

2. then one uses the algebraic structure (a Lie group) underlying the topological sector of the action to define a triangulation-independent state sum Z,

3. and finally, one imposes the simplicity constraints on the state sum, promoting it into a path integral for a physical theory.

This quantization prescription has been implemented for various choices of the action, the Lie group, and the spacetime dimension. For example, in 3 dimensions, the prototype spinfoam model is known as the Ponzano-Regge model [4]. In 4 dimensions there are multiple models, such as the Barrett-Crane model [5, 6], the Ooguri model [7], and the most sophisticated EPRL/FK model [8, 9]. All these models aim to define a viable theory of quantum gravity, with variable success. However, virtually all of them are focused on pure gravity, without matter fields. The attempts to include matter fields have had limited success [10], mainly because the mass terms could not be expressed in the theory due to the absence of the tetrad fields from the BF sector of the theory.

In order to resolve this issue, a new approach has been developed, using the categorical generalization of the BF action, within the framework of *higher gauge theory* (see [11] for a review). In particular, one uses the idea of a categorical ladder to promote the BF action, which is based on some Lie group, into a $2BF$ action, which is based on the so-called 2-group structure. If chosen in a suitable way, the 2-group structure should hopefully introduce the tetrad fields into the action. This approach has been successfully implemented [12], rewriting the action for general relativity as a constrained $2BF$ action, such that the tetrad fields are present in the topological sector. This result opened up a possibility to couple all matter fields to gravity in a straightforward way. Nevertheless, the matter fields could not be naturally expressed using the underlying algebraic structure of a 2-group, rendering the spinfoam quantization method only half-implementable, since the matter sector of the classical action could not be expressed as a topological term plus a simplicity constraint, which means that the steps 2 and 3 above could not be performed for the matter sector of the action.

We address this problem in this paper. As we will show, it turns out that it is necessary to perform one more step in the categorical ladder, generalizing the underlying algebraic structure from a 2-group to a 3-group. This generalization then naturally gives rise to the so-called $3BF$ action, which proves to be suitable for a unified description of both gravity and matter fields. The steps of the categorical ladder can be conveniently summarized in the following table:

categorical structure	algebraic structure	linear structure	topological action	degrees of freedom
Lie group	Lie group	Lie algebra	BF theory	gauge fields
Lie 2-group	Lie crossed module	differential Lie crossed module	$2BF$ theory	tetrad fields
Lie 3-group	Lie 2-crossed module	differential Lie 2-crossed module	$3BF$ theory	scalar and fermion fields

Once the suitable gauge 3-group has been specified and the corresponding $3BF$ action constructed, the most important thing that remains, in order to complete the step 1 of the spinfoam quantization programme, is to impose appropriate simplicity constraints onto the degrees of freedom present in the $3BF$ action, so that we obtain the desired classical dynamics of the gravitational and matter fields. Then one can proceed with steps 2 and 3 of the spinfoam quantization, hopefully ending up with a viable model of quantum gravity and matter.

In this paper, we restrict our attention to the first of the above steps: we will construct a constrained $3BF$ action for the cases of Klein-Gordon, Dirac, Weyl and Majorana fields, as well as Yang-Mills and Proca vector fields, all coupled to the Einstein-Cartan gravity in the standard way. This construction will lead us to an unexpected novel result. As we shall see, the scalar and fermion fields will be *naturally associated to a new gauge group*, generalizing the notion of a gauge group in the Yang-Mills theory, which describes vector bosons. This new group opens up a possibility to use it as an algebraic way of classifying matter fields, describing the structures such as quark and lepton families, and so on. The insight into the existence of this new gauge group is the consequence of the categorical ladder and is one of the main results of the paper. However, given the complexity of the algebraic properties of 3-groups, we will restrict ourselves only to the reconstruction of the already known theories, such as the Standard Model (SM), in the new framework. In this sense, any potential explanation of the spectrum of matter fields in the SM will be left for future work.

The layout of the paper is as follows. In subsection 2.1 we will give a short overview of the constrained BF actions, including the well-known example of the Plebanski action for general relativity, and a completely new example of the Yang-Mills theory rewritten as a constrained BF model. In the subsection 2.2 we also introduce the formalism of the constrained $2BF$ actions, reviewing the example of general relativity as a constrained $2BF$ action, first introduced in [12]. In addition, we will demonstrate how to couple gravity in a natural way within the formalism of 2-groups. Section 3 contains the main results of the paper and is split into 4 subsections. The subsection 3.1 introduces the formalism of 3-groups, and the definition and properties of a $3BF$ action, including the three types of gauge transformations. The subsection 3.2 focuses on the construction of a constrained $3BF$ action which describes a single real scalar field coupled to gravity. It provides the most elementary example of the insight that matter fields correspond to a gauge group. Encouraged by these results, in the subsection 3.3 we construct the constrained $3BF$ action for the Dirac field coupled to gravity and specify its gauge group. Finally, the subsection 3.4 deals with the construction of the constrained $3BF$ action for the Weyl and Majorana fields coupled to gravity, thereby covering all types of fields potentially relevant for the Standard Model and beyond. After the construction of all building blocks, in section 4 we apply the results of sections 2 and 3 to construct the constrained $3BF$ action corresponding to the full Standard Model coupled to Einstein-Cartan gravity. Finally, section 5 is devoted to the discussion of the results and the possible future lines of research. The appendices contain some mathematical reminders and technical details.

The notation and conventions are as follows. The local Lorentz indices are denoted by the Latin letters $a, b, c, \dots$, take values $0, 1, 2, 3$, and are raised and lowered using the

Minkowski metric η_{ab} with signature $(-,+,+,+)$. Spacetime indices are denoted by the Greek letters $\mu, \nu, \dots$, and are raised and lowered by the spacetime metric $g_{\mu\nu} = \eta_{ab} e^a{}_\mu e^b{}_\nu$, where $e^a{}_\mu$ are the tetrad fields. The inverse tetrad is denoted as $e^\mu{}_a$. All other indices that appear in the paper are dependent on the context, and their usage is explicitly defined in the text where they appear. A lot of additional notation is defined in appendix A. We work in the natural system of units where $c = \hbar = 1$, and $G = l_p^2$, where l_p is the Planck length.

2 BF and $2BF$ models, ordinary gauge fields and gravity

Let us begin by giving a short review of BF and $2BF$ theories in general. For additional information on these topics, see for example [11, 13–18].

2.1 BF theory

Given a Lie group G and its corresponding Lie algebra $\mathfrak{g}$, one can introduce the so-called BF action as

$$S_{BF} = \int_{\mathcal{M}_4} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} \,. \tag{2.1}$$

Here, $\mathcal{F} \equiv \mathrm{d}\alpha + \alpha \wedge \alpha$ is the curvature 2-form for the algebra-valued connection 1-form $\alpha \in \mathcal{A}^1(\mathcal{M}_4\,, \mathfrak{g})$ on some 4-dimensional spacetime manifold $\mathcal{M}_4$. In addition, $B \in \mathcal{A}^2(\mathcal{M}_4\,, \mathfrak{g})$ is a Lagrange multiplier 2-form, while $\langle \_\,, \_ \rangle_{\mathfrak{g}}$ denotes the G-invariant bilinear symmetric nondegenerate form.

From the structure of (2.1), one can see that the action is diffeomorphism invariant, and it is usually understood to be gauge invariant with respect to G. In addition to these properties, the BF action is topological, in the following sense. Varying the action (2.1) with respect to B^β and α^β, where the index β counts the generators of $\mathfrak{g}$ (see appendix A for notation and conventions), one obtains the equations of motion of the theory,

$$\mathcal{F} = 0\,, \qquad \nabla B \equiv \mathrm{d}B + \alpha \wedge B = 0\,. \tag{2.2}$$

From the first equation of motion, one immediately sees that α is a flat connection, which then together with the second equation of motion implies that B is constant. Therefore, there are no local propagating degrees of freedom in the theory, and one then says that the theory is topological.

Usually, in physics one is interested in theories which are nontopological, i.e., which have local propagating degrees of freedom. In order to transform the BF action into such a theory, one adds an additional term to the action, commonly called the *simplicity constraint*. A very nice example is the Yang-Mills theory for the $\mathrm{SU}(N)$ group, which can be rewritten as a constrained BF theory in the following way:

$$S = \int B_I \wedge F^I + \lambda^I \wedge \left(B_I - \frac{12}{g} M_{abI} \delta^a \wedge \delta^b \right) + \zeta^{abI} \left(M_{abI} \varepsilon_{cdef} \delta^c \wedge \delta^d \wedge \delta^e \wedge \delta^f - g_{IJ} F^J \wedge \delta_a \wedge \delta_b \right). \tag{2.3}$$

Here $F \equiv \mathrm{d}A + A \wedge A$ is again the curvature 2-form for the connection $A \in \mathcal{A}^1(\mathcal{M}_4\,, \mathfrak{su}(N))$, and $B \in \mathcal{A}^2(\mathcal{M}_4\,, \mathfrak{su}(N))$ is the Lagrange multiplier 2-form. The Killing form $g_{IJ} \equiv$

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$\langle\tau_I,\tau_J\rangle_{\mathfrak{su}(N)}\propto f_{IK}{}^L f_{JL}{}^K$ is used to raise and lower the indices $I,J,\dots$ which count the generators of $\mathrm{SU}(N)$, where $f_{IJ}{}^K$ are the structure constants for the $\mathfrak{su}(N)$ algebra. In addition to the topological $B\wedge F$ term, we also have two simplicity constraint terms, featuring the Lagrange multiplier 2-form λ^I and the Lagrange multiplier 0-form ζ^{abI}. The 0-form M_{abI} is also a Lagrange multiplier, while g is the coupling constant for the Yang-Mills theory.

Finally, δ^a is a nondynamical 1-form, such that there exists a global coordinate frame in which its components are equal to the Kronecker symbol $\delta^a{}_\mu$ (hence the notation δ^a). The 1-form δ^a plays the role of a background field, and defines the global spacetime metric, via the equation

$$\eta_{\mu\nu}=\eta_{ab}\delta^a{}_\mu\delta^b{}_\nu\,, \tag{2.4}$$

where $\eta_{ab}\equiv\mathrm{diag}(-1,+1,+1,+1)$ is the Minkowski metric. Since the coordinate system is global, the spacetime manifold $\mathcal{M}_4$ is understood to be flat. The indices $a,b,\dots$ are local Lorentz indices, taking values $0,\dots,3$. Note that the field δ^a has all the properties of the tetrad 1-form e^a in the flat Minkowski spacetime. Also note that the action (2.3) is manifestly diffeomorphism invariant and gauge invariant with respect to $\mathrm{SU}(N)$, but not background independent, due to the presence of δ^a.

The equations of motion are obtained by varying the action (2.3) with respect to the variables ζ^{abI}, M_{abI}, A^I, B_I, and λ^I, respectively (note that we do not take the variation of the action with respect to the background field δ^a):

$$M_{abI}\varepsilon_{cdef}\delta^c\wedge\delta^d\wedge\delta^e\wedge\delta^f-F_I\wedge\delta_a\wedge\delta_b=0\,, \tag{2.5}$$

$$-\frac{12}{g}\lambda^I\wedge\delta^a\wedge\delta^b+\zeta^{abI}\varepsilon_{cdef}\delta^c\wedge\delta^d\wedge\delta^e\wedge\delta^f=0\,, \tag{2.6}$$

$$-\mathrm{d}B_I+f_{JI}{}^K B_K\wedge A^J+\mathrm{d}(\zeta^{ab}{}_I\delta_a\wedge\delta_b)-f_{JI}{}^K\zeta^{ab}{}_K\delta_a\wedge\delta_b\wedge A^J=0\,, \tag{2.7}$$

$$F_I+\lambda_I=0\,, \tag{2.8}$$

$$B_I-\frac{12}{g}M_{abI}\delta^a\wedge\delta^b=0\,, \tag{2.9}$$

From the algebraic equations (2.5), (2.6), (2.8) and (2.9) one obtains the multipliers as functions of the dynamical field A^I:

$$M_{abI}=\frac{1}{48}\varepsilon_{abcd}F_I{}^{cd}\,,\quad \zeta^{abI}=\frac{1}{4g}\varepsilon^{abcd}F^I{}_{cd}\,,\quad \lambda_{Iab}=F_{Iab}\,,\quad B_{Iab}=\frac{1}{2g}\varepsilon_{abcd}F_I{}^{cd}\,. \tag{2.10}$$

Here we used the notation $F_{Iab}=F_{I\mu\nu}\delta_a{}^\mu\delta_b{}^\nu$, where we used the fact that $\delta^a{}_\mu$ is invertible, and similarly for other variables. Using these equations and the differential equation (2.7) one obtains the equation of motion for gauge field A^I,

$$\nabla_\rho F^{I\rho\mu}\equiv\partial_\rho F^{I\rho\mu}+f_{JK}{}^I A^J{}_\rho F^{K\rho\mu}=0\,. \tag{2.11}$$

This is precisely the classical equation of motion for the free Yang-Mills theory. Note that in addition to the Yang-Mills theory, one can easily extend the action (2.3) in order to describe the massive vector field and obtain the Proca equation of motion. This is done by adding a mass term

$$-\frac{1}{4!}m^2A_{I\mu}A^I{}_\nu\eta^{\mu\nu}\varepsilon_{abcd}\delta^a\wedge\delta^b\wedge\delta^c\wedge\delta^d \tag{2.12}$$

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to the action (2.3). Of course, this term explicitly breaks the SU(N) gauge symmetry of the action.

Another example of the constrained BF theory is the Plebanski action for general relativity [15], see also [13] for a recent review. Starting from a gauge group SO(3, 1), one constructs a constrained BF action as

$$S = \int_{\mathcal{M}_4} B_{ab} \wedge R^{ab} + \phi_{abcd} B^{ab} \wedge B^{cd} \,. \tag{2.13}$$

Here R^{ab} is the curvature 2-form for the spin connection ω^{ab}, B_{ab} is the usual Lagrange multiplier 2-form, while ϕ_{abcd} is the Lagrange multiplier 0-form corresponding to the simplicity constraint term $B^{ab} \wedge B^{cd}$. It can be shown that the variation of this action with respect to B_{ab}, ω^{ab} and ϕ_{abcd} gives rise to equations of motion which are equivalent to vacuum general relativity. However, the tetrad fields appear in the model as a solution to the simplicity constraint equation of motion $B^{ab} \wedge B^{cd} = 0$. Thus, being intrinsically on-shell objects, they are not present in the action and cannot be quantized. This renders the Plebanski model unsuitable for coupling of matter fields to gravity [10, 12, 19]. Nevertheless, as a model for pure gravity, the Plebanski model has been successfully quantized in the context of spinfoam models, see [1, 2, 8, 9] for details and references.

2.2 2BF theory

In order to circumvent the issue of coupling of matter fields, a recent promising approach has been developed [12, 19–23] in the context of higher category theory [11]. In particular, one employs the higher category theory construction to generalize the BF action to the so-called 2BF action, by passing from the notion of a gauge group to the notion of a gauge 2-group. In order to introduce it, let us first give a short review of the 2-group formalism.

In the framework of category theory, the group as an algebraic structure can be understood as a specific type of category, namely a category with only one object and invertible morphisms [11]. The notion of a category can be generalized to the so-called *higher categories*, which have not only objects and morphisms, but also 2-morphisms (morphisms between morphisms), and so on. This process of generalization is called the *categorical ladder*. Similarly to the notion of a group, one can introduce a 2-group as a 2-category consisting of only one object, where all the morphisms and 2-morphisms are invertible. It has been shown that every strict 2-group is equivalent to a crossed module $(H \stackrel{\partial}{\to} G\,, \triangleright)$, see appendix A for definition. Here G and H are groups, δ is a homomorphism from H to G, while $\triangleright : G \times H \to H$ is an action of G on H.

An important example of this structure is a vector space V equipped with an isometry group O. Namely, V can be regarded as an Abelian Lie group with addition as a group operation, so that a representation of O on V is an action $\triangleright$ of O on the group V, giving rise to the crossed module $(V \stackrel{\partial}{\to} O\,, \triangleright)$, where the homomorphism ∂ is chosen to be trivial, i.e., it maps every element of V into a unit of O. We will make use of this example below to introduce the Poincaré 2-group.

Similarly to the case of an ordinary Lie group G which has a naturally associated notion of a connection α, giving rise to a BF theory, the 2-group structure has a naturally associated notion of a 2-connection $(\alpha\,,\beta)$, described by the usual $\mathfrak{g}$-valued 1-form $\alpha \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{g})$ and an $\mathfrak{h}$-valued 2-form $\beta \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{h})$, where $\mathfrak{h}$ is a Lie algebra of the Lie group H. The 2-connection gives rise to the so-called *fake 2-curvature* $(\mathcal{F},\mathcal{G})$, given as

$$\mathcal{F} = \mathrm{d}\alpha + \alpha\wedge\alpha - \partial\beta\,, \qquad \mathcal{G} = d\beta + \alpha\wedge^{\triangleright}\beta\,. \tag{2.14}$$

Here $\alpha\wedge^{\triangleright}\beta$ means that α and β are multiplied as forms using $\wedge$, and simultaneously multiplied as algebra elements using $\triangleright$, see appendix A. The curvature pair $(\mathcal{F},\mathcal{G})$ is called fake because of the presence of the $\partial\beta$ term in the definition of $\mathcal{F}$, see [11] for details.

Using these variables, one can introduce a new action as a generalization of the BF action, such that it is gauge invariant with respect to both G and H groups. It is called the $2BF$ action and is defined in the following way [16, 17]:

$$S_{2BF} = \int_{\mathcal{M}_4} \langle B\wedge\mathcal{F}\rangle_{\mathfrak{g}} + \langle C\wedge\mathcal{G}\rangle_{\mathfrak{h}}\,, \tag{2.15}$$

where the 2-form $B \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{g})$ and the 1-form $C \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{h})$ are Lagrange multipliers. Also, $\langle\_\,,\_\rangle_{\mathfrak{g}}$ and $\langle\_\,,\_\rangle_{\mathfrak{h}}$ denote the G-invariant bilinear symmetric nondegenerate forms for the algebras $\mathfrak{g}$ and $\mathfrak{h}$, respectively. As a consequence of the axiomatic structure of a crossed module (see appendix A), the bilinear form $\langle\_\,,\_\rangle_{\mathfrak{h}}$ is H-invariant as well. See [16, 17] for review and references.

Similarly to the BF action, the $2BF$ action is also topological, which can be seen from equations of motion. Varying with respect to B and C one obtains

$$\mathcal{F} = 0\,, \qquad \mathcal{G} = 0\,, \tag{2.16}$$

while varying with respect to α and β one obtains the equations for the multipliers,

$$\mathrm{d}B_\alpha - g_{\alpha\beta}{}^{\gamma} B_\gamma \wedge \alpha^\beta - \triangleright_{\alpha a}{}^{b} C_b \wedge \beta^a = 0\,, \tag{2.17}$$

$$\mathrm{d}C_a - \partial_a{}^{\alpha} B_\alpha + \triangleright_{\alpha a}{}^{b} C_b \wedge \alpha^\alpha = 0\,. \tag{2.18}$$

One can either show that these equations have only trivial solutions, or one can use the Hamiltonian analysis to show that there are no local propagating degrees of freedom (see for example [21, 22]), demostrating the topological nature of the theory.

An example of a 2-group relevant for physics is the Poincaré 2-group, which is constructed using the aforementioned example of a vector space equipped with an isometry group. One constructs a crossed module by choosing

$$G = \mathrm{SO}(3,1)\,, \qquad H = \mathbb{R}^4\,, \tag{2.19}$$

while $\triangleright$ is a natural action of $\mathrm{SO}(3,1)$ on $\mathbb{R}^4$, and the map ∂ is trivial. The 2-connection (α,β) is given by the algebra-valued differential forms

$$\alpha = \omega^{ab} M_{ab}\,, \qquad \beta = \beta^a P_a\,, \tag{2.20}$$

where ω^{ab} is the spin connection, while M_{ab} and P_a are the generators of groups $\mathrm{SO}(3,1)$ and $\mathbb{R}^4$, respectively. The corresponding 2-curvature in this case is given by

$$\mathcal{F} = (\mathrm{d}\omega^{ab} + \omega^a{}_c\wedge\omega^{cb})M_{ab} \equiv R^{ab}M_{ab}\,, \quad \mathcal{G} = (\mathrm{d}\beta^a + \omega^a{}_b\wedge\beta^b)P_a \equiv \nabla\beta^a P_a \equiv G^a P_a\,, \tag{2.21}$$

where we have evaluated $\wedge^{\triangleright}$ using the equation $M_{ab} \triangleright P_c = \eta_{[bc}P_{a]}$. Note that, since ∂ is trivial, the fake curvature is the same as ordinary curvature. Using the bilinear forms

$$\langle M_{ab}, M_{cd} \rangle_{\mathfrak{g}} = \eta_{a[c}\eta_{bd]}\,, \qquad \langle P_a, P_b \rangle_{\mathfrak{h}} = \eta_{ab}\,, \tag{2.22}$$

one can show that 1-forms C^a transform in the same way as the tetrad 1-forms e^a under the Lorentz transformations and diffeomorphisms, so the fields C^a can be identified with the tetrads. Then one can rewrite the $2BF$ action (2.15) for the Poincaré 2-group as

$$S_{2BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a\,. \tag{2.23}$$

In order to obtain general relativity, the topological action (2.23) can be modified by adding a convenient simplicity constraint, like it is done in the BF case:

$$S = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right). \tag{2.24}$$

Here λ_{ab} is a Lagrange multiplier 2-form associated to the simplicity constraint term, and l_p is the Planck length. Varying the action (2.24) with respect to B_{ab}, e_a, ω_{ab}, β_a and λ_{ab}, one obtains the following equations of motion:

$$R_{ab} - \lambda_{ab} = 0\,, \tag{2.25}$$

$$\nabla \beta_a + \frac{1}{8\pi l_p^2} \varepsilon_{abcd} \lambda^{bc} \wedge e^d = 0\,, \tag{2.26}$$

$$\nabla B_{ab} - e_{[a} \wedge \beta_{b]} = 0\,, \tag{2.27}$$

$$\nabla e_a = 0\,, \tag{2.28}$$

$$B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d = 0\,. \tag{2.29}$$

The only dynamical fields are the tetrads e^a, while all other fields can be algebraically determined, as follows. From the equations (2.28) and (2.29) we obtain that $\nabla B^{ab} = 0$, from which it follows, using the equation (2.27), that $e_{[a} \wedge \beta_{b]} = 0$. Assuming that the tetrads are nondegenerate, $e \equiv \det(e^a{}_\mu) \neq 0$, it can be shown that this is equivalent to the condition $\beta^a = 0$ (for the proof see appendix in [12]). Therefore, from the equations (2.25), (2.27), (2.28) and (2.29) we obtain

$$\lambda^{ab}{}_{\mu\nu} = R^{ab}{}_{\mu\nu}\,, \quad \beta^a{}_{\mu\nu} = 0\,, \quad B_{ab\mu\nu} = \frac{1}{8\pi l_p^2} \varepsilon_{abcd} e^c{}_\mu e^d{}_\nu\,, \quad \omega^{ab}{}_\mu = \triangle^{ab}{}_\mu\,. \tag{2.30}$$

Here the Ricci rotation coefficients are defined as

$$\triangle^{ab}{}_\mu \equiv \frac{1}{2}(c^{abc} - c^{cab} + c^{bca}) e_{c\mu}\,, \tag{2.31}$$

where

$$c^{abc} = e^\mu{}_b e^\nu{}_c \left(\partial_\mu e^a{}_\nu - \partial_\nu e^a{}_\mu \right)\,. \tag{2.32}$$

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Finally, the remaining equation (2.26) reduces to

$$\varepsilon_{abcd} R^{bc} \wedge e^d = 0\,, \tag{2.33}$$

which is nothing but the vacuum Einstein field equation $R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 0$. Therefore, the action (2.24) is classically equivalent to general relativity.

The main advantage of the action (2.24) over the Plebanski model and similar approaches lies in the fact that the tetrad fields are explicitly present in the topological sector of the theory. This allows one to couple matter fields in a straightforward way, as demonstrated in [12]. However, one can do even better, and couple gauge fields to gravity within a unified framework of 2-group formalism.

Let us demonstrate this on the example of the SU(N) Yang-Mills theory. Begin by modifying the Poincaré 2-group structure to include the SU(N) gauge group, as follows. We choose the two Lie groups as

$$G = \mathrm{SO}(3,1) \times \mathrm{SU}(N)\,, \qquad H = \mathbb{R}^4\,, \tag{2.34}$$

and we define the action $\triangleright$ of the group G in the following way. As in the case of the Poincaré 2-group, it acts on itself via conjugation. Next, it acts on H such that the SO(3,1) subgroup acts on $\mathbb{R}^4$ via the vector representation, while the action of SU(N) subgroup is trivial. The map ∂ also remains trivial, as before. The 2-connection (α, β) now obtains the form which reflects the structure of the group G,

$$\alpha = \omega^{ab} M_{ab} + A^I \tau_I\,, \qquad \beta = \beta^a P_a\,, \tag{2.35}$$

where A^I is the gauge connection 1-form, while τ_I are the SU(N) generators. The curvature for α is thus

$$\mathcal{F} = R^{ab} M_{ab} + F^I \tau_I\,, \qquad F^I \equiv \mathrm{d}A^I + f_{JK}{}^I A^J \wedge A^K\,. \tag{2.36}$$

The curvature for β remains the same as before, since the action $\triangleright$ of SU(N) on $\mathbb{R}^4$ is trivial, i.e., $\tau_I \triangleright P_a = 0$. Finally, the product structure of the group G implies that its Killing form $\langle \_, \_ \rangle_{\mathfrak{g}}$ reduces to the Killing forms for the SO(3,1) and SU(N), along with the identity $\langle M_{ab}, \tau_I \rangle_{\mathfrak{g}} = 0$.

Given a crossed module defined in this way, its corresponding topological $2BF$ action (2.15) becomes

$$S_{2BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + B^I \wedge F_I + e_a \wedge \nabla \beta^a\,, \tag{2.37}$$

where $B^I \in \mathcal{A}^2(\mathcal{M}_4\,, \mathfrak{su}(N))$ is the new Lagrange multiplier. In order to transform this topological action into action with nontrivial dynamics, we again introduce the appropriate simplicity constraints. The constraint giving rise to gravity is the same as in (2.24), while the constraint for the gauge fields is given as in the action (2.3) with the substitution $\delta^a \to e^a$:

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + B^I \wedge F_I + e_a \wedge \nabla \beta^a - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right) \\ & + \lambda^I \wedge \left(B_I - \frac{12}{g} M_{abI} e^a \wedge e^b \right) + \zeta^{abI} \left(M_{abI} \varepsilon_{cdef} e^c \wedge e^d \wedge e^e \wedge e^f - g_{IJ} F^J \wedge e_a \wedge e_b \right). \end{aligned} \tag{2.38}$$

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It is crucial to note that the action (2.38) is a combination of the pure gravity action (2.24) and the Yang-Mills action (2.3), such that the nondynamical background field δ^a from (2.3) gets promoted to a dynamical field e^a. The relationship between these fields has already been hinted at in the equation (2.4), which describes the connection between δ^a and the flat spacetime metric $\eta_{\mu\nu}$. Once promoted to e^a, this field becomes dynamical, while the equation (2.4) becomes the usual relation between the tetrad and the metric,

$$g_{\mu\nu} = \eta_{ab} e^a{}_\mu e^b{}_\nu \,, \tag{2.39}$$

further confirming that the Lagrange multiplier C^a should be identified with the tetrad. Moreover, the total action (2.38) now becomes background independent, as expected in general relativity. All this is a consequence of the fact that the tetrad field is explicitly present in the topological sector of the action (2.24), establishing an improvement over the Plebanski model.

By varying the action (2.38) with respect to the variables B_{ab}, ω_{ab}, β_a, λ_{ab}, ζ^{abI}, M_{abI}, B_I, λ^I, A^I, and e^a, we obtain the following equations of motion, respectively:

$$R^{ab} - \lambda^{ab} = 0\,, \tag{2.40}$$

$$\nabla B^{ab} - e^{[a} \wedge \beta^{b]} = 0\,, \tag{2.41}$$

$$\nabla e^a = 0\,, \tag{2.42}$$

$$B_{ab} - \frac{1}{16\pi l_p^2} \varepsilon_{abcd} e^c \wedge e^d = 0\,, \tag{2.43}$$

$$M_{abI} \varepsilon_{cdef} e^c \wedge e^d \wedge e^e \wedge e^f - F_I \wedge e_a \wedge e_b = 0\,, \tag{2.44}$$

$$-\frac{12}{g} \lambda^I \wedge e^a \wedge e^b + \zeta^{abI} \varepsilon_{cdef} e^c \wedge e^d \wedge e^e \wedge e^f = 0\,, \tag{2.45}$$

$$F_I + \lambda_I = 0\,, \tag{2.46}$$

$$B_I - \frac{12}{g} M_{abI} e^a \wedge e^b = 0\,, \tag{2.47}$$

$$-\mathrm{d}B_I + B_K \wedge g_{JI}{}^K A^J + \mathrm{d}(\zeta_I^{ab} e_a \wedge e_b) - \zeta_K^{ab} e_a \wedge e_b \wedge g_{JI}{}^K A^J = 0\,, \tag{2.48}$$

$$\begin{aligned} &\nabla \beta_a + \frac{1}{8\pi l_p^2} \varepsilon_{abcd} \lambda^{bc} \wedge e^d - \frac{24}{g} M_{abI} \lambda^I \wedge e^b \\ &+ 4\zeta^{ef\,I} M_{ef\,I} \varepsilon_{abcd} e^b \wedge e^c \wedge e^d - 2\zeta_{ab}{}^I F_I \wedge e^b = 0\,. \end{aligned} \tag{2.49}$$

In the above system of equations, we have two dynamical equations for e^a and A^I, while all other variables are algebraically determined from these. In particular, from equations (2.40)–(2.47), we have:

$$\lambda_{ab\mu\nu} = R_{ab\mu\nu}\,, \quad \beta_{a\mu\nu} = 0\,, \quad \omega_{ab\mu} = \triangle_{ab\mu}\,, \quad \lambda_{abI} = F_{abI}\,, \quad B_{\mu\nu I} = -\frac{e}{2g} \varepsilon_{\mu\nu\rho\sigma} F^{\rho\sigma}{}_I\,, \tag{2.50}$$
$$B_{ab\mu\nu} = \frac{1}{8\pi l_p^2} \varepsilon_{abcd} e^c{}_\mu e^d{}_\nu\,, \quad M_{abI} = -\frac{1}{4eg} \varepsilon^{\mu\nu\rho\sigma} F_{\mu\nu}{}^I e^a{}_\rho e^b{}_\sigma\,, \quad \zeta^{abI} = \frac{1}{4eg} \varepsilon^{\mu\nu\rho\sigma} F_{\mu\nu}{}^I e^a{}_\rho e^b{}_\sigma\,.$$

Then, substituting all these into (2.48) and (2.49) we obtain the differential equation of motion for A^I,

$$\nabla_\rho F^{I\rho\mu} \equiv \partial_\rho F^{I\rho\mu} + \Gamma^\rho{}_{\lambda\rho} F^{I\lambda\mu} + f_{JK}{}^I A^J{}_\rho F^{K\rho\mu} = 0\,, \tag{2.51}$$

where $\Gamma^{\lambda}{}_{\mu\nu}$ is the standard Levi-Civita connection, and a differential equation of motion for e^a,

$$R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R = 8\pi l_p^2\, T^{\mu\nu}\,, \qquad T^{\mu\nu} \equiv -\frac{1}{4g}\left(F_{\rho\sigma}{}^{I}F^{\rho\sigma}{}_{I}g^{\mu\nu} + 4F^{\mu\rho}{}_{I}F_{\rho}{}^{\nu I}\right)\,. \tag{2.52}$$

The system of equations (2.50)–(2.52) is equivalent to the system (2.40)–(2.49). Note that we have again obtained that $\beta^a = 0$, as in the pure gravity case.

In this way, we see that both gravity and gauge fields can be represented within a unified framework of higher gauge theory based on a 2-group structure.

3 3BF models, scalar and fermion matter fields

While the structure of a 2-group can successfully accommodate both gravitational and gauge fields, unfortunately it cannot include other matter fields, such as scalars or fermions. In order to construct a unified description of all matter fields within the framework of higher gauge theory, we are led to make a further generalization, passing from the notion of a 2-group to the notion of a 3-group. As it turns out, the 3-group structure is a perfect fit for the description of all fields that are present in the Standard Model, coupled to gravity. Moreover, this structure gives rise to a new gauge group, which corresponds to the choice of the scalar and fermion fields present in the theory. This is a novel and unexpected result, which has the potential to open up a new avenue of research with the aim of explaining the structure of the matter sector of the Standard Model and beyond.

In order to demonstrate this in more detail, we first need to introduce the notion of a 3-group, which we will afterward use to construct constrained 3BF actions describing scalar and fermion fields on an equal footing with gravity and gauge fields.

3.1 3-groups and topological 3BF action

Similarly to the concepts of a group and a 2-group, one can introduce the notion of a 3-group in the framework of higher category theory, as a 3-category with only one object where all the morphisms, 2-morphisms and 3-morphisms are invertible. It has been proved that a strict 3-group is equivalent to a 2-*crossed module* [24], in the same way as a 2-group is equivalent to a crossed module.

A Lie 2-crossed module, denoted as $(L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G\,, \triangleright\,, \{\_\,,\_\})$, is a algebraic structure specified by three Lie groups G, H and L, together with the homomorphisms δ and ∂, an action $\triangleright$ of the group G on all three groups, and a G-equivariant map

$$\{\_\,,\_\} : H \times H \to L\,.$$

called the Peiffer lifting. See appendix A for more details.

In complete analogy to the construction of BF and 2BF topological actions, one can define a gauge invariant topological 3BF action for the manifold $\mathcal{M}_4$ and 2-crossed module $(L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G\,, \triangleright\,, \{\_\,,\_\})$. Given $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{l}$ as Lie algebras corresponding to the groups G, H and L, one can introduce a 3-connection (α, β, γ) given by the algebra-valued differential forms $\alpha \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{g})$, $\beta \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{h})$ and $\gamma \in \mathcal{A}^3(\mathcal{M}_4\,,\mathfrak{l})$. The corresponding fake 3-curvature $(\mathcal{F}\,,\mathcal{G}\,,\mathcal{H})$ is then defined as

$$\mathcal{F} = \mathrm{d}\alpha + \alpha\wedge\alpha - \partial\beta\,, \qquad \mathcal{G} = \mathrm{d}\beta + \alpha\wedge^{\triangleright}\beta - \delta\gamma\,, \qquad \mathcal{H} = \mathrm{d}\gamma + \alpha\wedge^{\triangleright}\gamma + \{\beta\wedge\beta\}\,. \tag{3.1}$$

see [24, 25] for details. Then, a $3BF$ action is defined as

$$S_{3BF} = \int_{\mathcal{M}_4} \langle B\wedge\mathcal{F}\rangle_{\mathfrak{g}} + \langle C\wedge\mathcal{G}\rangle_{\mathfrak{h}} + \langle D\wedge\mathcal{H}\rangle_{\mathfrak{l}}\,, \tag{3.2}$$

where $B \in \mathcal{A}^2(\mathcal{M}_4,\mathfrak{g})$, $C \in \mathcal{A}^1(\mathcal{M}_4,\mathfrak{h})$ and $D \in \mathcal{A}^0(\mathcal{M}_4,\mathfrak{l})$ are Lagrange multipliers. The forms $\langle \_,\_\rangle_{\mathfrak{g}}$, $\langle \_,\_\rangle_{\mathfrak{h}}$ and $\langle \_,\_\rangle_{\mathfrak{l}}$ are G-invariant bilinear symmetric nondegenerate forms on $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{l}$, respectively. Under certain conditions, the forms $\langle \_,\_\rangle_{\mathfrak{h}}$ and $\langle \_,\_\rangle_{\mathfrak{l}}$ are also H-invariant and L-invariant, see appendix B for details.

One can see that varying the action with respect to the variables B, C and D, one obtains the equations of motion

$$\mathcal{F} = 0\,, \qquad \mathcal{G} = 0\,, \qquad \mathcal{H} = 0\,, \tag{3.3}$$

while varying with respect to α, β, γ one obtains

$$\mathrm{d}B_\alpha - g_{\alpha\beta}{}^{\gamma} B_\gamma \wedge \alpha^\beta - \triangleright_{\alpha a}{}^{b} C_b \wedge \beta^a + \triangleright_{\alpha B}{}^{A} D_A \wedge \gamma^B = 0\,, \tag{3.4}$$

$$\mathrm{d}C_a - \partial_a{}^{\alpha} B_\alpha + \triangleright_{\alpha a}{}^{b} C_b \wedge \alpha^\alpha + 2X_{\{ab\}}{}^{A} D_A \wedge \beta^b = 0\,, \tag{3.5}$$

$$\mathrm{d}D_A - \triangleright_{\alpha A}{}^{B} D_B \wedge \alpha^\alpha + \delta_A{}^a C_a = 0\,. \tag{3.6}$$

Regarding the gauge transformations, the $3BF$ action is invariant with respect to three different types of transformations, generated by the groups G, H and L, respectively. Under the G-gauge transformations, the 3-connection transforms as

$$\alpha' = g^{-1}\alpha g + g^{-1}\mathrm{d}g\,, \qquad \beta' = g^{-1}\triangleright\beta\,, \qquad \gamma' = g^{-1}\triangleright\gamma\,, \tag{3.7}$$

where $g : \mathcal{M}_4 \to G$ is an element of the G-principal bundle over $\mathcal{M}_4$. Next, under the H-gauge transformations, generated by $\eta \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{h})$, the 3-connection transforms as

$$\alpha' = \alpha + \partial\eta\,, \qquad \beta' = \beta + \mathrm{d}\eta + \alpha'\wedge^{\triangleright}\eta - \eta\wedge\eta\,, \qquad \gamma' = \gamma - \{\beta'\wedge\eta\} - \{\eta\wedge\beta\}\,. \tag{3.8}$$

Finally, under the L-gauge transformations, generated by $\theta \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{l})$, the 3-connection transforms as

$$\alpha' = \alpha\,, \qquad \beta' = \beta - \delta\theta\,, \qquad \gamma' = \gamma - \mathrm{d}\theta - \alpha\wedge\theta\,. \tag{3.9}$$

As a consequence of the definition (3.1) and the above transformation rules, the curvatures transform under the G-gauge transformations as

$$\mathcal{F} \to g^{-1}\mathcal{F}g\,, \qquad \mathcal{G} \to g^{-1}\triangleright\mathcal{G}\,, \qquad \mathcal{H} \to g^{-1}\triangleright\mathcal{H}\,, \tag{3.10}$$

under the H-gauge transformations as

$$\mathcal{F} \to \mathcal{F}\,, \qquad \mathcal{G} \to \mathcal{G} + \mathcal{F}\wedge^{\triangleright}\eta\,, \qquad \mathcal{H} \to \mathcal{H} - \{\mathcal{G}'\wedge\eta\} + \{\eta\wedge\mathcal{G}\}\,, \tag{3.11}$$

and under the L-gauge transformations as

$$\mathcal{F} \to \mathcal{F}\,, \qquad \mathcal{G} \to \mathcal{G}\,, \qquad \mathcal{H} \to \mathcal{H} - \mathcal{F} \wedge^{\rhd} \theta\,. \tag{3.12}$$

For more details, the reader is referred to [25].

In order to make the action (3.2) gauge invariant with respect to the transformations (3.7), (3.8) and (3.9), the Lagrange multipliers B, C and D must transform under the G-gauge transformations as

$$B \to g^{-1} B g\,, \qquad C \to g^{-1} \rhd C\,, \qquad D \to g^{-1} \rhd D\,, \tag{3.13}$$

under the H-gauge transformations as

$$B \to B + C' \wedge^{\mathcal{T}} \eta - \eta \wedge^{\mathcal{D}} \eta \wedge^{\mathcal{D}} D\,, \qquad C \to C + D \wedge^{\mathcal{X}_1} \eta + D \wedge^{\mathcal{X}_2} \eta\,, \qquad D \to D\,, \tag{3.14}$$

while under the L-gauge transformations they transform as

$$B \to B - D \wedge^{\mathcal{S}} \theta\,, \qquad C \to C\,, \qquad D \to D\,. \tag{3.15}$$

See appendix B for details, for the definition of the maps $\mathcal{T}$, $\mathcal{D}$, $\mathcal{X}_1$, $\mathcal{X}_2$, $\mathcal{S}$, and for the notation of the $\wedge^{\mathcal{T}}$, $\wedge^{\mathcal{D}}$, $\wedge^{\mathcal{X}_1}$, $\wedge^{\mathcal{X}_2}$, and $\wedge^{\mathcal{S}}$ products.

3.2 Constrained 3BF action for a real Klein-Gordon field

Once the topological 3BF action is specified, we can proceed with the construction of the constrained 3BF action, describing a realistic case of a scalar field coupled to gravity. In order to perform this construction, we have to define a specific 2-crossed module which gives rise to the topological sector of the action, and then we have to impose convenient simplicity constraints.

We begin by defining a 2-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \rhd\,, \{\_\,,\_\})$, as follows. The groups are given as

$$G = \mathrm{SO}(3,1)\,, \qquad H = \mathbb{R}^4\,, \qquad L = \mathbb{R}\,. \tag{3.16}$$

The group G acts on itself via conjugation, on H via the vector representation, and on L via the trivial representation. This specifies the definition of the action $\rhd$. The map ∂ is chosen to be trivial, as before. The map δ is also trivial, that is, every element of L is mapped to the identity element of H. Finally, the Peiffer lifting is trivial as well, mapping every ordered pair of elements in H to an identity element in L. This specifies one concrete 2-crossed module.

Given this choice of a 2-crossed module, the 3-connection $(\alpha\,,\beta\,,\gamma)$ takes the form

$$\alpha = \omega^{ab} M_{ab}\,, \qquad \beta = \beta^a P_a\,, \qquad \gamma = \gamma \mathbb{I}\,, \tag{3.17}$$

where $\mathbb{I}$ is the sole generator of the Lie group $\mathbb{R}$. From (3.1), the fake 3-curvature $(\mathcal{F}\,,\mathcal{G}\,,\mathcal{H})$ reduces to the ordinary 3-curvature,

$$\mathcal{F} = R^{ab} M_{ab}\,, \qquad \mathcal{G} = \nabla \beta^a P_a\,, \qquad \mathcal{H} = \mathrm{d}\gamma\,, \tag{3.18}$$

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where we used the fact that G acts trivially on L, that is, $M_{ab} \rhd \mathbb{I} = 0$. The topological $3BF$ action (3.2) now becomes

$$S_{3BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla\beta^a + \phi \, \mathrm{d}\gamma \,, \tag{3.19}$$

where the bilinear form for L is $\langle \mathbb{I}, \mathbb{I} \rangle_{\mathfrak{l}} = 1$.

It is important to note that the Lagrange multiplier D in (3.2) is a 0-form and transforms trivially with respect to G, H and L gauge transformations for our choice of the 2-crossed module, as can be seen from (3.13), (3.14) and (3.15). Thus, D has all the *hallmark properties of a real scalar field*, allowing us to make identification between them, and conveniently relabel D into ϕ in (3.19). This is a crucial property of the 3-group structure in a 4-dimensional spacetime and is one of the main results of the paper. It follows the line of reasoning used in recognizing the Lagrange multiplier C^a in the $2BF$ action for the Poincaré 2-group as a tetrad field e^a. It is also important to stress that the choice of the third gauge group, L, dictates the number and the structure of the matter fields present in the action. In this case, $L = \mathbb{R}$ implies that we have only one real scalar field, corresponding to a single generator $\mathbb{I}$ of $\mathbb{R}$. The trivial nature of the action $\rhd$ of $\mathrm{SO}(3,1)$ on $\mathbb{R}$ also implies that ϕ transforms as a scalar field. Finally, the scalar field appears as a degree of freedom in the topological sector of the action, making the quantization procedure feasible.

As in the case of BF and $2BF$ theories, in order to obtain nontrivial dynamics, we need to impose convenient simplicity constraints on the variables in the action (3.19). Since we are interested in obtaining the scalar field ϕ of mass m coupled to gravity in the standard way, we choose the action in the form:

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + e_a \wedge \nabla\beta^a + \phi \, \mathrm{d}\gamma \\ & - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right) \\ & + \lambda \wedge \left(\gamma - \frac{1}{2} H_{abc} e^a \wedge e^b \wedge e^c \right) + \Lambda^{ab} \wedge \left(H_{abc} \varepsilon^{cdef} e_d \wedge e_e \wedge e_f - \mathrm{d}\phi \wedge e_a \wedge e_b \right) \\ & - \frac{1}{2 \cdot 4!} m^2 \phi^2 \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \,. \end{aligned} \tag{3.20}$$

Note that the first row is the topological sector (3.19), the second row is the familiar simplicity constraint for gravity from the action (2.24), the third row contains the new simplicity constraints corresponding to the Lagrange multiplier 1-forms λ and Λ^{ab} and featuring the Lagrange multiplier 0-form H_{abc}, while the fourth row is the mass term for the scalar field.

Varying the total action (3.20) with respect to the variables B_{ab}, ω_{ab}, β_a, λ_{ab}, Λ_{ab}, γ, λ, H_{abc}, ϕ and e^a one obtains the equations of motion:

$$R^{ab} - \lambda^{ab} = 0 \,, \tag{3.21}$$

$$\nabla B^{ab} - e^{[a} \wedge \beta^{b]} = 0 \,, \tag{3.22}$$

$$\nabla e^a = 0 \,, \tag{3.23}$$

$$B_{ab} - \frac{1}{16\pi l_p^2}\varepsilon_{abcd}e^c \wedge e^d = 0\,, \tag{3.24}$$

$$H_{abc}\varepsilon^{cdef} e_d \wedge e_e \wedge e_f - \mathrm{d}\phi \wedge e_a \wedge e_b = 0\,, \tag{3.25}$$

$$\mathrm{d}\phi - \lambda = 0\,, \tag{3.26}$$

$$\gamma - \frac{1}{2}H_{abc}e^a \wedge e^b \wedge e^c = 0\,, \tag{3.27}$$

$$-\frac{1}{2}\lambda \wedge e^a \wedge e^b \wedge e^c + \varepsilon^{cdef}\Lambda^{ab} \wedge e_d \wedge e_e \wedge e_f = 0\,, \tag{3.28}$$

$$\mathrm{d}\gamma - \mathrm{d}(\Lambda^{ab} \wedge e_a \wedge e_b) - \frac{1}{4!}m^2\phi\varepsilon_{abcd}e^a \wedge e^b \wedge e^c \wedge e^d = 0\,, \tag{3.29}$$

$$\nabla\beta_a + \frac{1}{8\pi l_p^2}\varepsilon_{abcd}\lambda^{bc} \wedge e^d + \frac{3}{2}H_{abc}\lambda \wedge e^b \wedge e^c + 3H^{def}\varepsilon_{abcd}\Lambda_{ef} \wedge e^b \wedge e^c$$
$$-2\Lambda_{ab} \wedge \mathrm{d}\phi \wedge e^b - 2\frac{1}{4!}m^2\phi\varepsilon_{abcd}e^b \wedge e^c \wedge e^d = 0\,. \tag{3.30}$$

The dynamical degrees of freedom are e^a and ϕ, while the remaining variables are algebraically determined in terms of them. Specifically, the equations (3.21)–(3.28) give

$$\begin{aligned}
&\lambda_{ab\mu\nu} = R_{ab\mu\nu}\,, && \omega^{ab}{}_\mu = \triangle^{ab}{}_\mu\,, \quad \gamma_{\mu\nu\rho} = -\frac{e}{2}\varepsilon_{\mu\nu\rho\sigma}\partial^\sigma\phi\,,\\
&\Lambda^{ab}{}_\mu = \frac{1}{12e}g_{\mu\lambda}\varepsilon^{\lambda\nu\rho\sigma}\partial_\nu\phi e^a{}_\rho e^b{}_\sigma\,, && \beta^a{}_{\mu\nu} = 0\,, \quad B_{ab\mu\nu} = \frac{1}{8\pi l_p^2}\varepsilon_{abcd}e^c{}_\mu e^d{}_\nu\,,\\
&H^{abc} = \frac{1}{6e}\varepsilon^{\mu\nu\rho\sigma}\partial_\mu\phi e^a{}_\nu e^b{}_\rho e^c{}_\sigma\,, && \lambda_\mu = \partial_\mu\phi\,.
\end{aligned} \tag{3.31}$$

Note that from the equations (3.22), (3.23) and (3.24) it follows that $\beta^a = 0$, as in the pure gravity case. The equation of motion (3.29) reduces to the covariant Klein-Gordon equation for the scalar field,

$$\left(\nabla_\mu\nabla^\mu - m^2\right)\phi = 0\,. \tag{3.32}$$

Finally, the equation of motion (3.30) for e^a becomes:

$$R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R = 8\pi l_p^2\, T^{\mu\nu}\,, \qquad T^{\mu\nu} \equiv \partial^\mu\phi\partial^\nu\phi - \frac{1}{2}g^{\mu\nu}\left(\partial_\rho\phi\partial^\rho\phi + m^2\phi^2\right)\,. \tag{3.33}$$

The system of equations (3.21)–(3.30) is equivalent to the system of equations (3.31)–(3.33). Note that in addition to the correct covariant form of the Klein-Gordon equation, we have also obtained the correct form of the stress-energy tensor for the scalar field.

3.3 Constrained 3BF action for the Dirac field

Now we pass to the more complicated case of the Dirac field. We first define a 2-crossed module $(L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G\,, \triangleright\,, \{\_\,,\_\})$ as follows. The groups are:

$$G = \mathrm{SO}(3,1)\,, \qquad H = \mathbb{R}^4\,, \qquad L = \mathbb{R}^8(\mathbb{G})\,, \tag{3.34}$$

where $\mathbb{G}$ is the algebra of complex Grassmann numbers. The maps ∂, δ and the Peiffer lifting are trivial. The action of the group G on itself is given via conjugation, on H via vector representation, and on L via spinor representation, as follows. Denoting the

8 generators of the Lie group $\mathbb{R}^8(\mathbb{G})$ as P_α and P^α, where the index α takes the values $1,\dots,4$, the action of G on L is thus given explicitly as

$$M_{ab} \triangleright P_\alpha = \frac{1}{2}(\sigma_{ab})^\beta{}_\alpha P_\beta\,, \qquad M_{ab} \triangleright P^\alpha = -\frac{1}{2}(\sigma_{ab})^\alpha{}_\beta P^\beta\,, \tag{3.35}$$

where $\sigma_{ab} = \frac{1}{4}[\gamma_a, \gamma_b]$, and γ_a are the usual Dirac matrices, satisfying the anticommutation rule $\{\gamma_a\,,\,\gamma_b\} = -2\eta_{ab}$.

As in the case of the scalar field, the choice of the group L dictates the matter content of the theory, while the action $\triangleright$ of G on L specifies its transformation properties. To see this explicitly, let us construct the corresponding $3BF$ action. The 3-connection $(\alpha\,,\beta\,,\gamma)$ now takes the form

$$\alpha = \omega^{ab}M_{ab}\,, \qquad \beta = \beta^a P_a\,, \qquad \gamma = \gamma^\alpha P_\alpha + \bar{\gamma}_\alpha P^\alpha\,, \tag{3.36}$$

while the 3-curvature $(\mathcal{F}\,,\mathcal{G}\,,\mathcal{H})$, defined in (3.1), is given as

$$\mathcal{F} = R^{ab}M_{ab}\,, \mathcal{G} = \nabla\beta^a P_a\,, \tag{3.37}$$
$$\mathcal{H} = \left(\mathrm{d}\gamma^\alpha + \frac{1}{2}\omega^{ab}(\sigma_{ab})^\alpha{}_\beta\gamma^\beta\right)P_\alpha + \left(\mathrm{d}\bar{\gamma}_\alpha - \frac{1}{2}\omega^{ab}\bar{\gamma}_\beta(\sigma_{ab})^\beta{}_\alpha\right)P^\alpha \equiv (\overset{\rightarrow}{\nabla}\gamma)^\alpha P_\alpha + (\bar{\gamma}\overset{\leftarrow}{\nabla})_\alpha P^\alpha\,,$$

where we have used (3.35). The bilinear form $\langle\_,\_\rangle_\mathfrak{l}$ is defined as

$$\langle P_\alpha, P_\beta\rangle_\mathfrak{l} = 0\,, \qquad \langle P^\alpha, P^\beta\rangle_\mathfrak{l} = 0\,, \qquad \langle P_\alpha, P^\beta\rangle_\mathfrak{l} = -\delta_\alpha^\beta\,, \qquad \langle P^\alpha, P_\beta\rangle_\mathfrak{l} = \delta^\alpha_\beta\,. \tag{3.38}$$

Note that, for general $A, B \in \mathfrak{l}$, we can write

$$\langle A, B\rangle_\mathfrak{l} = A^I B^J g_{IJ}\,, \qquad \langle B, A\rangle_\mathfrak{l} = B^J A^I g_{JI}\,. \tag{3.39}$$

Since we require the bilinear form to be symmetric, the two expressions must be equal. However, since the coefficients in $\mathfrak{l}$ are Grassmann numbers, we have $A^I B^J = -B^J A^I$, so it follows that $g_{IJ} = -g_{JI}$. Hence the antisymmetry of (3.38).

Now we use the properties of the group L and the action $\triangleright$ of G on L to recognize the physical nature of the Lagrange multiplier D in (3.2). Indeed, the choice of the group L dictates that D contains 8 independent complex Grassmannian matter fields as its components. Moreover, due to the fact that D is a 0-form and that it transforms according to the spinorial representation of SO(3,1), we can identify its components with the Dirac bispinor fields, and write

$$D = \psi^\alpha P_\alpha + \bar{\psi}_\alpha P^\alpha\,, \tag{3.40}$$

where it is assumed that ψ and $\bar{\psi}$ are independent fields, as usual. This is again an illustration of the fact that information about the structure of the matter sector in the theory is specified by the choice of the group L in the 2-crossed module, and another main result of the paper.

Given all of the above, now we can finally write the $3BF$ action (3.2) corresponding to this choice of the 2-crossed module as

$$S_{3BF} = \int_{\mathcal{M}_4} B^{ab}\wedge R_{ab} + e_a \wedge \nabla\beta^a + (\bar{\gamma}\overset{\leftarrow}{\nabla})_\alpha\psi^\alpha + \bar{\psi}_\alpha(\overset{\rightarrow}{\nabla}\gamma)^\alpha\,. \tag{3.41}$$

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In order to promote this action into a full theory of gravity coupled to Dirac fermions, we add the convenient constraint terms to the action, as follows:

$$
\begin{aligned}
S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a + (\bar{\gamma}\overleftarrow{\nabla})_\alpha \psi^\alpha + \bar{\psi}_\alpha (\overrightarrow{\nabla}\gamma)^\alpha \\
& - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right) \\
& - \lambda^\alpha \wedge \left(\bar{\gamma}_\alpha - \frac{i}{6} \varepsilon_{abcd} e^a \wedge e^b \wedge e^c (\bar{\psi}\gamma^d)_\alpha \right) + \bar{\lambda}_\alpha \wedge \left(\gamma^\alpha + \frac{i}{6} \varepsilon_{abcd} e^a \wedge e^b \wedge e^c (\gamma^d \psi)^\alpha \right) \\
& - \frac{1}{12} m \, \bar{\psi}\psi \, \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d + 2\pi i l_p^2 \, \bar{\psi}\gamma_5 \gamma^a \psi \, \varepsilon_{abcd} e^b \wedge e^c \wedge \beta^d \,.
\end{aligned} \tag{3.42}
$$

Here the first row is the topological sector, the second row is the gravitational simplicity constraint term from (2.24), while the third row contains the new simplicity constraints for the Dirac field corresponding to the Lagrange multiplier 1-forms λ^α and $\bar{\lambda}_\alpha$. The fourth row contains the mass term for the Dirac field, and a term which ensures the correct coupling between the torsion and the spin of the Dirac field, as specified by the Einstein-Cartan theory. Namely, we want to ensure that the torsion has the form

$$
T_a \equiv \nabla e_a = 2\pi l_p^2 s_a \,, \tag{3.43}
$$

where

$$
s_a = i \varepsilon_{abcd} e^b \wedge e^c \bar{\psi} \gamma_5 \gamma^d \psi \tag{3.44}
$$

is the spin 2-form. Of course, other couplings should also be straightforward to implement, but we choose this particular coupling because we are interested in reproducing the standard Einstein-Cartan gravity coupled to the Dirac field.

Varying the action (3.42) with respect to B_{ab}, λ^{ab}, $\bar{\gamma}_\alpha$, γ^α, λ^α, $\bar{\lambda}_\alpha$, $\bar{\psi}_\alpha$, ψ^α, e^a, β^a and ω^{ab} one obtains the equations of motion:

$$
R^{ab} - \lambda^{ab} = 0 \,, \tag{3.45}
$$

$$
B_{ab} - \frac{1}{16\pi l_p^2} \varepsilon_{abcd} e^c \wedge e^d = 0 \,, \tag{3.46}
$$

$$
(\overrightarrow{\nabla}\psi)^\alpha - \lambda^\alpha = 0 \,, \tag{3.47}
$$

$$
(\bar{\psi}\overleftarrow{\nabla})_\alpha - \bar{\lambda}_\alpha = 0 \,, \tag{3.48}
$$

$$
\bar{\gamma}_\alpha - \frac{i}{6} \varepsilon_{abcd} e^a \wedge e^b \wedge e^c (\bar{\psi}\gamma^d)_\alpha = 0 \,, \tag{3.49}
$$

$$
\gamma^\alpha + \frac{i}{6} \varepsilon_{abcd} e^a \wedge e^b \wedge e^c (\gamma^d \psi)^\alpha = 0 \,, \tag{3.50}
$$

$$
\begin{aligned}
\mathrm{d}\gamma^\alpha + \omega^\alpha{}_\beta \wedge \gamma^\beta + \frac{i}{6} \lambda^\beta \wedge \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \gamma^{d\alpha}{}_\beta + \frac{1}{12} m \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \psi^\alpha & \\
+ i 2\pi l_p^2 \varepsilon_{abcd} e^a \wedge e^b \wedge \beta^c (\gamma_5 \gamma^d \psi)^\alpha = 0 \,, &
\end{aligned} \tag{3.51}
$$

$$
\begin{aligned}
\mathrm{d}\bar{\gamma}_\alpha - \bar{\gamma}_\beta \wedge \omega^\beta{}_\alpha + \frac{i}{6} \bar{\lambda}_\beta \wedge \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \gamma^{d\beta}{}_\alpha - \frac{1}{12} m \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \bar{\psi}_\alpha & \\
- i 2\pi l_p^2 \varepsilon_{abcd} e^a \wedge e^b \wedge \beta^c (\bar{\psi} \gamma_5 \gamma^d)_\alpha = 0 \,, &
\end{aligned} \tag{3.52}
$$

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$$\nabla\beta_a + 2\varepsilon_{abcd}\lambda^{bc}\wedge e^d - \frac{i}{2}\varepsilon_{abcd}\lambda^\alpha \wedge e^b\wedge e^c(\bar\psi\gamma^d)_\alpha + \frac{i}{2}\varepsilon_{abcd}\bar\lambda_\alpha\wedge e^b\wedge e^c(\gamma^d\psi)^\alpha$$
$$-\frac{1}{3}\varepsilon_{abcd}e^b\wedge e^c\wedge e^d m\bar\psi\psi - 4\pi l_p^2 i\varepsilon_{abcd}e^b\wedge\beta^c\bar\psi\gamma_5\gamma^d\psi = 0\,, \quad (3.53)$$
$$\nabla e_a - i2\pi l_p^2\varepsilon_{abcd}e^b\wedge e^c\bar\psi\gamma_5\gamma^d\psi = 0\,, \quad (3.54)$$
$$\nabla B_{ab} - e_{[a}\wedge\beta_{b]} + \bar\gamma\frac{1}{8}[\gamma_a,\gamma_b]\psi + \bar\psi\frac{1}{8}[\gamma_a,\gamma_b]\gamma = 0\,. \quad (3.55)$$

The dynamical degrees of freedom are e^a, ψ^α and $\bar\psi_\alpha$, while the remaining variables are determined in terms of the dynamical variables, and are given as:

$$\begin{aligned}
&B_{ab\mu\nu} = \frac{1}{8\pi l_p^2}\varepsilon_{abcd}e^c{}_\mu e^d{}_\nu\,, && \lambda^\alpha{}_\mu = (\overrightarrow{\nabla}_\mu\psi)^\alpha\,, && \bar\lambda_{\alpha\mu} = (\bar\psi\overleftarrow{\nabla}_\mu)_\alpha\,,\\
&\bar\gamma_{\alpha\mu\nu\rho} = i\varepsilon_{abcd}e^a{}_\mu e^b{}_\nu e^c{}_\rho(\bar\psi\gamma^d)_\alpha\,, && \gamma^\alpha{}_{\mu\nu\rho} = -i\varepsilon_{abcd}e^a{}_\mu e^b{}_\nu e^c{}_\rho(\gamma^d\psi)^\alpha\,, && \\
&\lambda_{ab\mu\nu} = R_{ab\mu\nu}\,, && \omega^{ab}{}_\mu = \triangle^{ab}{}_\mu + K^{ab}{}_\mu\,. &&
\end{aligned} \quad (3.56)$$

Here $K^{ab}{}_\mu$ is the contorsion tensor, constructed in the standard way from the torsion tensor, whereas from (3.54) we have

$$T_a \equiv \nabla e_a = 2\pi l_p^2 s_a\,, \quad (3.57)$$

which is precisely the desired equation (3.43). Further, from the equation (3.46) one obtains

$$\nabla B^{ab} = -\frac{1}{8\pi l_p^2}\varepsilon^{abcd}\left(e_c\wedge\nabla e_d\right)\,. \quad (3.58)$$

Substituting this expression in the equation (3.55) it follows that

$$2\varepsilon_{abcd}e^c\wedge\left(-\frac{1}{16\pi l_p^2}\nabla e^d + \frac{1}{8}s^d\right) - e_{[a}\wedge\beta_{b]} = 0\,. \quad (3.59)$$

The expression in the parentheses is equal to zero, according to the equation (3.54). From the remaining term $e_{[a}\wedge\beta_{b]} = 0$ it again follows that

$$\beta = 0\,. \quad (3.60)$$

Using this result, the equation of motion (3.51) for fermions becomes

$$\frac{i}{6}\varepsilon_{abcd}e^a\wedge e^b\wedge\left(2e^c\wedge\gamma^d\overrightarrow{\nabla} + \frac{im}{2}e^c\wedge e^d - 3(\nabla e^c)\gamma^d\right)\psi = 0\,. \quad (3.61)$$

Using equation (3.54), the last term in the parentheses vanishes, and the equation reduces to the covariant Dirac equation,

$$(i\gamma^a e^\mu{}_a\overrightarrow{\nabla}_\mu - m)\psi = 0\,, \quad (3.62)$$

where $e^\mu{}_a$ is the inverse tetrad. Similarly, the equation (3.52) gives the conjugated Dirac equation:

$$\bar\psi(i\overleftarrow{\nabla}_\mu e^\mu{}_a\gamma^a + m) = 0\,. \quad (3.63)$$

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Finally, the equation of motion (3.53) for tetrad field reduces to

$$R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R = 8\pi l_p^2\, T^{\mu\nu}\,, \qquad T^{\mu\nu} \equiv \frac{i}{2}\bar{\psi}\gamma^{\nu}\overset{\leftrightarrow}{\nabla}{}^{a}e^{\mu}{}_{a}\psi - \frac{1}{2}g^{\mu\nu}\bar{\psi}\Big(i\gamma^{a}\overset{\leftrightarrow}{\nabla}_{\rho}e^{\rho}{}_{a} - 2m\Big)\psi\,, \tag{3.64}$$

Here, we used the notation $\overset{\leftrightarrow}{\nabla} = \overset{\rightarrow}{\nabla} - \overset{\leftarrow}{\nabla}$. The system of equations (3.45)–(3.55) is equivalent to the system of equations (3.56), (3.60), (3.62)–(3.64). As we expected, the equations of motion (3.57), (3.62), (3.63) and (3.64) are precisely the equations of motion of the Einstein-Cartan theory coupled to a Dirac field.

3.4 Constrained 3*BF* action for the Weyl and Majorana fields

A general solution of the Dirac equation is not an irreducible representation of the Lorentz group, and one can rewrite Dirac fermions as left-chiral and right-chiral fermion fields that both retain their chirality under Lorentz transformations, implying their irreducibility. Hence, it is useful to rewrite the action for left and right Weyl spinors as a constrained 3*BF* action. For simplicity, we will discuss only left-chiral spinor field, while the right-chiral field can be treated analogously. Both Weyl and Majorana fermions can be treated in the same way, the only difference being the presence of an additional mass term in the Majorana action.

We being by defining a 2-crossed module $(L \overset{\delta}{\to} H \overset{\partial}{\to} G\,, \triangleright\,, \{\_\,,\_\})$, as follows. The groups are:

$$G = \mathrm{SO}(3,1)\,, \qquad H = \mathbb{R}^4\,, \qquad L = \mathbb{R}^4(\mathbb{G})\,. \tag{3.65}$$

The maps ∂, δ and the Peiffer lifting are trivial. The action $\triangleright$ of the group G on G, H and L is given in the same way as for the Dirac case, whereas the spinorial representation reduces to

$$M_{ab} \triangleright P^{\alpha} = \frac{1}{2}(\sigma_{ab})^{\alpha}{}_{\beta}P^{\beta}\,, \qquad M_{ab} \triangleright P_{\dot{\alpha}} = \frac{1}{2}(\bar{\sigma}_{ab})^{\dot{\beta}}{}_{\dot{\alpha}}P_{\dot{\beta}}\,, \tag{3.66}$$

where $\sigma^{ab} = -\bar{\sigma}^{ab} = \frac{1}{4}(\sigma^a\bar{\sigma}^b - \sigma^b\bar{\sigma}^a)$, for $\sigma^a = (1, \vec{\sigma})$ and $\bar{\sigma}^a = (1, -\vec{\sigma})$, in which $\vec{\sigma}$ denotes the set of three Pauli matrices. The four generators of the group L are denoted as P^{α} and $P_{\dot{\alpha}}$, where the Weyl indices $\alpha, \dot{\alpha}$ take values $1, 2$.

The 3-connection $(\alpha\,, \beta\,, \gamma)$ now takes the form corresponding to this choice of Lie groups,

$$\alpha = \omega^{ab}M_{ab}\,, \qquad \beta = \beta^a P_a\,, \qquad \gamma = \gamma_{\alpha}P^{\alpha} + \bar{\gamma}^{\dot{\alpha}}P_{\dot{\alpha}}\,, \tag{3.67}$$

while the fake 3-curvature $(\mathcal{F}\,, \mathcal{G}\,, \mathcal{H})$ defined in (3.1) is

$$\mathcal{F} = R^{ab}M_{ab}\,, \qquad \mathcal{G} = \nabla\beta^a P_a\,, \tag{3.68}$$

$$\mathcal{H} = \Big(\mathrm{d}\gamma_{\alpha} + \frac{1}{2}\omega^{ab}(\sigma^{ab})^{\beta}{}_{\alpha}\gamma_{\beta}\Big)P^{\alpha} + \Big(\mathrm{d}\bar{\gamma}^{\dot{\alpha}} + \frac{1}{2}\omega_{ab}(\bar{\sigma}^{ab})^{\dot{\alpha}}{}_{\dot{\beta}}\bar{\gamma}^{\dot{\beta}}\Big)P_{\dot{\alpha}} \equiv (\overset{\rightarrow}{\nabla}\gamma)_{\alpha}P^{\alpha} + (\bar{\gamma}\overset{\leftarrow}{\nabla})^{\dot{\alpha}}P_{\dot{\alpha}}\,.$$

Introducing the spinor fields ψ_{α} and $\bar{\psi}^{\dot{\alpha}}$ via the Lagrange multiplier D as

$$D = \psi_{\alpha}P^{\alpha} + \bar{\psi}^{\dot{\alpha}}P_{\dot{\alpha}}\,, \tag{3.69}$$

and using the bilinear form $\langle\_,\_\rangle_{\mathfrak{l}}$ for the group L,

$$\langle P^{\alpha}, P^{\beta}\rangle_{\mathfrak{l}} = \varepsilon^{\alpha\beta}\,, \qquad \langle P_{\dot{\alpha}}, P_{\dot{\beta}}\rangle_{\mathfrak{l}} = \varepsilon_{\dot{\alpha}\dot{\beta}}\,, \qquad \langle P^{\alpha}, P_{\dot{\beta}}\rangle_{\mathfrak{l}} = 0\,, \qquad \langle P_{\dot{\alpha}}, P^{\beta}\rangle_{\mathfrak{l}} = 0\,, \tag{3.70}$$

where $\varepsilon^{\alpha\beta}$ and $\varepsilon_{\dot\alpha\dot\beta}$ are the usual two-dimensional antisymmetric Levi-Civita symbols, the topological $3BF$ action (3.2) for spinors coupled to gravity becomes

$$S_{3BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla\beta^a + \psi^\alpha \wedge (\overset{\rightarrow}{\nabla}\gamma)_\alpha + \bar\psi_{\dot\alpha} \wedge (\bar\gamma\overset{\leftarrow}{\nabla})^{\dot\alpha} . \tag{3.71}$$

In order to obtain the suitable equations of motion for the Weyl spinors, we again introduce appropriate simplicity constraints, so that the action becomes:

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + e_a \wedge \nabla\beta^a + \psi^\alpha \wedge (\overset{\rightarrow}{\nabla}\gamma)_\alpha + \bar\psi_{\dot\alpha} \wedge (\bar\gamma\overset{\leftarrow}{\nabla})^{\dot\alpha} \\ & - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2}\varepsilon^{abcd} e_c \wedge e_d \right) \\ & - \lambda^\alpha \wedge \left(\gamma_\alpha + \frac{i}{6}\varepsilon_{abcd} e^a \wedge e^b \wedge e^c \sigma^d{}_{\alpha\dot\beta}\bar\psi^{\dot\beta} \right) - \bar\lambda_{\dot\alpha} \wedge \left(\bar\gamma^{\dot\alpha} + \frac{i}{6}\varepsilon_{abcd} e^a \wedge e^b \wedge e^c \bar\sigma^{d\dot\alpha\beta}\psi_\beta \right) \\ & - 4\pi l_p^2 \varepsilon_{abcd} e^a \wedge e^b \wedge \beta^c (\bar\psi_{\dot\alpha}\bar\sigma^{d\dot\alpha\beta}\psi_\beta) . \end{aligned} \tag{3.72}$$

The new simplicity constraints are in the third row, featuring the Lagrange multiplier 1-forms λ_α and $\bar\lambda^{\dot\alpha}$. Also, using the coupling between the Dirac field and torsion from Einstein-Cartan theory as a model, the term in the fourth row is chosen to ensure that the coupling between the Weyl spin tensor

$$s_a \equiv i\varepsilon_{abcd} e^b \wedge e^c \, \psi^\alpha \sigma^d{}_{\alpha\dot\beta} \bar\psi^{\dot\beta} , \tag{3.73}$$

and torsion is given as:

$$T_a = 4\pi l_p^2 s_a . \tag{3.74}$$

The case of the Majorana field is introduced in exactly the same way, albeit with an additional mass term in the action, of the form:

$$-\frac{1}{12} m \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d (\psi^\alpha\psi_\alpha + \bar\psi_{\dot\alpha}\bar\psi^{\dot\alpha}) . \tag{3.75}$$

Varying the action (3.72) with respect to the variables B_{ab}, λ^{ab}, γ_α, $\bar\gamma^{\dot\alpha}$, λ_α, $\bar\lambda^{\dot\alpha}$, ψ_α, $\bar\psi^{\dot\alpha}$, e^a, β^a and ω^{ab} one again obtains the complete set of equations of motion, displayed in the appendix C. The only dynamical degrees of freedom are ψ_α, $\bar\psi^{\dot\alpha}$ and e^a, while the remaining variables are algebraically determined in terms of these as:

$$\lambda^{ab}{}_{\mu\nu} = R^{ab}{}_{\mu\nu} , \quad B_{ab\mu\nu} = \frac{1}{8\pi l_p^2}\varepsilon_{abcd} e^c{}_\mu e^d{}_\nu , \quad \lambda_{\alpha\mu} = \nabla_\mu\psi_\alpha , \quad \bar\lambda^{\dot\alpha}{}_\mu = \nabla_\mu\bar\psi^{\dot\alpha} , \tag{3.76}$$

$$\gamma_{\alpha\mu\nu\rho} = i\varepsilon_{abcd} e^a{}_\mu e^b{}_\nu e^c{}_\rho \sigma^d{}_{\alpha\dot\beta}\bar\psi^{\dot\beta} , \quad \bar\gamma^{\dot\alpha}{}_{\mu\nu\rho} = i\varepsilon_{abcd} e^a{}_\mu e^b{}_\nu e^c{}_\rho \bar\sigma^{d\dot\alpha\beta}\psi_\beta , \quad \omega_{ab\mu} = \triangle_{ab\mu} + K_{ab\mu} .$$

In addition, one also maintains the result $\beta = 0$ as before. Finally, the equations of motion for the dynamical fields are

$$\bar\sigma^{a\dot\alpha\beta} e^\mu{}_a \nabla_\mu\psi_\beta = 0 , \qquad \sigma^a{}_{\alpha\dot\beta} e^\mu{}_a \nabla_\mu\bar\psi^{\dot\beta} = 0 , \tag{3.77}$$

and

$$R^{\mu\nu} - \frac{1}{2} g^{\mu\nu} R = 8\pi l_p^2 \, T^{\mu\nu} , \tag{3.78}$$

where

$$T^{\mu\nu} \equiv \frac{i}{2}\bar{\psi}\bar{\sigma}^b e^\nu{}_b \nabla^\mu \psi + \frac{i}{2}\psi\sigma^b e^\nu{}_b \nabla^\mu \bar{\psi} - g^{\mu\nu}\frac{1}{2}\Big(i\bar{\psi}\bar{\sigma}^a e^\lambda{}_a \nabla_\lambda \psi + i\psi\sigma^a e^\lambda{}_a \nabla_\lambda \bar{\psi}\Big)\,. \tag{3.79}$$

Here we have suppressed the spinor indices. In the case of the Majorana field, the equations of motion (3.76) remain the same, while the equations of motion for ψ_α and $\bar{\psi}^{\dot{\alpha}}$ take the form

$$i\sigma^a{}_{\alpha\dot{\beta}} e^\mu{}_a \nabla_\mu \bar{\psi}^{\dot{\beta}} - m\psi_\alpha = 0\,, \qquad i\bar{\sigma}^{a\dot{\alpha}\beta} e^\mu{}_a \nabla_\mu \psi_\beta - m\bar{\psi}^{\dot{\alpha}} = 0\,, \tag{3.80}$$

whereas the stress-energy tensor takes the form

$$\begin{aligned} T^{\mu\nu} \equiv\; & \frac{i}{2}\bar{\psi}\bar{\sigma}^b e^\nu{}_b \nabla^\mu \psi + \frac{i}{2}\psi\sigma^b e^\nu{}_b \nabla^\mu \bar{\psi} \\ & - g^{\mu\nu}\frac{1}{2}\left[i\bar{\psi}\bar{\sigma}^a e^\lambda{}_a \nabla_\lambda \psi + i\psi\sigma^a e^\lambda{}_a \nabla_\lambda \bar{\psi} - \frac{1}{2}m\left(\psi\psi + \bar{\psi}\bar{\psi}\right)\right]. \end{aligned} \tag{3.81}$$

4 The Standard Model

The Standard Model 3-group can be defined as:

$$G = \mathrm{SO}(3,1)\times\mathrm{SU}(3)\times\mathrm{SU}(2)\times\mathrm{U}(1)\,, \quad H = \mathbb{R}^4\,, \quad L = \mathbb{R}^4(\mathbb{C})\times\mathbb{R}^{64}(\mathbb{G})\times\mathbb{R}^{64}(\mathbb{G})\times\mathbb{R}^{64}(\mathbb{G})\,, \tag{4.1}$$

where $\mathbb{C}$ denotes the field of complex numbers. The motivation for this choice of the group L is given in the table below.

1. lepton generation	red color 1. quark generation	green color 1. quark generation	blue color 1. quark generation
$\begin{pmatrix}\nu_e \\ e^-\end{pmatrix}_L$	$\begin{pmatrix}u_r \\ d_r\end{pmatrix}_L$	$\begin{pmatrix}u_g \\ d_g\end{pmatrix}_L$	$\begin{pmatrix}u_b \\ d_b\end{pmatrix}_L$
$(\nu_e)_R$	$(u_r)_R$	$(u_g)_R$	$(u_b)_R$
$(e^-)_R$	$(d_r)_R$	$(d_g)_R$	$(d_b)_R$

We see that in order to introduce one generation of matter one needs to provide 16 spinors, or equivalently the group L has to be chosen as $L = \mathbb{R}^{64}(\mathbb{G})$. As there are three generations of matter, the part of the group L that corresponds to the fermion fields in the theory is chosen to be $L = \mathbb{R}^{64}(\mathbb{G}) \times \mathbb{R}^{64}(\mathbb{G}) \times \mathbb{R}^{64}(\mathbb{G})$. To define the Higgs sector one needs two complex scalar fields $\begin{pmatrix}\phi^+ \\ \phi_0\end{pmatrix}$, or equivalently the scalar sector of the group L is given as $L = \mathbb{R}^4(\mathbb{C})$.

The maps ∂, δ and the Peiffer lifting are trivial. The action of the group G on itself is given via conjugation. The action of the $\mathrm{SO}(3,1)$ subgroup of G on H is via vector representation and the action of $\mathrm{SU}(3) \times \mathrm{SU}(2) \times \mathrm{U}(1)$ subgroup on H is via trivial representation. The action of the $\mathrm{SO}(3,1)$ on L is via trivial representation for the generators corresponding to the scalar fields, i.e. the $\mathbb{R}^4(\mathbb{C})$ subgroup of L, and via spinor representation for the every quadruple of generators corresponding to the fermion fields, given as in the section 3. The information how spinors transform under the $SU(3) \times SU(2) \times U(1)$ group is encoded in the action of that subgroup of G on L, as specified in the table above. For simplicity, in the following, only one family of the lepton sector and only electroweak part of the gauge sector of the Standard model is considered.

The groups are chosen as:

$$G = SO(3,1) \times SU(2) \times U(1)\,, \quad H = \mathbb{R}^4\,, \quad L^{\text{leptons}} = \mathbb{R}^{16}(\mathbb{G}) \times \mathbb{R}^4(\mathbb{C})\,. \tag{4.2}$$

The 3-connection then takes the form

$$\begin{aligned} &\alpha = \omega^{ab} M_{ab} + W^I T_I + AY\,, && \beta = \beta^a P_a\,, \\ &\gamma = \gamma_\alpha{}^{\tilde{L}} P^\alpha{}_{\tilde{L}} + \gamma^{\dot\alpha}{}_{\tilde{L}} P_{\dot\alpha}{}^{\tilde{L}} + \gamma_\alpha{}^{\tilde{R}} P^\alpha{}_{\tilde{R}} + \gamma^{\dot\alpha}{}_{\tilde{R}} P_{\dot\alpha}{}^{\tilde{R}} + \gamma^{\tilde{a}} P_{\tilde{a}}\,. \end{aligned} \tag{4.3}$$

Here the indices $I, J, \dots$ take the values $1,2,3$ and counts the Pauli matrices, generators of the group SU(2), the indices $\tilde{L}, \tilde{L}', \dots$ take the values $1,2$ and count the components of left doublet, $\tilde{R}$ denotes the right singlet $(e^-)_R$ and right singlet $(\nu_e)_R$, and indices $\tilde{a}, \tilde{b}, \dots$ take values $1,2$ and count the components of the scalar doublet. It is also useful to define $\tilde{i} = (\tilde{L}, \tilde{R})$ which takes values $1, \dots, 4$.

The action of the group G on L is defined as:

$$\begin{aligned} &M_{ab} \rhd P^\alpha{}_i = \frac{1}{2}(\sigma_{ab})^\alpha{}_\beta P^\beta{}_i\,, \qquad M_{ab} \rhd P_{\dot\alpha i} = \frac{1}{2}(\bar\sigma_{ab})^{\dot\beta}{}_{\dot\alpha} P_{\dot\beta i}\,, \qquad M_{ab} \rhd P_{\tilde{a}} = 0\,, \\ &T_I \rhd P^\alpha{}_{\tilde{L}} = \frac{1}{2}(\sigma_I)^{\tilde{L}'}{}_{\tilde{L}} P^\alpha{}_{\tilde{L}'}\,, \qquad T_I \rhd P_{\dot\alpha \tilde{L}} = \frac{1}{2}(\sigma_I)^{\tilde{L}'}{}_{\tilde{L}} P_{\dot\alpha \tilde{L}'}\,, \\ &T_I \rhd P^\alpha{}_{\tilde{R}} = 0\,, \qquad T_I \rhd P_{\dot\alpha \tilde{R}} = 0\,, \qquad T_I \rhd P_{\tilde{a}} = \frac{1}{2}(\sigma_I)^{\tilde{b}}{}_{\tilde{a}} P_{\tilde{b}}\,, \\ &Y \rhd P^\alpha{}_{\tilde{L}} = -P^\alpha{}_{\tilde{L}}\,, \quad Y \rhd P^\alpha{}_{e_R} = -2P^\alpha{}_{e_R}\,, \quad Y \rhd P^\alpha{}_{\nu_R} = -2P^\alpha{}_{\nu_R}\,, \quad Y \rhd P_{\tilde{a}} = P_{\tilde{a}}\,, \\ &Y \rhd P_{\dot\alpha \tilde{L}} = -P_{\dot\alpha \tilde{L}}\,, \qquad Y \rhd P_{\dot\alpha e_R} = -2P_{\dot\alpha e_R}\,, \qquad Y \rhd P_{\dot\alpha \nu_R} = -2P_{\dot\alpha \nu_R}\,. \end{aligned} \tag{4.4}$$

The 3-curvatures are given as:

$$\begin{aligned} &\mathcal{F} = R^{ab} M_{ab} + F^I T_I + FY\,, \qquad \mathcal{G} = \nabla \beta^a P_a\,, \\ &\mathcal{H} = (\overrightarrow{\nabla}\gamma^{\tilde{L}})_\alpha P^\alpha{}_{\tilde{L}} + (\bar\gamma_{\tilde{L}} \overleftarrow{\nabla})^{\dot\alpha} P_{\dot\alpha}{}^{\tilde{L}} + (\overrightarrow{\nabla}\gamma^{\tilde{R}})_\alpha P^\alpha{}_{\tilde{R}} + (\bar\gamma_{\tilde{R}} \overleftarrow{\nabla})^{\dot\alpha} P_{\dot\alpha}{}^{\tilde{R}} + \mathrm{d}\gamma^{\tilde{a}} P_{\tilde{a}}\,. \end{aligned} \tag{4.5}$$

The topological $3BF$ action is defined as:

$$S = \int B_{ab} R^{ab} + B_I F^I + BF + e_a \nabla \beta^a + \psi^\alpha{}_{\tilde{i}} (\overrightarrow{\nabla}\gamma^{\tilde{i}})_\alpha + \bar\psi_{\dot\alpha}{}^{\tilde{i}} (\bar\gamma_{\tilde{i}} \overleftarrow{\nabla})^{\dot\alpha} + \phi^{\tilde{a}} \mathrm{d}\gamma_{\tilde{a}}\,. \tag{4.6}$$

At this point, it is useful to simplify the notation and denote all indices of the group G by $\hat\alpha$, of the group H by $\hat{a}$ and L by $\hat{A}$. In order to promote this action to a full theory of first lepton family coupled to electroweak gauge fields, Higgs field, and gravity, we again introduce the appropriate simplicity constraint, as follows

$$
\begin{aligned}
S = \int & B_{\hat\alpha} \wedge \mathcal{F}^{\hat\alpha} + e_{\hat a} \wedge \mathcal{G}^{\hat a} + D_{\hat A} \wedge \mathcal{H}^{\hat A} \\
& + \left(B_{\hat\alpha} - C_{\hat\alpha}{}^{\hat\beta} M_{cd\hat\beta} e^c \wedge e^d \right) \wedge \lambda^{\hat\alpha} - \left(\gamma_{\hat A} - e^a \wedge e^b \wedge e^c C_{\hat A}{}^{\hat B} M_{abc\hat B} \right) \wedge \lambda^{\hat A} \\
& + \zeta^{ab}{}_{\hat\alpha} \wedge \left(M_{ab}{}^{\hat\alpha} \varepsilon^{cdef} e_c \wedge e_d \wedge e_e \wedge e_f - F^{\hat\alpha} \wedge e_c \wedge e_d \right) \\
& + \zeta^{ab}{}_{\hat A} \wedge \left(M_{abc}{}^{\hat A} \varepsilon^{cdef} e_d \wedge e_e \wedge e_f - F^{\hat A} \wedge e_a \wedge e_b \right) \\
& - \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \; \left(Y_{\hat A\hat B\hat C} D^{\hat A} D^{\hat B} D^{\hat C} + M_{\hat A\hat B} D^{\hat A} D^{\hat B} + L_{\hat A\hat B\hat C\hat D} D^{\hat A} D^{\hat B} D^{\hat C} D^{\hat D} \right) \\
& - 4\pi i \, l_p^2 \, \varepsilon_{abcd} e^a \wedge e^b \wedge \beta^c D_{\hat A} T^{d\hat A}{}_{\hat B} D^{\hat B} \,,
\end{aligned}
\tag{4.7}
$$

where:

$$
\begin{aligned}
& B_{\hat\alpha} = \begin{bmatrix} B_{ab} & B_I & B \end{bmatrix}, \qquad \mathcal{F}^{\hat\alpha} = \begin{bmatrix} R_{ab} & F_I & F \end{bmatrix}^T, \qquad D_{\hat A} = \begin{bmatrix} \psi^\alpha{}_{\tilde L} & \bar\psi_{\dot\alpha \tilde L} & \psi^\alpha{}_R & \bar\psi_{\dot\alpha R} & \phi_{\tilde a} \end{bmatrix}, \\
& \mathcal{H}^{\hat A} = \begin{bmatrix} (\overrightarrow{\nabla}\gamma_{\tilde L})_\alpha & (\bar\gamma_{\tilde L}\overleftarrow{\nabla})^{\dot\alpha} & (\overrightarrow{\nabla}\gamma_{\tilde R})_\alpha & (\bar\gamma_{\tilde R}\overleftarrow{\nabla})^{\dot\alpha} & \mathrm{d}\gamma_{\tilde a} \end{bmatrix}^T, \quad \gamma_{\hat A} = \begin{bmatrix} \gamma^\alpha{}_{\tilde L} & \bar\gamma_{\dot\alpha \tilde L} & \gamma^\alpha{}_{\tilde R} & \bar\gamma_{\dot\alpha \tilde R} & \gamma_{\tilde a} \end{bmatrix}, \\
& \lambda^{\hat\alpha} = \begin{bmatrix} -\lambda^{ab} & \lambda^I & \lambda \end{bmatrix}^T, \qquad \zeta^{cd}{}_{\hat\alpha} = \begin{bmatrix} 0 & \zeta^{cd}{}_I & \zeta^{cd} \end{bmatrix}, \qquad \zeta^{ab}{}_{\hat A} = \begin{bmatrix} \zeta^{ab} & 0 & 0 \end{bmatrix}, \\
& \lambda^{\hat A} = \begin{bmatrix} \lambda_{\alpha L} & \bar\lambda^{\dot\alpha}{}_L & \lambda_{\alpha R} & \bar\lambda^{\dot\alpha}{}_R & \lambda^{\tilde a} \end{bmatrix}^T, \qquad M_{cd\hat\alpha} = \begin{bmatrix} \varepsilon_{abcd} & M_{cdI} & M_{cd} \end{bmatrix}, \\
& M_{abc\hat A} = \begin{bmatrix} \varepsilon_{abcd}\sigma^d{}_{\alpha\dot\beta}\bar\psi^{\dot\beta}{}_L & \varepsilon_{abcd}\bar\sigma^{d\dot\alpha\beta}\psi_{\beta L} & \varepsilon_{abcd}\sigma^d{}_{\alpha\dot\beta}\bar\psi^{\dot\beta}{}_R & \varepsilon_{abcd}\bar\sigma^{d\dot\alpha\beta}\psi_{\beta R} & M_{abc\tilde a} \end{bmatrix}.
\end{aligned}
$$

The matrices $C^{\hat\alpha}{}_{\hat\beta}$, $C^{\hat A}{}_{\hat B}$, $M_{\hat A\hat B}$, $Y_{\hat A\hat B\hat C}$, $L_{\hat A\hat B\hat C\hat D}$ and $T^{d\hat A}{}_{\hat B}$ are constant matrices, and carry the information about gauge coupling constants, mass of the Higgs field, Yukawa couplings and mixing angles, Higgs self-coupling constant and torsion coupling, respectively.

5 Conclusions

Let us summarize the results of the paper. In section 2 we have given a short reminder of the BF theory and described how one can use it to construct the action for general relativity (the well known Plebanski model), and the action for the Yang-Mills theory in flat spacetime, in a novel way. Passing on to higher gauge theory, we have reviewed the formalism of 2-groups and the corresponding $2BF$ theory, using it again to construct the action for general relativity (a model first described in [12]), and the unified action of general relativity and Yang-Mills theory, both naturally described using the 2-group formalism. With this background material in hand, in section 3 we have used the idea of a categorical ladder yet again, generalizing the $2BF$ theory to $3BF$ theory, with the underlying structure of a 3-group instead of a 2-group. This has led us to the main insight that the *scalar and fermion fields can be specified using a gauge group*, namely the third gauge group, denoted L, present in the 2-crossed module corresponding to a given 3-group. This has allowed us to single out specific gauge groups corresponding to the Klein-Gordon, Dirac, Weyl and Majorana fields, and to construct the relevant constrained $3BF$ actions that describe all these fields coupled to gravity in the standard way.

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The obtained results represent the fundamental building blocks for the construction of the complete Standard Model of elementary particles coupled to Einstein-Cartan gravity as a $3BF$ action with suitable simplicity constraints, as demonstrated in section 4. In this way, we can complete the first step of the spinfoam quantization programme for the complete theory of gravity and all matter fields, as specified in the Introduction. This is a clear improvement over the ordinary spinfoam models based on an ordinary constrained BF theory.

In addition to this, the gauge group which determines the matter spectrum of the theory is a completely novel structure, not present in the Standard Model. This new gauge group stems from the 3-group structure of the theory, so it is not surprising that it is invisible in the ordinary formulation of the Standard Model, since the latter does not use any 3-group structure in an explicit way. In this paper, we have discussed the choices of this group which give rise to all relevant matter fields, and these can simply be directly multiplied to give the group corresponding to the full Standard Model, encoding the quark and lepton families and all other structure of the matter spectrum. However, the true potential of the matter gauge group lies in a possibility of nontrivial unification of matter fields, by choosing it to be something other than the ordinary product of its component groups. For example, instead of choosing $\mathbb{R}^8(\mathbb{G})$ for the Dirac field, one can try a noncommutative SU(3) group, which also contains 8 generators, but its noncommutativity requires that the maps δ and $\{\_\,,\_\}$ be nontrivial, in order to satisfy the axioms of a 2-crossed module. This, in turn, leads to a distinction between 3-curvature and fake 3-curvature, which can have consequences for the dynamics of the theory. In this way, by studying nontrivial choices of a 3-group, one can construct various different 3-group-unified models of gravity and matter fields, within the context of higher gauge theory. This idea resembles the ordinary grand unification programme within the framework of the standard gauge theory, where one constructs various different models of vector fields by making various choices for the Yang-Mills gauge group. The detailed discussion of these 3-group unified models is left for future work.

As far as the spinfoam quantization programme is concerned, having completed the step 1 (as outlined in the Introduction), there is a clear possibility to complete the steps 2 and 3 as well. First, the fact that the full action is written completely in terms of differential forms of various degrees, allows us to adapt it to a triangulated spacetime manifold, in the sense of Regge calculus. In particular, all fields and their field strengths present in the $3BF$ action can be naturally associated to the appropriate d-dimensional simplices of a 4-dimensional triangulation, by matching 0-forms to vertices, 1-forms to edges, etc. This leads us to the following table:

d	triangulation	dual triangulation	form	fields	field strengths
0	vertex	4-polytope	0-form	ϕ, $\psi_{\tilde{\alpha}}$, $\bar{\psi}^{\tilde{\alpha}}$	
1	edge	3-polyhedron	1-form	ω^{ab}, A^I, e^a	
2	triangle	face	2-form	β^a, B^{ab}	R^{ab}, F^I, T^a
3	tetrahedron	edge	3-form	γ, $\gamma_{\tilde{\alpha}}$, $\bar{\gamma}^{\tilde{\alpha}}$	$\mathcal{G}^a$
4	4-simplex	vertex	4-form		$\mathcal{H}$, $\mathcal{H}_{\tilde{\alpha}}$, $\bar{\mathcal{H}}^{\tilde{\alpha}}$

Once the classical Regge-discretized topological $3BF$ action is constructed, one can attempt to construct a state sum Z which defines the path integral for the theory. The topological nature of the pure $3BF$ action, together with the underlying structure of the 3-group, should ensure that such a state sum Z is a topological invariant, in the sense that it is triangulation independent. Unfortunately, in order to perform this step precisely, one needs a generalization of the Peter-Weyl and Plancharel theorems to 2-groups and 3-groups, a mathematical result that is presently still missing. The purpose of the Peter-Weyl theorem is to provide a decomposition of a function on a group into a sum over the corresponding irreducible representations, which ultimately specifies the appropriate spectrum of labels for the d-simplices in the triangulation, fixing the domain of values for the fields living on those d-simplices. In the case of 2-groups and especially 3-groups, the representation theory has not been developed well enough to allow for such a construction, with a consequence of the missing Peter-Weyl theorem for 2-groups and 3-groups. However, until the theorem is proved, we can still try to *guess* the appropriate structure of the irreducible representations of the 2- and 3-groups, as was done for example in [12], leading to the so-called *spincube model* of quantum gravity.

Finally, if we remember that for the purpose of physics we are not really interested in a topological theory, but instead in one which contains local propagating degrees of freedom, we are therefore not really engaged in constructing a topological invariant Z, but rather a state sum which describes nontrivial dynamics. In particular, we need to impose the simplicity constraints onto the state sum Z, which is the step 3 of the spinfoam quantization programme. In light of that, one of the main motivations and also main results of our paper was to rewrite the action for gravity and matter in a way that explicitly distinguishes the topological sector from the simplicity constraints. Imposing the constraints is therefore straightforward in the context of a 3-group gauge theory, and completing this step would ultimately lead us to a state sum corresponding to a tentative theory of quantum gravity with matter. This is also a topic for future work.

In the end, let us also mention that aside from the unification and quantization programmes, there is also a plethora of additional studies one can perform with the constrained $3BF$ action, such as the analysis of the Hamiltonian structure of the theory (suitable for a potential canonical quantization programme), the idea of imposing the simplicity constraints using a spontaneous symmetry breaking mechanism, and finally a detailed study of the mathematical structure and properties of the simplicity constraints. This list is of course not conclusive, and there may be many more interesting related topics to study in both physics and mathematics.

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A Category theory, 2-groups and 3-groups

Definition 1 (Pre-crossed module and crossed module) *A pre-crossed module* $(H \stackrel{\partial}{\to} G\,, \rhd)$ *of groups G and H, is given by a group map $\partial : H \to G$, together with a left action $\rhd$ of G on H, by automorphisms, such that for each $h_1\,, h_2 \in H$ and $g \in G$ the following identity hold:*

$$g \partial h g^{-1} = \partial(g \rhd h)\,.$$

In a pre-crossed module the **Peiffer commutator** *is defined as:*

$$\langle h_1\,, h_2 \rangle_{\mathrm{p}} = h_1 h_2 h_1^{-1} \partial(h_1) \rhd h_2^{-1}\,.$$

A pre-crossed module is said to be a **crossed module** *if all of its Peiffer commutators are trivial, which is to say that*

$$(\partial h) \rhd h' = h h' h^{-1}\,,$$

i.e. the **Peiffer identity** *is satisfied.*

Definition 2 (2-crossed module) *A 2-crossed module* $(L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G, \rhd, \{-,-\})$ *is given by three groups G, H and L, together with maps ∂ and δ such that:*

$$L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G\,,$$

where $\partial\delta = 1$, an action $\rhd$ of the group G on all three groups, and an G-equivariant map called the **Peiffer lifting***:*

$$\{-\,,-\} : H \times H \to L\,.$$

The following identities are satisfied:

1. *The maps ∂ and δ are G-equivariant, i.e. for each $g \in G$ and $h \in H$:*

$$g \rhd \partial(h) = \partial(g \rhd h)\,, \qquad g \rhd \delta(l) = \delta(g \rhd l)\,,$$

the action of the group G on the groups H and L is a smooth left action by automorphisms, i.e. for each $g, g_1, g_2 \in G$, $h_1, h_2 \in H$, $l_1, l_2 \in L$ and $e \in H, L$:

$$g_1 \rhd (g_2 \rhd e) = (g_1 g_2) \rhd e\,, \quad g \rhd (h_1 h_2) = (g \rhd h_1)(g \rhd h_2)\,, \quad g \rhd (l_1 l_2) = (g \rhd l_1)(g \rhd l_2)\,,$$

and the Peiffer lifting is G-equivariant, i.e. for each h_1, $h_2 \in H$ and $g \in G$:

$$g \rhd \{h_1\,, h_2\} = \{g \rhd h_1,\, g \rhd h_2\}\,;$$

2. *the action of the group G on itself is via conjugation, i.e. for each $g\,, g_0 \in G$:*

$$g \rhd g_0 = g\, g_0\, g^{-1}\,;$$

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3. *In a* 2*-crossed module the structure* $(L \xrightarrow{\delta} H, \triangleright')$ *is a crossed module, with action of the group* H *on the group* L *is defined for each* $h \in H$ *and* $l \in L$ *as:*

$$h \triangleright' l = l\,\{\delta(l)^{-1},\, h\}\,,$$

but $(H \xrightarrow{\partial} G\,, \triangleright)$ *may not be one, and the Peiffer identity does not necessary hold. However, when* ∂ *is chosen to be trivial and group* H *Abelian, the Peiffer identity is satisfied, i.e. for each* $h,\, h' \in H$*:*

$$\delta(h) \triangleright h' = h\, h'\, h^{-1}\,;$$

4. $\delta(\{h_1, h_2\}) = \langle h_1\,, h_2\rangle_{\rm p}, \qquad \forall h_1, h_2 \in H,$
5. $[l_1, l_2] = \{\delta(l_1)\,, \delta(l_2)\}, \qquad \forall l_1\,, l_2 \in L.$ *Here, the notation* $[l,k] = lkl^{-1}k^{-1}$ *is used;*
6. $\{h_1 h_2, h_3\} = \{h_1, h_2 h_3 h_2^{-1}\}\partial(h_1) \triangleright \{h_2, h_3\}, \qquad \forall h_1, h_2, h_3 \in H;$
7. $\{h_1, h_2 h_3\} = \{h_1, h_2\}\{h_1, h_3\}\{\langle h_1, h_3\rangle_{\rm p}^{-1}, \partial(h_1) \triangleright h_2\}, \qquad \forall h_1, h_2, h_3 \in H;$
8. $\{\delta(l), h\}\{h, \delta(l)\} = l(\partial(h) \triangleright l^{-1}), \qquad \forall h \in H\,, \quad \forall l \in L.$

Definition 3 (Differential pre-crossed module, differential crossed module) *A differential pre-crossed module* $(\mathfrak{h} \xrightarrow{\partial} \mathfrak{g}\,, \triangleright)$ *of algebras* $\mathfrak{g}$ *and* $\mathfrak{h}$ *is given by a Lie algebra map* $\partial : \mathfrak{h} \to \mathfrak{g}$ *together with an action* $\triangleright$ *of* $\mathfrak{g}$ *on* $\mathfrak{h}$ *such that for each* $\underline{h} \in \mathfrak{h}$ *and* $\underline{g} \in \mathfrak{g}$*:*

$$\partial(\underline{g} \triangleright \underline{h}) = [\underline{g}, \partial(\underline{h})]\,.$$

The action $\triangleright$ *of* $\mathfrak{g}$ *on* $\mathfrak{h}$ *is on left by derivations, i.e. for each* $\underline{h}_1, \underline{h}_2 \in \mathfrak{h}$ *and each* $\underline{g} \in \mathfrak{g}$*:*

$$\underline{g} \triangleright [\underline{h}_1,\, \underline{h}_2] = [\underline{g} \triangleright \underline{h}_1,\, \underline{h}_2] + [\underline{h}_1,\, \underline{g} \triangleright \underline{h}_2]\,.$$

In a differential pre-crossed module, the Peiffer commutators are defined for each $\underline{h}_1, \underline{h}_2 \in \mathfrak{h}$ *as:*

$$\langle \underline{h}_1,\, \underline{h}_2\rangle_{\rm p} = [\underline{h}_1, \underline{h}_2] - \partial(\underline{h}_1) \triangleright \underline{h}_2\,.$$

The map $(\underline{h}_1,\, \underline{h}_2) \in \mathfrak{h} \times \mathfrak{h} \to \langle \underline{h}_1,\, \underline{h}_2\rangle_{\rm p} \in \mathfrak{h}$ *is bilinear* $\mathfrak{g}$*-equivariant map called the* **Peiffer paring***, i.e. all* $\underline{h}_1\,, \underline{h}_2 \in \mathfrak{h}$ *and* $\underline{g} \in \mathfrak{g}$ *satisfy the following identity:*

$$\underline{g} \triangleright \langle \underline{h}_1\,, \underline{h}_2\rangle_{\rm p} = \langle \underline{g} \triangleright \underline{h}_1\,, \underline{h}_2\rangle + \langle \underline{h}_1\,, \underline{g} \triangleright \underline{h}_2\rangle_{\rm p}\,.$$

A differential pre-crossed module is said to be a **differential crossed module** *if all of its Peiffer commutators vanish, which is to say that for each* $\underline{h}_1, \underline{h}_2 \in \mathfrak{h}$*:*

$$\partial(\underline{h}_1) \triangleright \underline{h}_2 = [\underline{h}_1,\, \underline{h}_2]\,.$$

Definition 4 (Differential 2-crossed module) *A differential* 2*-crossed module is given by a complex of Lie algebras:*

$$\mathfrak{l} \xrightarrow{\delta} \mathfrak{h} \xrightarrow{\partial} \mathfrak{g}\,,$$

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together with left action $\triangleright$ of $\mathfrak{g}$ on $\mathfrak{h}$, $\mathfrak{l}$, by derivations, and on itself via adjoint representation, and a $\mathfrak{g}$-equivariant bilinear map called the **Peiffer lifting***:*

$$\{-\,,\,-\}:\mathfrak{h}\times\mathfrak{h}\to\mathfrak{l}$$

Fixing the basis in algebra $T_A\in\mathfrak{l}$, $t_a\in\mathfrak{h}$ and $\tau_\alpha\in\mathfrak{g}$:

$$[T_A,T_B]=f_{AB}{}^C\,T_C\,,\qquad [t_a,t_b]=f_{ab}{}^c\,t_c\,,\qquad [\tau_\alpha,\tau_\beta]=f_{\alpha\beta}{}^\gamma\,\tau_\gamma\,,$$

one defines the maps ∂ and δ as:

$$\partial(t_a)=\partial_a{}^\alpha\,\tau_\alpha\,,\qquad \delta(T_A)=\delta_A{}^a\,t_a\,,$$

and action of $\mathfrak{g}$ on the generators of $\mathfrak{l}$, $\mathfrak{h}$ and $\mathfrak{g}$ is, respectively:

$$\tau_\alpha\triangleright T_A=\triangleright_{\alpha A}{}^B\,T_B\,,\qquad \tau_\alpha\triangleright t_a=\triangleright_{\alpha a}{}^b\,t_b\,,\qquad \tau_\alpha\triangleright\tau_\beta=\triangleright_{\alpha\beta}{}^\gamma\,\tau_\gamma\,.$$

Note that when η is $\mathfrak{g}$-valued differential form and ω is $\mathfrak{l}$, $\mathfrak{h}$ or $\mathfrak{g}$ valued differential form the previous action is defined as:

$$\eta\triangleright\omega=\eta^\alpha\wedge\omega^A\,\triangleright_{\alpha A}{}^B\,T_B\,,\qquad \eta\triangleright\omega=\eta^\alpha\wedge\omega^a\,\triangleright_{\alpha a}{}^b\,t_b\,,\qquad \eta\triangleright\omega=\eta^\alpha\wedge\omega^\beta f_{\alpha\beta}{}^\gamma\,\tau_\gamma\,.$$

The coefficients $X_{ab}{}^A$ are introduced as:

$$\{t_a,\,t_b\}=X_{ab}{}^A T_A\,.$$

The following identities are satisfied:

1. *In the differential crossed module $(L\xrightarrow{\delta}H\,,\triangleright')$ the action $\triangleright'$ of $\mathfrak{h}$ on $\mathfrak{l}$ is defined for each $\underline{h}\in\mathfrak{h}$ and $\underline{l}\in\mathfrak{l}$ as:*

   $$\underline{h}\triangleright'\underline{l}=-\{\delta(\underline{l}),\,\underline{h}\}\,,$$

   or written in the basis where $t_a\triangleright' T_A=\triangleright'{}_{aA}{}^B T_B$ the previous identity becomes:

   $$\triangleright'{}_{aA}{}^B=-\delta_A{}^b X_{ba}{}^B\,;$$

2. *The action of $\mathfrak{g}$ on itself is via adjoint representation:*

   $$\triangleright_{\alpha\beta}{}^\gamma=f_{\alpha\beta}{}^\gamma\,;$$

3. *The action of $\mathfrak{g}$ on $\mathfrak{h}$ and $\mathfrak{l}$ is equivariant, i.e. the following identities are satisfied:*

   $$\partial_a{}^\beta f_{\alpha\beta}{}^\gamma=\triangleright_{\alpha a}{}^b\partial_b{}^\gamma\,,\qquad \delta_A{}^a\,\triangleright_{\alpha a}{}^b=\triangleright_{\alpha A}{}^B\delta_B{}^b\,;$$

4. *The Peiffer lifting is $\mathfrak{g}$-equivariant, i.e. for each $\underline{h}_1,\underline{h}_2\in\mathfrak{h}$ and $\underline{g}\in\mathfrak{g}$:*

   $$\underline{g}\triangleright\{\underline{h}_1,\underline{h}_2\}=\{\underline{g}\triangleright\underline{h}_1,\underline{h}_2\}+\{\underline{h}_1,\,\underline{g}\triangleright\underline{h}_2\}\,,$$

   or written in the basis:

   $$X_{ab}{}^B\triangleright_{\alpha B}{}^A=\triangleright_{\alpha a}{}^c X_{cb}{}^A+\triangleright_{\alpha b}{}^c X_{ac}{}^A\,;$$

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5. $\delta(\{\underline{h}_1, \underline{h}_2\}) = \langle \underline{h}_1, \underline{h}_2 \rangle_{\mathrm{p}}$, $\quad \forall \underline{h}_1, \underline{h}_2 \in \mathfrak{h}$, *i.e.*

$$X_{ab}{}^A \delta_A{}^c = f_{ab}{}^c - \partial_a{}^\alpha \triangleright_{\alpha b}{}^c ;$$

6. $[\underline{l}_1, \underline{l}_2] = \{\delta(\underline{l}_1), \delta(\underline{l}_2)\}$, $\quad \forall \underline{l}_1, \underline{l}_2 \in \mathfrak{l}$, *i.e.*

$$f_{AB}{}^C = \delta_A{}^a \delta_B{}^b X_{ab}{}^C ;$$

7. $\{[\underline{h}_1, \underline{h}_2], \underline{h}_3\} = \partial(\underline{h}_1) \triangleright \{\underline{h}_2, \underline{h}_3\} + \{\underline{h}_1, [\underline{h}_2, \underline{h}_3]\} - \partial(\underline{h}_2) \triangleright \{\underline{h}_1, \underline{h}_3\} - \{\underline{h}_2, [\underline{h}_1, \underline{h}_3]\}$, $\forall \underline{h}_1, \underline{h}_2, \underline{h}_3 \in \mathfrak{h}$, *i.e.*

$$\{[\underline{h}_1, \underline{h}_2], \underline{h}_3\} = \{\partial(\underline{h}_1) \triangleright \underline{h}_2, \underline{h}_3\} - \{\partial(\underline{h}_2) \triangleright \underline{h}_1, \underline{h}_3\} - \{\underline{h}_1, \delta\{\underline{h}_2, \underline{h}_3\}\} + \{\underline{h}_2, \delta\{\underline{h}_1, q, \underline{h}_3\}\},$$

$$f_{ab}{}^d X_{dc}{}^B = \partial_a{}^\alpha X_{bc}{}^A \triangleright_{\alpha A}{}^B + X_{ad}{}^B f_{bc}{}^d - \partial_b{}^\alpha \triangleright_{\alpha A}{}^B X_{ac}{}^A - X_{bd}{}^B f_{ac}{}^d ;$$

8. $\{\underline{h}_1, [\underline{h}_2, \underline{h}_3]\} = \{\delta\{\underline{h}_1, \underline{h}_2\}, \underline{h}_3\} - \{\delta\{\underline{h}_1, \underline{h}_3\}, \underline{h}_2\}$, $\quad \forall \underline{h}_1, \underline{h}_2, \underline{h}_3 \in \mathfrak{h}$, *i.e.*

$$X_{ad}{}^A f_{bc}{}^d = X_{ab}{}^B \delta_B{}^d X_{dc}{}^A - X_{ac}{}^B \delta_B{}^d X_{db}{}^A ;$$

9. $\{\delta(\underline{l}), \underline{h}\} + \{\underline{h}, \delta(\underline{l})\} = -\partial(\underline{h}) \triangleright \underline{l}$, $\quad \forall \underline{l} \in \mathfrak{l}$, $\quad \forall \underline{h} \in \mathfrak{h}$, *i.e.*

$$\delta_A{}^a X_{ab}{}^B + \delta_A{}^a X_{ba}{}^B = -\partial_b{}^\alpha \triangleright_{\alpha A}{}^B .$$

Note that the property 6. implies that either trivial map δ or the trivial Peiffer lifting imply that L is an Abelian group. Conversely, if L is Abelian, property 6. implies that either the map δ or the Peiffer lifting is trivial, or both.

In the case of an Abelian group H and trivial map ∂, among the aforementioned properties the only non-trivial remaining are:

1. $\delta\{\underline{h}_1, \underline{h}_2\} = 0$, $\quad \forall \underline{h}_1, \underline{h}_2 \in \mathfrak{h}$;
2. $[\underline{l}_1, \underline{l}_2] = \{\delta(\underline{l}_1), \delta(\underline{l}_2)\}$, $\quad \forall \underline{l}_1, \underline{l}_2 \in \mathfrak{l}$;
3. $\{\delta(\underline{l}), \underline{h}\} = -\{\underline{h}, \delta(\underline{l})\}$, $\quad \forall \underline{h} \in \mathfrak{h}$, $\quad \forall \underline{l} \in \mathfrak{l}$.

A reader intrested in more details about 3-groups is referred to [25].

B The construction of gauge-invariant actions for $3BF$ theory

Symmetric bilinear invariant nondegenerate forms are defined as:

$$\langle T_A , T_B \rangle_{\mathfrak{l}} = g_{AB} , \qquad \langle t_a , t_b \rangle_{\mathfrak{h}} = g_{ab} , \qquad \langle \tau_\alpha , \tau_\beta \rangle_{\mathfrak{g}} = g_{\alpha\beta} .$$

They satisfy the following properties:

- $\langle \_ , \_ \rangle_{\mathfrak{g}}$ is G-invariant:

$$\langle g \tau_\alpha g^{-1} , g \tau_\beta g^{-1} \rangle_{\mathfrak{g}} = \langle \tau_\alpha , \tau_\beta \rangle_{\mathfrak{g}} , \quad \forall g \in G ;$$

- $\langle \_ , \_ \rangle_{\mathfrak{h}}$ is G-invariant:

$$\langle g \rhd t_a \,, g \rhd t_b \rangle_{\mathfrak{h}} = \langle t_a \,, t_b \rangle_{\mathfrak{h}} \,, \quad \forall g \in G \,,$$

  and, when $(H \stackrel{\partial}{\to} G \,, \rhd)$ is a crossed module, consequently H-invariant:

$$\langle h t_a h^{-1} \,, h t_b h^{-1} \rangle_{\mathfrak{h}} = \langle \partial(h) \rhd t_a \,, \partial(h) \rhd t_b \rangle_{\mathfrak{h}} = \langle t_a \,, t_b \rangle_{\mathfrak{h}} \,, \quad \forall h \in H \,;$$

- $\langle \_ , \_ \rangle_{\mathfrak{l}}$ is G-invariant:

$$\langle g \rhd T_A \,, g \rhd T_B \rangle_{\mathfrak{l}} = \langle T_A \,, T_B \rangle_{\mathfrak{l}} \,, \quad \forall g \in G \,,$$

  and in the case when the Peiffer lifting or the map δ is trivial consequently H-invariant:

$$\langle h \rhd' T_A \,, h \rhd' T_B \rangle_{\mathfrak{l}} = \langle T_A - \{\delta(T_A), h\} \,, T_B - \{\delta(T_B), h\} \rangle_{\mathfrak{l}} = \langle T_A \,, T_B \rangle_{\mathfrak{l}} \,, \quad \forall h \in H \,.$$

  From the H-invariance of $\langle \_ , \_ \rangle_{\mathfrak{l}}$ and properties of a crossed module $(L \stackrel{\delta}{\to} H \,, \rhd')$ follows L-invariance:

$$\langle l T_A l^{-1} \,, l T_B l^{-1} \rangle_{\mathfrak{l}} = \langle \delta(l) \rhd' T_A \,, \delta(l) \rhd' T_B \rangle_{\mathfrak{l}} = \langle T_A \,, T_B \rangle_{\mathfrak{l}} \,, \quad \forall l \in L \,.$$

From the invariance of the bilinear forms follows the existence of gauge-invariant topological $3BF$ action of the form:

$$S_{3BF} = \int_{\mathcal{M}_4} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} + \langle \mathcal{C} \wedge \mathcal{G} \rangle_{\mathfrak{h}} + \langle \mathcal{D} \wedge \mathcal{H} \rangle_{\mathfrak{l}} \,, \tag{B.1}$$

where $B \in \mathcal{A}^2(\mathcal{M}_4 \,, \mathfrak{g})$, $C \in \mathcal{A}^1(\mathcal{M}_4 \,, \mathfrak{h})$ and $D \in \mathcal{A}^0(\mathcal{M}_4 \,, \mathfrak{l})$ are Lagrange multipliers, and $\mathcal{F} \in \mathcal{A}^2(\mathcal{M}_4 \,, \mathfrak{g})$, $\mathcal{G} \in \mathcal{A}^3(\mathcal{M}_4 \,, \mathfrak{h})$ and $\mathcal{H} \in \mathcal{A}^4(\mathcal{M}_4 \,, \mathfrak{l})$ are curvatures defined as in (3.1). Written in the basis:

$$\begin{aligned}
&\mathcal{F} = \frac{1}{2} \mathcal{F}^{\alpha}{}_{\mu\nu} \tau_\alpha \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \,, \qquad \mathcal{G} = \frac{1}{3!} \mathcal{G}^{a}{}_{\mu\nu\rho} t_a \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho \,, \\
&\mathcal{H} = \frac{1}{4!} \mathcal{H}^{A}{}_{\mu\nu\rho\sigma} T_A \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho \wedge \mathrm{d}x^\sigma \,,
\end{aligned}$$

the coefficients are:

$$\begin{aligned}
\mathcal{F}^{\alpha}{}_{\mu\nu} &= \partial_\mu \alpha^\alpha{}_\nu - \partial_\nu \alpha^\alpha{}_\mu + f_{\beta\gamma}{}^{\alpha} \alpha^\beta{}_\mu \alpha^\gamma{}_\nu - \beta^a{}_{\mu\nu} \partial_a{}^{\alpha} \,, \\
\mathcal{G}^{a}{}_{\mu\nu\rho} &= \partial_\mu \beta^a{}_{\nu\rho} + \partial_\nu \beta^a{}_{\rho\mu} + \partial_\rho \beta^a{}_{\mu\nu} \\
&\quad + \alpha^\alpha{}_\mu \beta^b{}_{\nu\rho} \rhd_{\alpha b}{}^{a} + \alpha^\alpha{}_\nu \beta^b{}_{\rho\mu} \rhd_{\alpha b}{}^{a} + \alpha^\alpha{}_\rho \beta^b{}_{\mu\nu} \rhd_{\alpha b}{}^{a} - \gamma^A{}_{\mu\nu\rho} \delta_A{}^{a} \,, \\
\mathcal{H}^{A}{}_{\mu\nu\rho\sigma} &= \partial_\mu \gamma^A{}_{\nu\rho\sigma} - \partial_\nu \gamma^A{}_{\rho\sigma\mu} + \partial_\rho \gamma^A{}_{\sigma\mu\nu} - \partial_\sigma \gamma^A{}_{\mu\nu\rho} \\
&\quad + 2\beta^a{}_{\mu\nu} \beta^b{}_{\rho\sigma} X_{\{ab\}}{}^{A} - 2\beta^a{}_{\mu\rho} \beta^b{}_{\nu\sigma} X_{\{ab\}}{}^{A} + 2\beta^a{}_{\mu\sigma} \beta^b{}_{\nu\rho} X_{\{ab\}}{}^{A} \\
&\quad + \alpha^\alpha{}_\mu \gamma^B{}_{\nu\rho\sigma} \rhd_{\alpha B}{}^{A} - \alpha^\alpha{}_\nu \gamma^B{}_{\rho\sigma\mu} \rhd_{\alpha B}{}^{A} + \alpha^\alpha{}_\rho \gamma^B{}_{\sigma\mu\nu} \rhd_{\alpha B}{}^{A} - \alpha^\alpha{}_\sigma \gamma^B{}_{\mu\nu\rho} \rhd_{\alpha B}{}^{A} \,.
\end{aligned}$$

Note that the wedge product $A \wedge B$ when A is a 0-form and B is a p-form is defined as $A \wedge B = \frac{1}{p!} A B_{\mu_1 \dots \mu_p} \mathrm{d}x^{\mu_1} \wedge \dots \wedge x^{\mu_p}$.

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Given G-invariant symmetric non-degenerate bilinear forms in $\mathfrak{g}$ and $\mathfrak{h}$, one can define a bilinear antisymmetric map $\mathcal{T} : \mathfrak{h} \times \mathfrak{h} \to \mathfrak{g}$ by the rule:

$$\langle \mathcal{T}(\underline{h}_1, \underline{h}_2)\,, \underline{g} \rangle_{\mathfrak{g}} = -\langle \underline{h}_1, \underline{g} \rhd \underline{h}_2 \rangle_{\mathfrak{h}}, \qquad \forall \underline{h}_1, \underline{h}_2 \in \mathfrak{h}\,, \quad \forall \underline{g} \in \mathfrak{g}\,.$$

See [17] for more properties and the construction of $2BF$ invariant topological action using this map. To define $3BF$ invariant topological action one has to first define a bilinear antisymmetric map $\mathcal{S} : \mathfrak{l} \times \mathfrak{l} \to \mathfrak{g}$ by the rule:

$$\langle \mathcal{S}(\underline{l}_1, \underline{l}_2), \underline{g} \rangle_{\mathfrak{g}} = -\langle \underline{l}_1, \underline{g} \rhd \underline{l}_2 \rangle_{\mathfrak{l}}\,, \qquad \forall \underline{l}_1, \forall \underline{l}_2 \in \mathfrak{l}\,, \quad \forall \underline{g} \in \mathfrak{g}\,.$$

Note that $\langle \_\,, \_\rangle_{\mathfrak{g}}$ is non-degenerate and

$$\langle \underline{l}_1, \underline{g} \rhd \underline{l}_2 \rangle_{\mathfrak{l}} = -\langle \underline{g} \rhd \underline{l}_1, \underline{l}_2 \rangle_{\mathfrak{l}} = -\langle \underline{l}_2, \underline{g} \rhd \underline{l}_1 \rangle_{\mathfrak{l}}\,, \qquad \forall \underline{g} \in \mathfrak{g}, \quad \forall \underline{l}_1, \underline{l}_2 \in \mathfrak{l}\,.$$

Morever, given $g \in G$ and $\underline{l}_1, \underline{l}_2 \in \mathfrak{l}$ one has:

$$\mathcal{S}(g \rhd \underline{l}_1, g \rhd \underline{l}_2) = g\, \mathcal{S}(\underline{l}_1, \underline{l}_2)\, g^{-1}\,,$$

since for each $\underline{g} \in \mathfrak{g}$ and $\underline{l}_1, \underline{l}_2 \in \mathfrak{l}$:

$$\begin{aligned}\langle \underline{g}, g^{-1} \mathcal{S}(g \rhd \underline{l}_1\,, g \rhd \underline{l}_2) g \rangle_{\mathfrak{g}} &= \langle g \underline{g} g^{-1}, \mathcal{S}(g \rhd \underline{l}_1, g \rhd \underline{l}_2) \rangle_{\mathfrak{g}} \\ &= -\langle (g\, \underline{g}\, g^{-1}) \rhd g \rhd \underline{l}_1, g \rhd \underline{l}_2 \rangle_{\mathfrak{l}} \\ &= -\langle \underline{g} \rhd \underline{l}_1\,, \underline{l}_2 \rangle_{\mathfrak{l}} = \langle \underline{g}\,, \mathcal{S}(\underline{l}_1, \underline{l}_2) \rangle_{\mathfrak{g}}\,,\end{aligned}$$

where the following mixed relation has been used:

$$g \rhd (\underline{g} \rhd \underline{l}) = (g\, \underline{g}\, g^{-1}) \rhd g \rhd \underline{l}\,. \tag{B.2}$$

We thus have the following identity:

$$\mathcal{S}(\underline{g} \rhd \underline{l}_1, \underline{l}_2) + \mathcal{S}(\underline{l}_1, \underline{g} \rhd \underline{l}_2) = [\underline{g}, \mathcal{S}(\underline{l}_1, \underline{l}_2)]\,.$$

As far as the bilinear antisymmetric map $\mathcal{S} : l \times l \to g$, one can write it in the basis:

$$\mathcal{S}(T_A, T_B) = \mathcal{S}_{AB}{}^{\alpha} \tau_{\alpha}\,,$$

so that the defining relation for $\mathcal{S}$ becomes the relation:

$$\mathcal{S}_{AB}{}^{\alpha} g_{\alpha\beta} = -\rhd_{\alpha[B}{}^{C} g_{A]C}\,.$$

Given two $\mathfrak{l}$-valued forms η and ω, one can define a $\mathfrak{g}$-valued form:

$$\omega \wedge^{\mathcal{S}} \eta = \omega^A \wedge \eta^B \mathcal{S}_{AB}{}^{\alpha} \tau_{\alpha}\,.$$

Now one can define the transformations of the Lagrange multipliers under L-gauge transformations (3.15).

Further, to define the transformations of the Lagrange multipliers under H-gauge transformations one needs to define the bilinear map $\mathcal{X}_1 : \mathfrak{l} \times \mathfrak{h} \to \mathfrak{h}$ by the rule:

$$\langle \mathcal{X}_1(\underline{l},\, \underline{h}_1),\, \underline{h}_2 \rangle_{\mathfrak{h}} = -\langle \underline{l},\, \{\underline{h}_1,\, \underline{h}_2\} \rangle_{\mathfrak{l}}\,, \qquad \forall \underline{h}_1,\, \underline{h}_2 \in \mathfrak{h}\,, \quad \forall \underline{l} \in \mathfrak{l}\,,$$

and bilinear map $\mathcal{X}_2 : \mathfrak{l} \times \mathfrak{h} \to \mathfrak{h}$ by the rule:

$$\langle \mathcal{X}_2(\underline{l},\, \underline{h}_2),\, \underline{h}_1 \rangle_{\mathfrak{h}} = -\langle \underline{l},\, \{\underline{h}_1,\, \underline{h}_2\} \rangle_{\mathfrak{l}}\,, \qquad \forall \underline{h}_1,\, \underline{h}_2 \in \mathfrak{h}\,, \quad \forall \underline{l} \in \mathfrak{l}\,.$$

As far as the bilinear maps $\mathcal{X}_1$ and $\mathcal{X}_2$ one can define the coefficients in the basis as:

$$\mathcal{X}_1(T_A, t_a) = \mathcal{X}_{1Aa}{}^b\, t_b\,, \qquad \mathcal{X}_2(T_A, t_a) = \mathcal{X}_{2Aa}{}^b\, t_b\,.$$

When written in the basis the defining relations for the maps $\mathcal{X}_1$ and $\mathcal{X}_2$ become:

$$\mathcal{X}_{1Ab}{}^c g_{ac} = -X_{ba}{}^B g_{AB}\,, \qquad \mathcal{X}_{2Ab}{}^c g_{ac} = -X_{ab}{}^B g_{AB}\,.$$

Given $\mathfrak{l}$-valued differential form ω and $\mathfrak{h}$-valued differential form η, one defines a $\mathfrak{h}$-valued form as:

$$\omega \wedge^{\mathcal{X}_1} \eta = \omega^A \wedge \eta^a \mathcal{X}_{1Aa}{}^b t_b\,, \qquad \omega \wedge^{\mathcal{X}_2} \eta = \omega^A \wedge \eta^a \mathcal{X}_{2Aa}{}^b t_b\,.$$

Given any $g \in G$, $\underline{l} \in \mathfrak{l}$ and $\underline{h} \in \mathfrak{h}$ one has:

$$\mathcal{X}_1(g \triangleright \underline{l},\, g^{-1} \triangleright \underline{h}) = g \triangleright \mathcal{X}_1(\underline{l},\, \underline{h})\,, \qquad \mathcal{X}_2(g \triangleright \underline{l},\, g \triangleright \underline{h}) = g^{-1} \triangleright \mathcal{X}_2(\underline{l},\, \underline{h})\,,$$

since for each $\underline{h}_1, \underline{h}_2 \in \mathfrak{h}$ and $\underline{l} \in \mathfrak{l}$:

$$\begin{aligned}\langle \underline{h}_2,\, g^{-1} \triangleright \mathcal{X}_1(g \triangleright \underline{l},\, g \triangleright \underline{h}_1) \rangle_{\mathfrak{h}} &= \langle g \triangleright \underline{h}_2,\, \mathcal{X}_1(g \triangleright \underline{l},\, g \triangleright \underline{h}_1) \rangle_{\mathfrak{h}} = \langle g \triangleright \underline{l},\, \{g \triangleright \underline{h}_1,\, g \triangleright \underline{h}_2\} \rangle_{\mathfrak{l}} \\ \langle g \triangleright \underline{l},\, g \triangleright \{\underline{h}_1,\, \underline{h}_2\} \rangle_{\mathfrak{l}} &= \langle \underline{l},\, \{\underline{h}_1,\, \underline{h}_2\} \rangle_{\mathfrak{l}} = \langle \underline{h}_2,\, \mathcal{X}_1(l,\, \underline{h}_1) \rangle_{\mathfrak{h}}\,,\end{aligned}$$

and similarly for $\mathcal{X}_2$. Finaly, one needs to define a trilinear map $\mathcal{D} : \mathfrak{h} \times \mathfrak{h} \times \mathfrak{l} \to \mathfrak{g}$ by the rule:

$$\langle \mathcal{D}(\underline{h}_1,\, \underline{h}_2,\, \underline{l}),\, \underline{g} \rangle_{\mathfrak{g}} = -\langle \underline{l},\, \{\underline{g} \triangleright \underline{h}_1,\, \underline{h}_2\} \rangle_{\mathfrak{l}}\,, \qquad \forall \underline{h}_1,\, \underline{h}_2 \in \mathfrak{h}\,, \quad \forall \underline{l} \in \mathfrak{l}, \quad \forall \underline{g} \in \mathfrak{g}\,,$$

One can define the coefficients of the trilinear map as:

$$\mathcal{D}(t_a,\, t_b,\, T_A) = \mathcal{D}_{abA}{}^{\alpha} \tau_\alpha\,,$$

and the defining relation for the map $\mathcal{D}$ expressed in terms of coefficients becomes:

$$\mathcal{D}_{abA}{}^{\beta} g_{\alpha\beta} = - \triangleright_{\alpha a}{}^c X_{cb}{}^B g_{AB}\,.$$

Given two $\mathfrak{h}$-valued forms ω and η, and $\mathfrak{l}$-valued form ξ, the g-valued form is given by the formula:

$$\omega \wedge^{\mathcal{D}} \eta \wedge^{\mathcal{D}} \xi = \omega^a \wedge \eta^b \wedge \xi^A \mathcal{D}_{abA}{}^{\beta} \tau_\beta\,.$$

The following compatibility relation between the maps $\mathcal{X}_1$ and $\mathcal{D}$ hold:

$$\langle \mathcal{D}(\underline{h}_1,\, \underline{h}_2,\, \underline{l}),\, \underline{g} \rangle_{\mathfrak{g}} = \langle \mathcal{X}_1(\underline{l},\, \underline{g} \triangleright \underline{h}_1),\, \underline{h}_2 \rangle_{\mathfrak{h}}\,, \qquad \forall \underline{h}_1,\, \underline{h}_2 \in \mathfrak{h}\,, \quad \forall \underline{l} \in \mathfrak{l}, \quad \forall \underline{g} \in \mathfrak{g}\,, \qquad \text{(B.3)}$$

which one can prove valid from the defining relations in terms of the coefficients. One can demonstrate that for each $\underline{h}_1,\, \underline{h}_2 \in \mathfrak{h}$, $\underline{l} \in \mathfrak{l}$ and $g \in G$:

$$\mathcal{D}(g \rhd \underline{h}_1,\, g \rhd \underline{h}_2,\, g \rhd \underline{l}) = g\, \mathcal{D}(\underline{h}_1,\, \underline{h}_2,\, \underline{l})\, g^{-1}\,,$$

since for each $\underline{h}_1,\, \underline{h}_2 \in \mathfrak{h}$, $\underline{l} \in \mathfrak{l}$, $\underline{g} \in \mathfrak{g}$ and $g \in G$:

$$\begin{aligned}
\langle g^{-1}\mathcal{D}(g \rhd \underline{h}_1,\, g \rhd \underline{h}_2,\, g \rhd \underline{l})g,\, \underline{g}\rangle_{\mathfrak{g}} &= \langle \mathcal{D}(g \rhd \underline{h}_1,\, g \rhd \underline{h}_2,\, g \rhd \underline{l}),\, g\underline{g}g^{-1}\rangle_{\mathfrak{g}} \\
&= \langle \mathcal{X}_1(g \rhd \underline{l},\, g\underline{g}g^{-1} \rhd g \rhd \underline{h}_1),\, g \rhd \underline{h}_2\rangle_{\mathfrak{h}} \\
&= \langle \mathcal{X}_1(g \rhd \underline{l},\, g \rhd \underline{g} \rhd \underline{h}_1),\, g \rhd \underline{h}_2\rangle_{\mathfrak{h}} \\
&= \langle g \rhd \mathcal{X}_1(\underline{l},\, \underline{g} \rhd \underline{h}_1),\, g \rhd \underline{h}_2\rangle_{\mathfrak{h}} \\
&= \langle \mathcal{X}_1(\underline{l},\, \underline{g} \rhd \underline{h}_1),\, \underline{h}_2\rangle_{\mathfrak{h}} \\
&= \langle \mathcal{D}(\underline{h}_1,\, \underline{h}_2,\, \underline{l})\,,\underline{g}\rangle_{\mathfrak{g}}\,,
\end{aligned}$$

where the relation (B.2) and the compatibility relation (B.3) were used. We thus have for each $\underline{h}_1,\, \underline{h}_2 \in \mathfrak{h}$, $\underline{l} \in \mathfrak{l}$ and $\underline{g} \in \mathfrak{g}$ the following identity:

$$\mathcal{D}(\underline{g} \rhd \underline{h}_1,\, \underline{h}_2,\, \underline{l}) + \mathcal{D}(\underline{h}_1,\, \underline{g} \rhd \underline{h}_2,\, \underline{l}) + \mathcal{D}(\underline{h}_1,\, \underline{h}_2,\, \underline{g} \rhd \underline{l}) = [\underline{g},\, \mathcal{D}(\underline{h}_1,\, \underline{h}_2,\, \underline{l})]\,.$$

Now one can define the transformations of the Lagrange multipliers under H-gauge transformations as in (3.14).

C The equations of motion for the Weyl and Majorana fields

The action for the Weyl spinor field coupled to gravity is given by (3.72). The variation of this action with respect to the variables B_{ab}, λ^{ab}, γ_α, $\bar{\gamma}^{\dot\alpha}$, λ_α, $\bar{\lambda}^{\dot\alpha}$, ψ_α, $\bar{\psi}^{\dot\alpha}$, e^a, β^a and ω^{ab} one obtains the complete set of equations of motion, as follows:

$$\begin{aligned}
R^{ab} - \lambda^{ab} &= 0\,, \\
B_{ab} - \frac{1}{16\pi l_p^2}\varepsilon_{abcd}e^c \wedge e^d &= 0\,, \\
\nabla\psi_\alpha + \lambda_\alpha &= 0\,, \\
\nabla\bar{\psi}^{\dot\alpha} + \bar{\lambda}^{\dot\alpha} &= 0\,, \\
-\gamma_\alpha + \frac{i}{6}\varepsilon_{abcd}e^a \wedge e^b \wedge e^c \sigma^d{}_{\alpha\dot\beta}\bar{\psi}^{\dot\beta} &= 0\,, \\
-\bar{\gamma}^{\dot\alpha} + \frac{i}{6}\varepsilon_{abcd}e^a \wedge e^b \wedge e^c \bar{\sigma}^{d\dot\alpha\beta}\psi_\beta &= 0\,, \\
\nabla\gamma_\alpha - \frac{i}{6}\varepsilon_{abcd}e^a \wedge e^b \wedge e^c \sigma^d{}_{\alpha\dot\beta}\bar{\lambda}^{\dot\beta} &= 0\,, \\
\nabla\bar{\gamma}^{\dot\alpha} - \frac{i}{6}\varepsilon_{abcd}e^a \wedge e^b \wedge e^c \bar{\sigma}^{d\dot\alpha\beta}\lambda_\beta &= 0\,, \\
\nabla\beta_a + \frac{1}{8\pi l_p^2}\varepsilon_{abcd}\lambda^{bc} \wedge e^d + \frac{i}{2}\varepsilon_{abcd}e^b \wedge e^c \wedge (\bar{\lambda}_{\dot\alpha}\bar{\sigma}^{d\dot\alpha\beta}\psi_\beta + \lambda^\alpha \sigma^d{}_{\alpha\dot\beta}\bar{\psi}^{\dot\beta})& \\
-8\pi i l_p^2 \varepsilon_{abcd}e^b\beta^c\big(\psi^\alpha(\sigma^d)_{\alpha\dot\beta}\bar{\psi}^{\dot\beta}\big) &= 0\,,
\end{aligned}$$

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$$\nabla e_a - 4\pi l_p^2 \varepsilon_{abcd} e^b \wedge e^c \wedge (\bar{\psi}_{\dot{\alpha}} \bar{\sigma}^{d\dot{\alpha}\beta} \psi_\beta) = 0\,,$$
$$\nabla B_{ab} - e_{[a} \wedge \beta_{b]} - \frac{1}{2}\gamma \sigma^{ab}{}_\alpha{}^\beta \psi_\beta - \frac{1}{2}\bar{\gamma}_{\dot{\alpha}} \bar{\sigma}^{ab\dot{\alpha}}{}_{\dot{\beta}} \bar{\psi}^{\dot{\beta}} = 0\,.$$

In the case of the Majorana field, one adds the mass term (3.75) to the action (3.72). Then, the variation of the action with respect to B_{ab}, ψ^{ab}, γ^α, $\bar{\gamma}_{\dot{\alpha}}$, λ_α, $\bar{\lambda}^{\dot{\alpha}}$, ψ_α, $\bar{\psi}^{\dot{\alpha}}_I$, e^a, β^a and ω_{ab} gives the equations of motion for the Majorana case, as follows:

$$R^{ab} - \lambda^{ab} = 0\,,$$
$$B_{ab} - \frac{1}{16\pi l_p^2}\varepsilon_{abcd} e^c \wedge e^d = 0\,,$$
$$-\nabla \psi_\alpha + \lambda_\alpha = 0\,,$$
$$-\nabla \bar{\psi}^{\dot{\alpha}} + \lambda^{\dot{\alpha}} = 0\,,$$
$$\gamma^\alpha - \frac{i}{6}\varepsilon_{abcd} e^a \wedge e^b \wedge e^c \bar{\psi}_{\dot{\beta}} (\bar{\sigma}^d)^{\dot{\beta}\alpha} = 0\,,$$
$$\bar{\gamma}_{\dot{\alpha}} - \frac{i}{6}\varepsilon_{abcd} e^a \wedge e^b \wedge e^c \psi^\beta (\sigma^d)_{\beta\dot{\alpha}} = 0\,,$$
$$\nabla \gamma^\alpha + \frac{i}{6}\varepsilon_{abcd} \lambda^{\dot{\beta}} \wedge e^a \wedge e^b \wedge e^c (\sigma^d)^\alpha{}_{\dot{\beta}} - \frac{1}{6}\, m \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \psi^\alpha$$
$$-4i\pi l_p^2 \varepsilon_{abcd} e^a \wedge e^b \wedge \beta^c \bar{\psi}_{\dot{\beta}} (\bar{\sigma}^d)^{\dot{\beta}\alpha} = 0\,,$$
$$\nabla \bar{\gamma}_{\dot{\alpha}} + \frac{i}{6}\varepsilon_{abcd} \lambda_\beta \wedge e^a \wedge e^b \wedge e^c (\bar{\sigma}^d)_{\dot{\alpha}}{}^\beta - \frac{1}{6} m \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \psi_{\dot{\alpha}}$$
$$-4i\pi l_p^2 \varepsilon_{abcd} e^a \wedge e^b \wedge \beta^c \psi^\beta (\sigma^d)_{\beta\dot{\alpha}} = 0\,,$$
$$\nabla \beta^a + \frac{1}{8\pi l_p^2}\varepsilon_{abcd} \lambda^{bc} \wedge e^d + \frac{i}{2}\varepsilon_{abcd} \lambda_\alpha \wedge e^b \wedge e^c \bar{\psi}_{\dot{\beta}} (\bar{\sigma}^d)^{\dot{\beta}\alpha} + \frac{i}{2}\varepsilon_{abcd} \lambda^{\dot{\alpha}} \wedge e^b \wedge e^c \psi^\beta (\sigma^d)_{\beta\dot{\alpha}}$$
$$-\frac{1}{3} m \varepsilon_{abcd} e^b \wedge e^c \wedge e^d (\psi^\alpha \psi_\alpha + \bar{\psi}_{\dot{\alpha}} \bar{\psi}^{\dot{\alpha}}) - 8\pi i l_p^2 \varepsilon_{abcd} e^b \beta^c \big(\psi^\alpha (\sigma^d)_{\alpha\dot{\beta}} \bar{\psi}^{\dot{\beta}}\big) = 0\,,$$
$$\nabla e_a - 4i\pi l_p^2 \varepsilon_{abcd} e^b \wedge e^c \big(\psi^\alpha (\sigma^d)_{\alpha\dot{\beta}} \bar{\psi}^{\dot{\beta}}\big) = 0\,,$$
$$\nabla B_{ab} - e_{[a} \wedge \beta_{b]} - \frac{1}{2}\psi^\alpha (\sigma^{ab})_\alpha{}^\beta \gamma_\beta - \frac{1}{2}\bar{\psi}_{\dot{\alpha}} (\bar{\sigma}^{ab})^{\dot{\alpha}}{}_{\dot{\beta}} \bar{\gamma}^{\dot{\beta}} = 0\,.$$

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Entanglement-induced deviation from the geodesic motion in quantum gravity

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Abstract. We study the derivation of the effective equation of motion for a pointlike particle in the framework of quantum gravity. Just like the geodesic motion of a classical particle is a consequence of classical field theory coupled to general relativity, we introduce the similar notion of an effective equation of motion, but starting from an abstract quantum gravity description. In the presence of entanglement between gravity and matter, quantum effects give rise to modifications of the geodesic trajectory, primarily as a consequence of the interference between various coherent states of the gravity-matter system. Finally, we discuss the status of the weak equivalence principle in quantum gravity and its possible violation due to the nongeodesic motion.

Keywords: gravity, quantum field theory on curved space, quantum gravity phenomenology

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Contents

1 Introduction

The formulation of the theory of quantum gravity (QG) is one of the most fundamental open problems in modern theoretical physics. In models of QG, as in any quantum theory, superpositions of states are allowed. In a tentative "theory of everything", which includes both gravity and matter at a fundamental quantum level, superpositions of product gravity-matter states are particularly interesting. Entangled states are highly nonclassical, and as such are especially relevant because they give rise to a drastically different behavior of matter from what one would expect based on classical intuition, as confirmed by numerous examples from the standard quantum mechanics (QM). Therefore, it is interesting to study such states in the context of a QG coupled to matter, in particular the Schrödinger cat-like states. Moreover, a recent study [1] suggests that physically allowed states of a gravity-matter system are generically entangled due to gauge invariance, providing additional motivation for our study.

In standard QM, entanglement is generically a consequence of the interaction. Nevertheless, there exist situations which give rise to entanglement even without interaction. For example, the Pauli exclusion principle in the case of identical particles generates entanglement without an interaction, giving rise to an effective force (also called the "exchange interaction"). We investigate in detail whether an entanglement between gravity and matter could also be described as a certain type of an effective interaction, and if so, what are its aspects and details. In order to study this problem, we analyze the motion of a free test particle in a gravitational field. In general relativity (GR), this motion is described by a geodesic trajectory. However, we show that in the presence of the gravity-matter entanglement, the resulting effective interaction causes a deviation from a classical geodesic trajectory. In particular, we generalize the standard derivation of a geodesic equation from the case of classical gravity to the case of a full QG model, and derive the equation of motion for a particle which contains a non-geodesic term, reflecting the presence of the entanglement-induced effective interaction. The effects we discuss are purely quantum with respect to both gravity and matter, unlike previous studies of quantum matter in classical curved spacetime [2–5].

As a consequence of the modified equation of motion for a particle, we also discuss the status of the equivalence principle in the context of QG, and a possible violation of its weak flavor.

The paper is organized as follows. Section 2 is devoted to a review of the derivation of the geodesic equation in classical gravity, particularly in GR. The multipole formalism is employed and the geodesic equation for a particle is derived from the covariant conservation of the stress-energy tensor. In section 3 we generalize this procedure and derive our main results. Subsection 3.1 contains the general setup, the abstract quantum gravity framework that will be used, and the main assumptions. In subsection 3.2 we discuss the effective covariant conservation equation, which receives a correction to the classical one, due to the quantum gravity effects. In subsection 3.3 we put everything together and derive our main result — the effective equation of motion for a point particle, with the leading quantum correction. In subsection 3.4 we discuss the consistency of the assumptions that enter the approximation scheme used to derive the effective equation of motion. Section 4 is devoted to the discussion of the consequences of our results in the context of the weak equivalence principle. For the purpose of clarity, in subsection 4.1 we first provide the definitions of various flavors of the equivalence principle. Then, in subsection 4.2 we discuss the status of the equivalence principle in the context of quantum gravity and the results obtained in section 3. Subsection 4.3 provides further analysis of universality and equality between inertial and gravitational masses, in the context of the Newtonian approximation. Finally, section 5 contains our conclusions, discussion of the results and possible lines of further research. In the Appendix we give a short review of the multipole formalism used in the main text, with some mathematical details.

Our notation and conventions are as follows. We will work in the natural system of units in which $c = \hbar = 1$ and $G = l_p^2$, where l_p is the Planck length and G is the Newton's gravitational constant. By convention, the metric of spacetime will have the spacelike Lorentz signature $(-,+,+,+)$. The spacetime indices are denoted with lowercase Greek letters $\mu, \nu, \dots$ and take the values $0,1,2,3$. These can be split into the timelike index 0 and the spacelike indices denoted with lowercase Latin letters $i, j, k, \dots$ which take the values $1,2,3$. The Lorentz-invariant metric tensor is denoted as $\eta_{\mu\nu}$. Quantum operators always carry a hat, $\hat{\phi}(x)$, $\hat{g}(x)$, etc. The parentheses around indices indicate symmetrization with respect to those indices, while brackets indicate antisymmetrization:

$$A_{(\mu\nu)} \equiv \frac{1}{2}\left(A_{\mu\nu} + A_{\nu\mu}\right) , \qquad A_{[\mu\nu]} \equiv \frac{1}{2}\left(A_{\mu\nu} - A_{\nu\mu}\right) .$$

Finally, we will systematically denote the values of functions with parentheses, $f(x)$, while functionals will be denoted with brackets, $F[\phi]$.

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2 Geodesic equation in general relativity

In the context of the classical theories of gravity, like GR, the question of deriving the geodesic equation for a particle has initially been studied by Einstein, Infeld and Hoffmann [6], Mathisson [7], Lubánski [8], Fock [9], and others. Slightly later, the question was revisited in the seminal paper by Papapetrou [10], with generalizations followed by a number of authors [11–22], developing the so-called *multipole formalism*, see the appendix A. Recently, the multipole formalism has been reformulated in a manifestly covariant language and extended from pointlike objects to strings, membranes and further to p-branes, with general equations of motion studied in Riemann and Riemann-Cartan spaces [23–28]. Today, the multipole formalism and the resulting classes of effective equations of motion have found applications in a wide range of topics, from string theory [29] to cosmology [30] to blackbrane dynamics [31–33] to elasticity and the studies of the shape of red blood cells in biological systems [34].

In this section we will demonstrate the application of the multipole formalism in its crudest *single pole* approximation, and employ it to derive the geodesic equation of motion for a point particle in classical Riemannian spacetime. The results presented in this section are well known in the literature, and illustrate the derivation procedure of the geodesic motion for a point particle. After reviewing the standard results in this section, in section 3 the same procedure will be utilized to study the quantum gravity case.

The derivation procedure is based on two main assumptions. The first assumption is that the matter fields have internal dynamics such that they form particle-like kink solutions which are stable (i.e., non-decaying) across the spacetime regions under consideration. If that is the case, one can employ the multipole formalism and expand the stress-energy tensor into a series of derivatives of the Dirac δ function as (see the appendix A for details):

$$T^{\mu\nu}(x) = \int_{\mathcal{C}} d\tau \left[B^{\mu\nu}(\tau) \frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}} + \nabla_\rho \left(B^{\mu\nu\rho}(\tau) \frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}} \right) + \dots \right] . \tag{2.1}$$

Here we assume that the stress-energy tensor of matter fields has nonzero value only near some timelike curve $\mathcal{C}$ represented by parametric equations $x^\mu = z^\mu(\tau)$, where τ is a parameter counting the points along the curve $\mathcal{C}$. In that case, the B-coefficients in the δ series will be smaller and smaller with each new term in the series. We introduce a series of smallness scales for the coefficients,

$$B^{\mu\nu} \sim \mathcal{O}_0 \,, \qquad B^{\mu\nu\rho} \sim \mathcal{O}_1 \,, \qquad B^{\mu\nu\rho\sigma} \sim \mathcal{O}_2 \,, \qquad \dots$$

such that one can consider the multipole scales to behave as

$$\mathcal{O}_0 \gg \mathcal{O}_1 \gg \mathcal{O}_2 \gg \dots \tag{2.2}$$

Next we choose to work in the so-called *single pole* approximation, in which all quantities of order $\mathcal{O}_1$ and higher can be neglected. It is also assumed that the typical radius of curvature of spacetime near the curve $\mathcal{C}$ will be large enough not to interfere in the internal dynamics of the matter fields along $\mathcal{C}$ and break the kink configuration apart. Physically speaking, the sequence of inequalities (2.2) states that one can systematically approximate the full solution of the matter field equations of motion by neglecting various degrees of freedom which describe the "size" and "shape" of the kink compared to its orbital motion (i.e., motion along the curve $\mathcal{C}$). Given this setup, in the single pole approximation the matter

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fields are in a configuration that looks like a point particle traveling along a worldline curve $\mathcal{C}$, and terms of order $\mathcal{O}_1$ and higher can be dropped from the stress-energy tensor, giving:

$$T^{\mu\nu}(x) = \int_{\mathcal{C}} d\tau\, B^{\mu\nu}(\tau) \frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}} \,. \tag{2.3}$$

The second assumption is the validity of the local Poincaré invariance for the matter field equations. Namely, the classical action which describes the gravity-matter system can be generally written as

$$S[g, \phi] = S_G[g] + S_M[g, \phi] \,,$$

where g and ϕ denote gravitational and matter degrees of freedom, respectively, and it is generally considered to feature local Poincaré invariance. Our assumption is that the matter action S_M and the gravitational action S_G are invariant even taken separately. If this is the case, the Noether theorem gives us the covariant conservation of the stress-energy tensor of matter fields,

$$\nabla_\nu T^{\mu\nu} = 0 \,. \tag{2.4}$$

Taken together, assumptions (2.3) and (2.4) are sufficient to establish two results:

(a) that the parametric functions $z(\tau)$ of the curve $\mathcal{C}$ satisfy the geodesic equation,

$$\frac{d^2 z^\lambda(\tau)}{d\tau^2} + \varGamma^\lambda{}_{\mu\nu} \frac{dz^\mu(\tau)}{d\tau} \frac{dz^\nu(\tau)}{d\tau} = 0 \,, \tag{2.5}$$

where $\varGamma^\lambda{}_{\mu\nu}$ is the Christoffel connection for the background spacetime metric $g_{\mu\nu}$, and

(b) that the leading order coefficient $B^{\mu\nu}(\tau)$ in the stress-energy tensor for the particle has the form

$$B^{\mu\nu}(\tau) = m\, u^\mu(\tau) u^\nu(\tau) \,, \tag{2.6}$$

where $m \in \mathbb{R}\backslash\{0\}$ is an arbitrary constant parameter, while u^μ is the normalized tangent vector to the curve $\mathcal{C}$,

$$u^\mu \equiv \frac{dz^\mu(\tau)}{d\tau} \,, \qquad u^\mu u^\nu g_{\mu\nu} = -1 \,.$$

In order to demonstrate these two statements, we start from (2.4), contract it with an arbitrary test function $f_\mu(x)$ of compact support, and integrate over the whole spacetime,

$$\int_{\mathcal{M}_4} d^4x \sqrt{-g}\, f_\mu \nabla_\nu T^{\mu\nu} = 0 \,.$$

Then we perform the partial integration to move the covariant derivative from the stress-energy tensor to the test function. The boundary term vanishes since the test function has compact support, giving

$$\int_{\mathcal{M}_4} d^4x \sqrt{-g}\, T^{\mu\nu} \nabla_\nu f_\mu = 0 \,.$$

Then we substitute (2.3), switch the order of integrations and perform the integral over spacetime $\mathcal{M}_4$, ending up with

$$\int_{\mathcal{C}} d\tau B^{\mu\nu} \nabla_\nu f_\mu = 0 \,. \tag{2.7}$$

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The spacetime covariant derivative of the test function can be split into a component tangent to the curve $\mathcal{C}$ and a component orthogonal to it, in the following way. Using the identity

$$\delta^{\lambda}_{\mu} = -u^{\lambda}u_{\mu} + P^{\lambda}_{\perp\mu} \,, \tag{2.8}$$

where $-u^{\lambda}u_{\mu}$ and $P^{\lambda}_{\perp\mu}$ are projectors along u^{μ} and orthogonal to u^{μ}, respectively, we rewrite the derivative of f_{ν} as

$$\nabla_{\nu} f_{\mu} = -u_{\nu}\nabla f_{\mu} + f^{\perp}_{\nu\mu} \,, \tag{2.9}$$

where $\nabla \equiv u^{\lambda}\nabla_{\lambda}$ is the covariant derivative in the direction of the curve $\mathcal{C}$, while $f^{\perp}_{\nu\mu} \equiv P^{\lambda}_{\perp\nu}\nabla_{\lambda} f_{\mu}$ is a quantity orthogonal to the curve $\mathcal{C}$ with respect to its first index. Substituting (2.9) into (2.7), and performing another partial integration, we find

$$\int_{\mathcal{C}} d\tau \Big[f_{\mu}\nabla(B^{\mu\nu}u_{\nu}) + B^{\mu\nu} f^{\perp}_{\nu\mu} \Big] = 0 \,,$$

where the boundary term again vanishes due to the compact support of the test function.

Given that the values of f_{μ} and $f^{\perp}_{\nu\mu}$ are both arbitrary and mutually independent along the curve $\mathcal{C}$, the coefficients multiplying them must each be zero. The first term gives us

$$\nabla(B^{\mu\nu}u_{\nu}) = 0 \,, \tag{2.10}$$

while the second term, knowing that $f^{\perp}_{\nu\mu}$ is orthogonal to the curve $\mathcal{C}$ in its first index, gives

$$B^{\mu\nu} P^{\lambda}_{\perp\nu} = 0 \,. \tag{2.11}$$

Focus first on (2.11). Knowing that $B^{\mu\nu}$ is symmetric, we can use (2.8) to decompose it into orthogonal and parallel components with respect to its two indices,

$$B^{\mu\nu} = B^{\mu\nu}_{\perp} + B^{\mu}_{\perp}u^{\nu} + B^{\nu}_{\perp}u^{\mu} + Bu^{\mu}u^{\nu} \,,$$

where $B^{\mu\nu}_{\perp}$, $B^{\mu}_{\perp}$ and B are unknown coefficients, the first two being orthogonal to the curve $\mathcal{C}$ in all their indices. Substituting this expansion into (2.11), one finds that

$$B^{\mu\nu}_{\perp} = 0 \,, \qquad B^{\mu}_{\perp} = 0 \,,$$

leaving the scalar B as the only nonzero component of $B^{\mu\nu}$. Changing the notation from B to m, one obtains

$$B^{\mu\nu}(\tau) = m(\tau)u^{\mu}u^{\nu} \,. \tag{2.12}$$

This equation looks very similar to (2.6) but is still not equivalent to it, since the coefficient $m(\tau)$ is still not known to be a constant.

Next, focus on (2.10). Substituting (2.12), it reduces to

$$\nabla(mu^{\mu}) = 0 \,. \tag{2.13}$$

Projecting onto the tangent direction u_{μ} and using the identity $u_{\mu}\nabla u^{\mu} = 0$, one obtains

$$\nabla m \equiv \frac{dm}{d\tau} = 0 \,, \tag{2.14}$$

establishing that the parameter m is actually a constant. Given this, equation (2.13) reduces to

$$\nabla u^{\mu} = 0 \,. \tag{2.15}$$

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Remembering that $\nabla \equiv u^\lambda \nabla_\lambda$ and expanding the covariant derivative, we see that this is the geodesic equation (2.5). Finally, (2.14) and (2.12) together give (2.6), which completes the proof of statements (a) and (b).

There are three general remarks one should make regarding the above procedure. The first remark is about the physical interpretation and properties of the free parameter m. Namely, it can be given the interpretation of the total mass of the particle — substituting (2.6) into the stress-energy tensor (2.3) and integrating the T^{00} component over the volume of the spatial hypersurface orthogonal to u^μ, one can easily verify that the total rest-energy of the matter fields at a given time is equal to m. Note, however, that the sign of m is not fixed to be positive. This is not surprising, since the covariant conservation equation (2.4) and the stress-energy tensor (2.3) do not contain any information (or assumption) about the positivity of energy. Instead, the positive energy condition $m > 0$ has to be established from the full matter field equations, which take into account the internal dynamics of the matter fields that make up the particle.

The second remark is about the metric $g_{\mu\nu}$ of the background geometry. When discussing the motion of a particle, the background geometry is usually assumed to be fixed, and backreaction of the gravitational field of the particle itself is not taken into account, leading to the notion of a "test particle". However, ignoring the backreaction is not a necessary assumption. Namely, one can take the full stress-energy tensor of the matter fields which form the kink solution (as opposed to the approximate single pole stress-energy tensor (2.3)), put it as a source into the Einstein's field equations and solve for the metric $g_{\mu\nu}$. The resulting metric does include the backreaction, and can then be reinserted into the geodesic equation for the particle. Note that this procedure is self-consistent, since the geodesic motion of the particle is a consequence of the covariant conservation equation (2.4) which is in turn itself a consequence of Einstein's field equations. Also note that the metric $g_{\mu\nu}$ obtained in this way does not necessarily give rise to the black hole geometry in the neighborhood of the particle. This is because the Schwarzschild radius of the kink may be (and usually is) much smaller than the scale $\mathcal{O}_1$ which defines the precision of the single pole approximation (2.3). A simple example would be the motion of a planet around the Sun — in the single pole approximation, the radius of the planet (itself far larger than the planet's gravitational radius) is considered to be of the order $\mathcal{O}_1$ and the planet is treated as a pointlike object, but the spacetime metric used in the geodesic equation can still take into account the planet's gravitational field in addition to the field of the Sun.

The third remark is about going beyond the single pole approximation. This has been studied in detail in the literature [10–21, 25–28], so here we merely point out the main physical interpretation. Namely, keeping the second term in the multipole expansion (2.1) physically amounts to giving the particle a nonzero "thickness", in the sense that its internal angular momentum can be considered nonzero. In the resulting equation of motion for the particle, this angular momentum couples to the spacetime curvature tensor, giving rise to a deviation from the geodesic motion. This can intuitively be understood as an effect of tidal forces acting across the scale of the kink's width, pushing it off the geodesic trajectory. Similarly, including quadrupole and higher order terms in (2.1) takes into account additional internal degrees of freedom of the kink, which also couple to spacetime geometry and produce a further deviation from geodesic motion.

The above review of the multipole formalism, and its application to the derivation of the geodesic equation in GR, will be used in the next section to discuss the corrections to the motion of a particle stemming from quantum gravity. As we shall see, these quantum corrections will give rise to additional terms in the effective equation of motion for a particle, pushing it slightly off the geodesic trajectory, even in the single pole approximation.

3 Geodesic equation in quantum gravity

In this section we discuss the motion of a particle within the framework of quantum gravity. The exposition is structured into four parts — first, we introduce the abstract quantum gravity formalism, and give some technical details about the description of the states. In the second part, we discuss the quantum version of the covariant conservation equation of the stress-energy tensor. In the third part we adapt the derivation presented in section 2 to the quantum formalism, and obtain the effective equation of motion for the particle. Finally, in the fourth part we discuss the self-consistency assumptions that go into the calculation.

3.1 Preliminaries and the setup

We work in the so-called generic abstract quantum gravity setup, as follows. Starting from the Heisenberg picture for the description of quantum systems, we assume that gravitational degrees of freedom are described by some gravitational field operators $\hat{g}(x)$, while matter degrees of freedom are described by matter field operators $\hat{\phi}(x)$, where x represents the coordinates of some point on a 4-dimensional spacetime manifold $\mathcal{M}_4$. Both sets of operators have their corresponding canonically conjugate momentum operators, $\hat{\pi}_g(x)$ and $\hat{\pi}_\phi(x)$, such that the usual canonical commutation relations hold. The total (kinematical) Hilbert space of the theory is $\mathcal{H}_{\text{kin}} = \mathcal{H}_G \otimes \mathcal{H}_M$, where the gravitational and matter Hilbert spaces $\mathcal{H}_G$ and $\mathcal{H}_M$ are spanned by the bases of eigenvectors for the operators $\hat{g}$ and $\hat{\phi}$, respectively. The total state of the system, $|\Psi\rangle \in \mathcal{H}_{\text{kin}}$, does not depend on x, in line with the Heisenberg picture framework.

There are several important points that need to be emphasized regarding the above setup. First, we do not explicitly state what are the fundamental degrees of freedom $\hat{g}$ for the gravitational field. They can be chosen in many different ways, giving rise to different models of quantum gravity. Since we aim to present the analysis of geodesic motion which is model-independent, we refrain from specifying what are the fundamental degrees of freedom $\hat{g}$. Instead, we merely assume that the operators describing the spacetime geometry, i.e., the metric, connection, curvature, etc., depend somehow on $\hat{g}$ and $\hat{\pi}_g$, and are expressible as operator functions in terms of them:

$$\hat{g}_{\mu\nu} = \hat{g}_{\mu\nu}(\hat{g}, \hat{\pi}_g)\,, \qquad \hat{\Gamma}^\lambda{}_{\mu\nu} = \hat{\Gamma}^\lambda{}_{\mu\nu}(\hat{g}, \hat{\pi}_g)\,, \qquad \hat{R}^\lambda_{\mu\nu\rho} = \hat{R}^\lambda_{\mu\nu\rho}(\hat{g}, \hat{\pi}_g)\,, \qquad \dots$$

When discussing these geometric operators, for simplicity we will usually not explicitly write their $(\hat{g}, \hat{\pi}_g)$-dependence.

Second, in order for any operator function to be well defined, some operator ordering has to be assumed. However, since we aim to work in an abstract model-independent QG formalism, we do not choose any particular ordering, but merely assume that one such ordering has been fixed. In a similar fashion, we also simply assume that all operators and spaces are well defined, convergent, and otherwise specified in enough mathematical detail to have a well defined and unique QG model. In a nutshell, our calculations are formal, in the sense that one should be able to repeat them in a detailed fashion if one is given a specific model of QG. This also means that our analysis and results should not depend on any of these details, but are rather common to a large class of QG models, and are based only on very few assumptions given above.

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Third, we employ a natural distinction between gravitational and matter degrees of freedom. Namely, whereas geometric operators such as metric, curvature, and so on, depend only on $\hat{g}$ and $\hat{\pi}_g$, matter operators like field strengths, stress-energy tensor, etc., will generically be operator functions of both $\hat{g}$, $\hat{\pi}_g$, and the fundamental matter degrees of freedom $\hat{\phi}$ and $\hat{\pi}_\phi$. In other words, we assume that the separation between gravity and matter present in the classical theory, described by an action of the form

$$S_{\text{total}}[g,\phi] = S_{\text{gravity}}[g] + S_{\text{matter}}[g,\phi] \,,$$

remains present also in the full quantum regime. That is to say, we assume that one can construct a theory of quantum gravity without matter fields, using only gravitational degrees of freedom g, so that this theory gives sourceless Einstein's equations of GR in the classical limit. Once such a pure-QG model has been constructed, we assume one can couple matter ϕ to it without changing the structure of the gravitational sector, obtaining the full QG model which features Einstein's equations with appropriate matter sources in the classical limit. While we do not consider this to be a strong assumption, we feel that it is nevertheless important to spell it out explicitly, since there may exist some QG models which fail to satisfy it, and our analysis may be inapplicable to such models.

After the introduction of the above conceptual setup, we turn to some more practical details. For the purpose of discussing geodesic motion, we are mostly interested in the effective classical theory of the abstract QG introduced above. To that end, the main objects of attention are *classical states* of gravity and matter, denoted by $|\Psi\rangle \in \mathcal{H}_G \otimes \mathcal{H}_M$. By classical, we mean that the "effective classical" values for the metric tensor and the matter stress-energy tensor, given by the expectation values of the corresponding operators

$$g_{\mu\nu} = \langle \Psi | \hat{g}_{\mu\nu} | \Psi \rangle \,, \qquad T_{\mu\nu} = \langle \Psi | \hat{T}_{\mu\nu} | \Psi \rangle \tag{3.1}$$

satisfy classical Einstein equations of the GR. A recent study suggests that physical states of gravity and matter are generically entangled [1]. For our analysis, we do not need to assume that the overall gravity-matter state is separable, and thus we will work with a generic state $|\Psi\rangle$ (see appendix B for the discussion of the separable case).

For the purpose of our paper, we will consider a *toy example state*, defined as

$$|\mathbf{\Psi}\rangle = \alpha|\Psi\rangle + \beta|\tilde{\Psi}\rangle \,, \tag{3.2}$$

where $|\tilde{\Psi}\rangle$ is some other classical state analogous to $|\Psi\rangle$, but giving different expectation values for the classical metric and stress-energy tensors:

$$\tilde{g}_{\mu\nu} = \langle \tilde{\Psi} | \hat{g}_{\mu\nu} | \tilde{\Psi} \rangle \,, \qquad \tilde{T}_{\mu\nu} = \langle \tilde{\Psi} | \hat{T}_{\mu\nu} | \tilde{\Psi} \rangle \,. \tag{3.3}$$

One can see that our toy-example state (3.2) is a Schrödinger-cat type of state, describing a coherent superposition of two classical configurations of gravitational and matter fields. It will become evident later on that qualitative conclusions of the paper do not depend on the fact that (3.2) has precisely two terms in the sum. Choosing the state with three, four or more terms will lead to analogous conclusions, although quantitative details of the computation may become technically more involved.

Given that (3.2) is a Schrödinger-cat type of state, there are some phenomenological restrictions on the values of the independent parameters β and $S \equiv \langle \Psi | \tilde{\Psi} \rangle$. Namely, in the ordinary experimental situations we basically never observe this kind of states, which means that the overall entangled state $|\boldsymbol{\Psi}\rangle$ looks pretty much like a classical state, say the state $|\Psi\rangle$. In other words, we want the fidelity between these two states to be large, $F(|\Psi\rangle, |\boldsymbol{\Psi}\rangle) = |\langle\Psi|\boldsymbol{\Psi}\rangle| \approx 1$. From (3.2) we obtain

$$\langle\Psi|\boldsymbol{\Psi}\rangle = \alpha + \beta S \equiv \kappa\,.$$

Define $|\Psi^\perp\rangle$, such that

$$|\tilde{\Psi}\rangle = S|\Psi\rangle + \epsilon|\Psi^\perp\rangle\,,$$

$\langle\Psi|\Psi^\perp\rangle = 0$ and $\epsilon = \sqrt{1-|S|^2}$. Thus,

$$F^2 = |\langle\Psi|\boldsymbol{\Psi}\rangle|^2 = 1 - \eta^2\,, \tag{3.4}$$

where we introduce the small parameter

$$\eta \equiv \beta\epsilon\,.$$

Here, we have used the normalization condition for the entangled state (3.2),

$$\langle\boldsymbol{\Psi}|\boldsymbol{\Psi}\rangle = \alpha^2 + \beta^2 + 2\alpha\beta\,\mathrm{Re}(S) = 1\,.$$

Given the above definitions for κ and η, we can rewrite the total state (3.2) as

$$|\boldsymbol{\Psi}\rangle = \kappa|\Psi\rangle + \eta|\Psi^\perp\rangle\,, \tag{3.5}$$

where $|\kappa|^2 = F^2 = 1 - \eta^2$. The physical requirement of large fidelity implies that we study the limit $|\kappa| \approx 1$, $\eta \to 0$. We will therefore systematically expand the expectation values of all operators into power series in η, up to order $\mathcal{O}(\eta^2)$.

At this point we can evaluate the expectation values for the metric and stress-energy operators in the state (3.5), obtaining

$$\boldsymbol{g}_{\mu\nu} = \langle\boldsymbol{\Psi}|\hat{g}_{\mu\nu}|\boldsymbol{\Psi}\rangle = (1-\eta^2)g_{\mu\nu} + \eta^2\langle\Psi^\perp|\hat{g}_{\mu\nu}|\Psi^\perp\rangle + 2\eta\,\mathrm{Re}\left(\kappa\langle\Psi^\perp|\hat{g}_{\mu\nu}|\Psi\rangle\right)\,, \tag{3.6}$$

$$\boldsymbol{T}_{\mu\nu} = \langle\boldsymbol{\Psi}|\hat{T}_{\mu\nu}|\boldsymbol{\Psi}\rangle = (1-\eta^2)T_{\mu\nu} + \eta^2\langle\Psi^\perp|\hat{T}_{\mu\nu}|\Psi^\perp\rangle + 2\eta\,\mathrm{Re}\left(\kappa\langle\Psi^\perp|\hat{T}_{\mu\nu}|\Psi\rangle\right)\,. \tag{3.7}$$

It is easy to see that interference terms from the above expressions are generically nonvanishing. Indeed, even if, say, $\kappa\langle\Psi^\perp|\hat{g}_{\mu\nu}|\Psi\rangle$ were purely imaginary, a simple change of relative phase between $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$ would give rise to a nontrivial real part. Namely, given a fixed choice of $|\tilde{\Psi}\rangle$, the set of choices for $|\Psi\rangle$ for which the interference term is purely imaginary is of measure zero compared to the full set of possible phase shifts of $|\Psi\rangle$. An analogous argument applies for $\kappa\langle\Psi^\perp|\hat{T}_{\mu\nu}|\Psi\rangle$ as well. For a detailed analysis, see appendix C.

Let us denote the metric and stress-energy interference terms as $\bar{g}_{\mu\nu}$ and $\bar{T}_{\mu\nu}$, respectively. Since we want to expand (3.6) and (3.7) into power series in η up to linear order, we can write

$$\bar{g}_{\mu\nu} \equiv 2\,\mathrm{Re}\left(\kappa\langle\Psi^\perp|\hat{g}_{\mu\nu}|\Psi\rangle\right) = h_{\mu\nu} + \mathcal{O}(\eta)\,, \tag{3.8}$$

$$\bar{T}_{\mu\nu} \equiv 2\,\mathrm{Re}\left(\kappa\langle\Psi^\perp|\hat{T}_{\mu\nu}|\Psi\rangle\right) = t_{\mu\nu} + \mathcal{O}(\eta)\,. \tag{3.9}$$

Here, $h_{\mu\nu}$ and $t_{\mu\nu}$ are η-independent parts of $\bar{g}_{\mu\nu}$ and $\bar{T}_{\mu\nu}$. Thus, we can finally write:

$$\boldsymbol{g}_{\mu\nu} = g_{\mu\nu} + \eta\,h_{\mu\nu} + \mathcal{O}(\eta^2)\,, \tag{3.10}$$

$$\boldsymbol{T}_{\mu\nu} = T_{\mu\nu} + \eta\,t_{\mu\nu} + \mathcal{O}(\eta^2)\,. \tag{3.11}$$

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In what follows, we will refer to the classical state $|\Psi\rangle$ as the *dominant state*, while the other classical state $|\tilde{\Psi}\rangle$ will be called the *sub-dominant state*. To justify this terminology, recall the above requirement (3.4) that the overall entangled state $|\boldsymbol{\Psi}\rangle$ looks like the classical state $|\Psi\rangle$, i.e., $F^2 = 1 - \eta^2$, with the parameter $\eta \equiv \beta\epsilon$ being small. Therefore, in the case $\beta \to 0$ and ϵ finite, the state $|\tilde{\Psi}\rangle$ enters (3.2) with a very small contribution, and is thus sub-dominant. On the other hand, in the case when β is finite and $\epsilon \to 0$, the states $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$ are essentially indistinguishable, and their roles can be exchanged, as either can be considered sub-dominant to the other. By convention, we choose $|\tilde{\Psi}\rangle$ to again play the role of the sub-dominant state.

While in any quantum theory entangled states are allowed, note that when considering a product state of the gravity-matter system (i.e., the case $\eta = 0$), there is a danger that such a state may fail to be gauge invariant, as argued in [1]. So we need to introduce at least a small sub-dominant state, in order to ensure the gauge invariance of the total state. The simplest possible candidate state which describes the classical physics sufficiently well, and simultaneously stands a chance of being gauge invariant, is the genuinely entangled state (3.2), with $\beta \neq 0$ and $|\tilde{\Psi}\rangle \neq |\Psi\rangle$, leading to η being very small, but nonzero.

Regarding the effective entangled metric and stress-energy tensors (3.10) and (3.11), it is important to stress that they do not satisfy classical Einstein's equations of GR. Namely, we assume that Einstein's equations are separately satisfied by the metric and stress-energy tensors (3.1) coming from the classical state $|\Psi\rangle$, and by the metric and stress-energy tensors (3.3) coming from the other classical state $|\tilde{\Psi}\rangle$, as two different classical solutions:

$$R_{\mu\nu}(g) - \frac{1}{2} g_{\mu\nu} R(g) = 8\pi l_p^2 \, T_{\mu\nu} \,, \qquad R_{\mu\nu}(\tilde{g}) - \frac{1}{2} \tilde{g}_{\mu\nu} R(\tilde{g}) = 8\pi l_p^2 \, \tilde{T}_{\mu\nu} \,.$$

However, due to the nonlinearity of Einstein's equations, and due to the presence of the interference terms $h_{\mu\nu}$ and $t_{\mu\nu}$ in (3.10) and (3.11), quantities $\boldsymbol{g}_{\mu\nu}$ and $\boldsymbol{T}_{\mu\nu}$ do not satisfy Einstein's equations, as long as $\eta \neq 0$. This leads us to the following physical interpretation. First, it is natural to expand all quantities as corrections to the dominant classical configuration $(g_{\mu\nu}, T_{\mu\nu})$, including the equation of motion for a point particle. Second, as we shall see in the remainder of the text, given that $(\boldsymbol{g}_{\mu\nu}, \boldsymbol{T}_{\mu\nu})$ contains quantum gravity corrections through the interference terms, the presence of these quantum corrections in (3.10) and (3.11) will introduce an "effective force" term into the effective equation of motion for the particle. Finally, this effective force term will be pushing the particle off the geodesic trajectory defined by the classical dominant metric $g_{\mu\nu}$.

3.2 Effective covariant conservation equation

After the discussion of the general QG setup and the state (3.2), we move on to the discussion of the quantum analog of the covariant conservation equation (2.4). As in the classical theory, our basic assumption is that the matter sector of our QG model features local Poincaré invariance, i.e., that this symmetry is preserved at the quantum level. This assumption gives rise to a Gupta-Bleuler-like condition on the physical states, in the form

$$\langle \boldsymbol{\Psi} | \hat{\nabla}_\nu \hat{T}^{\mu\nu} | \boldsymbol{\Psi} \rangle = 0 \,, \tag{3.12}$$

where $\hat{\nabla}_\mu$ is the covariant derivative operator, defined by promoting the metric appearing in the Christoffel symbols into a corresponding operator. In general, the action of the stress-energy operator on the state $|\boldsymbol{\Psi}\rangle$ can be written[1] as

$$\hat{T}^{\mu\nu}|\boldsymbol{\Psi}\rangle = \boldsymbol{T}^{\mu\nu}|\boldsymbol{\Psi}\rangle + \boldsymbol{\Delta T}^{\mu\nu}|\boldsymbol{\Psi}^{\perp}\rangle\,, \tag{3.13}$$

where $\boldsymbol{T}^{\mu\nu}$ and $\boldsymbol{\Delta T}^{\mu\nu}$ are the expectation value and the uncertainty of the operator $\hat{T}^{\mu\nu}$ in the state $|\boldsymbol{\Psi}\rangle$, respectively,

$$\boldsymbol{T}^{\mu\nu} \equiv \langle\boldsymbol{\Psi}|\hat{T}^{\mu\nu}|\boldsymbol{\Psi}\rangle\,, \qquad \boldsymbol{\Delta T}^{\mu\nu} \equiv \sqrt{\langle\boldsymbol{\Psi}|\left(\hat{T}^{\mu\nu}\right)^2|\boldsymbol{\Psi}\rangle - \left(\langle\boldsymbol{\Psi}|\hat{T}^{\mu\nu}|\boldsymbol{\Psi}\rangle\right)^2}\,,$$

while $|\boldsymbol{\Psi}^{\perp}\rangle$ is some state orthogonal to $|\boldsymbol{\Psi}\rangle$. Note that the equation of the form (3.13) is completely general, holding for any stress-energy operator acting on an arbitrary state. Substituting (3.13) into (3.12), we obtain

$$\boldsymbol{\nabla}_{\nu}\boldsymbol{T}^{\mu\nu} + \langle\boldsymbol{\Psi}|\hat{\nabla}_{\nu}|\boldsymbol{\Psi}^{\perp}\rangle\boldsymbol{\Delta T}^{\mu\nu} = 0\,, \tag{3.14}$$

where $\boldsymbol{\nabla}_{\nu}$ is the expectation value of the operator $\hat{\nabla}_{\nu}$,

$$\boldsymbol{\nabla}_{\nu} \equiv \langle\boldsymbol{\Psi}|\hat{\nabla}_{\nu}|\boldsymbol{\Psi}\rangle\,.$$

At this point we need to make one more assumption. Namely, we assume that the error scale of the single pole approximation is bigger than the uncertainty of the stress-energy operator, $\boldsymbol{\Delta T}^{\mu\nu}$. Symbolically,

$$\mathcal{O}_1 \gtrsim \boldsymbol{\Delta T}^{\mu\nu}\,. \tag{3.15}$$

This means that in the single pole approximation we do not see the effects of the quantum fluctuations of matter fields. Intuitively, this is a reasonable assumption in most cases. For example, in the case of the kink solution describing the hydrogen atom, the scale on which one can detect quantum fluctuations (i.e., the Lamb shift effects) is much smaller than the size of the atom itself (i.e., the radius of the first Bohr orbit). Therefore, we expect that if our single pole approximation ignores the size of the atom itself, it also ignores the corresponding quantum fluctuations. An analogous assumption is made in relation to the uncertainty of the metric operator $\hat{g}_{\mu\nu}$,

$$\mathcal{O}_1 \gtrsim \boldsymbol{\Delta g}_{\mu\nu}\,, \tag{3.16}$$

given that the quantum gravity fluctuations can arguably also be ignored in the single pole approximation.

Applying (3.15) to (3.14), in the single pole approximation the second term can be dropped, leading to the effective classical covariant conservation equation,

$$\boldsymbol{\nabla}_{\nu}\boldsymbol{T}^{\mu\nu} = 0\,. \tag{3.17}$$

In a similar fashion, one can employ (3.16) to drop the off-diagonal components in the Christoffel symbol operators, leading to an effective classical expression

$$\boldsymbol{\Gamma}^{\lambda}{}_{\mu\nu} = \frac{1}{2}\boldsymbol{g}^{\lambda\sigma}\left(\partial_{\mu}\boldsymbol{g}_{\sigma\nu} + \partial_{\nu}\boldsymbol{g}_{\sigma\mu} - \partial_{\sigma}\boldsymbol{g}_{\mu\nu}\right)\,, \tag{3.18}$$

where $\boldsymbol{g}_{\mu\nu} \equiv \langle\boldsymbol{\Psi}|\hat{g}_{\mu\nu}|\boldsymbol{\Psi}\rangle$ is the effective classical metric and $\boldsymbol{g}^{\mu\nu}$ is its inverse matrix.

[1]Given any self-adjoint operator $\hat{A}$ and any state $|\Psi\rangle$, one can write

$$\hat{A}|\Psi\rangle = a|\Psi\rangle + b|\Psi^{\perp}\rangle\,,$$

where $\langle\Psi|\Psi^{\perp}\rangle \equiv 0$ and $a, b \in \mathbb{C}$. Multiplying this equation by $\langle\Psi|$ and by $\langle\Psi|\hat{A}$ from the left, one easily obtains that a and b are the expectation value and the uncertainty of the operator $\hat{A}$ in the state $|\Psi\rangle$, respectively.

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With effective classical expressions (3.17) and (3.18) in hand, we can now employ (3.10) and (3.11) to expand them into the dominant and correction parts. First we use (3.10) and $\boldsymbol{g}_{\mu\lambda}\boldsymbol{g}^{\lambda\nu} = \delta^\nu_\mu$ to find the inverse entangled metric $\boldsymbol{g}^{\mu\nu} = g^{\mu\nu} - \eta g^{\mu\rho}g^{\nu\sigma}h_{\rho\sigma} + \mathcal{O}(\eta^2)$, and then substitute into (3.18) to obtain

$$\boldsymbol{\Gamma}^\lambda{}_{\mu\nu} = \Gamma^\lambda{}_{\mu\nu} + \frac{\eta}{2} g^{\lambda\sigma} \left(\nabla_\mu h_{\sigma\nu} + \nabla_\nu h_{\sigma\mu} - \nabla_\sigma h_{\mu\nu} \right) + \mathcal{O}(\eta^2) \,, \tag{3.19}$$

where the Christoffel symbols in ordinary ∇_μ are defined with respect to the dominant classical metric $g_{\mu\nu}$. Then, expanding (3.17) into the form

$$\partial_\nu \boldsymbol{T}^{\mu\nu} + \boldsymbol{\Gamma}^\mu{}_{\sigma\nu}\boldsymbol{T}^{\sigma\nu} + \boldsymbol{\Gamma}^\nu{}_{\sigma\nu}\boldsymbol{T}^{\mu\sigma} = 0 \,,$$

we substitute (3.11) and (3.19), and after a bit of algebra we rewrite it as:

$$\nabla_\nu T^{\mu\nu} + \eta \left[\nabla_\nu t^{\mu\nu} + T^{\sigma\nu} \left(\nabla_\sigma h^\mu{}_\nu - \frac{1}{2}\nabla^\mu h_{\nu\sigma} \right) + \frac{1}{2} T^{\mu\sigma} \nabla_\sigma h^\nu{}_\nu \right] + \mathcal{O}(\eta^2) = 0 \,. \tag{3.20}$$

This equation is the one we sought out — it represents the analog of the classical covariant conservation equation (2.4), while taking into account the interference terms between the two classical states in (3.2), approximated to the linear order in η.

As a final step, (3.20) can be rewritten in a more compact form. For convenience, introduce the following shorthand notation (see our conventions from the last paragraph of the Introduction),

$$F^\mu{}_{\nu\sigma} \equiv \nabla_{(\sigma} h^\mu{}_{\nu)} - \frac{1}{2}\nabla^\mu h_{\nu\sigma} \,, \tag{3.21}$$

and also note that

$$F^\nu{}_{\nu\sigma} = \frac{1}{2}\nabla_\sigma h^\nu{}_\nu + \frac{1}{2}\nabla_\nu h^\nu{}_\sigma - \frac{1}{2}\nabla^\nu h_{\nu\sigma} = \frac{1}{2}\nabla_\sigma h^\nu{}_\nu \,,$$

so that, dropping the term $\mathcal{O}(\eta^2)$, equation (3.20) is rewritten as:

$$\nabla_\nu \left(T^{\mu\nu} + \eta t^{\mu\nu} \right) + 2\eta F^{(\mu}{}_{\nu\sigma} T^{\nu)\sigma} = 0 \,. \tag{3.22}$$

The equation (3.22) represents the effective classical covariant conservation law for the stress-energy tensor, with the included quantum correction, represented to first order in η. It is the starting point for the remainder of our analysis, and replaces equation (2.4) in the derivation of the equation of motion for a point particle.

Finally, note that the quantum correction term in (3.22) has two distinct parts — one part comes from the quantum correction to the dominant classical stress-energy tensor, i.e., the interference term $t^{\mu\nu}$, while the other part comes from the quantum correction to the dominant classical metric, i.e., the interference term $h_{\mu\nu}$. This latter quantum correction enters through the Christoffel connection terms present in the covariant derivative. As we shall see in the next subsection, its presence will be crucial for the "force term" in the equation of motion for the particle, responsible for the deviation from the classical geodesic trajectory.

3.3 Effective equation of motion

We are now ready to derive the equation of motion for a particle in the single pole approximation, using the technique presented in section 2. However, instead of (2.4), we start from the effective covariant conservation law (3.22), which contains the quantum correction terms. Throughout, we assume the following relation of scales,

$$\mathcal{O}(\eta) > \mathcal{O}_1 \geq \mathcal{O}(\eta^2)\,.$$

In other words, we assume that the quantum correction terms linear in η are not smaller than the width of our particle, since otherwise one could simply ignore them and recover the classical geodesic motion for the particle.

Repeating the method of section 2, we begin by contracting (3.22) with an arbitrary test function $f_\mu(x)$ of compact support, and integrating over the whole spacetime,

$$\int_{\mathcal{M}_4} d^4x\sqrt{-g}\, f_\mu \Big[\nabla_\nu \left(T^{\mu\nu} + \eta t^{\mu\nu}\right) + 2\eta F^{(\mu}{}_{\nu\sigma}T^{\nu)\sigma}\Big] = 0\,.$$

We then perform the partial integration to move the covariant derivative from the stress-energy tensors to the test function. As before, the boundary term vanishes since the test function has compact support, giving

$$\int_{\mathcal{M}_4} d^4x\sqrt{-g}\,\Big[-\left(T^{\mu\nu} + \eta t^{\mu\nu}\right)\nabla_\nu f_\mu + 2\eta F^{(\mu}{}_{\nu\sigma}T^{\nu)\sigma} f_\mu\Big] = 0\,. \tag{3.23}$$

Now we need to model the dominant and correction parts of the stress-energy tensor. For the dominant part, it is straightforward to assume the single pole approximation, as was done in the classical case:

$$T^{\mu\nu}(x) = \int_{\mathcal{C}} d\tau B^{\mu\nu}(\tau)\frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}}\,. \tag{3.24}$$

Regarding the correction term, we also use the single pole approximation,

$$t^{\mu\nu}(x) = \int_{\mathcal{C}} d\tau \bar{B}^{\mu\nu}(\tau)\frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}}\,, \tag{3.25}$$

but one should note that in the case of $t^{\mu\nu}$ it is less obvious why this approximation is adequate, and requires some justification. However, in order to focus on the derivation of the particle equation of motion, for the moment we simply adopt (3.25), and postpone the analysis and the meaning of this approximation for subsection 3.4.

Then we substitute (3.24) and (3.25) into (3.23), switch the order of integrations and perform the integral over spacetime $\mathcal{M}_4$, ending up with

$$\int_{\mathcal{C}} d\tau\Big[-\left(B^{\mu\nu} + \eta\bar{B}^{\mu\nu}\right)\nabla_\nu f_\mu + 2\eta F^{(\mu}{}_{\nu\sigma}B^{\nu)\sigma} f_\mu\Big] = 0\,. \tag{3.26}$$

The next step is to employ the identity (2.9) to separate the tangential and orthogonal components of the derivative of the test function. Substituting it into (3.26), and performing another partial integration, we find

$$\int_{\mathcal{C}} d\tau\Big[\left(B^{\mu\nu} + \eta\bar{B}^{\mu\nu}\right) f^{\perp}_{\nu\mu} + \Big[\nabla\left(B^{\mu\nu}u_\nu + \eta\bar{B}^{\mu\nu}u_\nu\right) - 2\eta F^{(\mu}{}_{\nu\sigma}B^{\nu)\sigma}\Big] f_\mu\Big] = 0\,,$$

where the boundary term again vanishes due to the compact support of the test function.

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After these transformations, we make use of the same argument that both f_μ and $f^\perp_{\nu\mu}$ are arbitrary and mutually independent along the curve $\mathcal{C}$, concluding that the coefficients multiplying them must each be zero. The first term gives us

$$\nabla \left(B^{\mu\nu} u_\nu + \eta \bar{B}^{\mu\nu} u_\nu \right) - 2\eta F^{(\mu}{}_{\nu\sigma} B^{\nu)\sigma} = 0\,, \tag{3.27}$$

while the second term, knowing that $f^\perp_{\nu\mu}$ is orthogonal to the curve $\mathcal{C}$ in its first index, gives

$$\left(B^{\mu\nu} + \eta \bar{B}^{\mu\nu} \right) P_\perp{}^\lambda{}_\nu = 0\,.$$

As in the previous case, given that $B^{\mu\nu}$ and $\bar{B}^{\mu\nu}$ are symmetric, one can decompose them into tangential and orthogonal components using (2.8), and then from (2.11) read off that all orthogonal components must be zero, concluding that

$$B^{\mu\nu} + \eta \bar{B}^{\mu\nu} = (B + \eta \bar{B}) u^\mu u^\nu \equiv m(\tau) u^\mu u^\nu\,, \tag{3.28}$$

where again we emphasized that the parameter m may depend on the particle's proper time τ.

Next, substituting this into (3.27) and neglecting the term $\mathcal{O}(\eta^2)$, we obtain

$$\nabla (m u^\mu) + \eta m u^\sigma \left(F^\mu{}_{\nu\sigma} u^\nu + F^\nu{}_{\nu\sigma} u^\mu \right) = 0\,. \tag{3.29}$$

Projecting onto the tangent direction u_μ and using the identity $u_\mu \nabla u^\mu = 0$, one obtains

$$\nabla m = \eta m u^\sigma \left(u^\nu u_\lambda F^\lambda{}_{\nu\sigma} - F^\nu{}_{\nu\sigma} \right)\,, \tag{3.30}$$

establishing that, in contrast to the classical case, here the parameter m fails to be constant. Substituting this back into the equation (3.29), after some simple algebra we obtain

$$\nabla u^\mu + \eta u^\nu u^\sigma P_\perp{}^\mu{}_\lambda F^\lambda{}_{\nu\sigma} = 0\,,$$

where the parameter m cancels out of the equation. As a final step, introducing the shorthand notation $F_\perp{}^\mu{}_{\nu\sigma} \equiv P_\perp{}^\mu{}_\lambda F^\lambda{}_{\nu\sigma}$, we can rewrite the equation of motion in its final form

$$\nabla u^\mu + \eta u^\nu u^\sigma F_\perp{}^\mu{}_{\nu\sigma} = 0\,. \tag{3.31}$$

The presence of the orthogonal projector in the second term should not be surprising. Namely, since acceleration must always be orthogonal to the velocity, the second term in the equation must also be orthogonal to velocity, and this is guaranteed by the presence of the orthogonal projector.

Equations (3.28), (3.30) and (3.31) are the main result of this paper, and we discuss them in turn. Equation (3.28) determines the structure of the stress-energy tensor describing the point particle, as a function of tangent vectors of its world line and a scalar parameter $m(\tau)$. Formally, it has the same form as its classical counterpart (2.12), and provisionally the parameter m may be even called *effective mass*. Namely, in the rest frame of the particle, integration of the $\boldsymbol{T}^{00}$ component of the entangled stress-energy tensor over the 3-dimensional spatial hypersurface can be interpreted as the total rest-energy of the kink configuration of fields that represents the particle. This terminology is of course provisional, since all these notions are merely a part of the semiclassical approximation of the full quantum gravity description.

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Equation (3.30) determines the proper time evolution of the parameter $m(\tau)$. In contrast to the classical case, where $m(\tau)$ was determined by (2.14) to be a constant, here we see that its time derivative is proportional to (covariant derivatives of) the interference term $h_{\mu\nu}$ between the dominant and sub-dominant classical geometry, via (3.21). If one puts $\eta = 0$, (3.30) reduces to the classical case, as expected. The interference between the two geometries gives rise to an effective force that is responsible for the change in time of the particle's effective mass. Since the particle is (effectively) not isolated, its total energy is therefore not conserved, in the sense of equation (3.30).

Finally, and most importantly, equation (3.31) represents the effective equation of motion of the particle, determining its world line. It has the form of the classical geodesic equation (2.15) with an additional correction term proportional to η and to the interference term $h_{\mu\nu}$. This additional term represents an *effective force*, pushing the particle off the classical geodesic trajectory. It is analogous to the notion of the "exchange interaction" force in molecular physics, in the region where the wavefunctions of the two electrons in a molecule overlap.

In our case, however, the force term is determined by the interference between the two classical spacetime and matter configurations superposed in the state (3.2), and in particular by the off-diagonal components of the metric operator $\hat{g}_{\mu\nu}$, see (3.8). It is thus a *pure quantum gravity effect*, a consequence of the nontrivial structure of the metric operator. Of course, the detailed properties and the magnitude of the force term depend on the choice of the two classical gravity-matter configurations and on the details of the quantization of the gravitational field.

3.4 Consistency of the approximation scheme

Regarding the analysis and the derivation of the effective equation of motion for a particle discussed in the previous subsection, there is one issue that we should reflect on. It is related to the additional consistency conditions that stem from our assumption that the quantum correction to the stress-energy tensor is approximated with a single pole term (3.25).

Namely, the two stress-energy tensors that enter the derivation of the effective equation of motion — the classical dominant stress-energy tensor $T^{\mu\nu}$, and the interference stress-energy tensor $t^{\mu\nu}$ — can in general be written in the single pole approximation as:

$$T^{\mu\nu} = \int_{\mathcal{C}} d\tau \, B^{\mu\nu}(\tau) \frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}} + \mathcal{O}_1(T) \,, \tag{3.32}$$

$$t^{\mu\nu} = \int_{\mathcal{C}} d\tau \, \bar{B}^{\mu\nu}(\tau) \frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}} + \mathcal{O}_1(t) \,. \tag{3.33}$$

Note that we have introduced two different $\mathcal{O}_1$ scales, one for each tensor. This is because, although we assume that both can be expanded into the δ series around the same curve $\mathcal{C}$, each tensor may have different "width", or in other words, the two configurations of matter fields may be such that they can be well approximated with a single pole term up to a priori two different $\mathcal{O}_1$ scales. In particular, if one chooses the $\mathcal{O}_1$ scale to write $T^{\mu\nu}$ in a single pole approximation, $\mathcal{O}_1 = \mathcal{O}_1(T)$, it is not obvious that $t^{\mu\nu}$ can also be approximated by a single pole term, compared to the same scale, and vice versa. Therefore, there is an assumption about the relationship between scales that we have made when we used expressions (3.24) and (3.25) in the derivation of the effective equation of motion.

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Looking at the structure of the equation (3.23) into which (3.24) and (3.25) have been substituted, the consistency condition for the approximation scheme can be written as

$$\mathcal{O}_1 \equiv \mathcal{O}_1(T) \geq \eta \mathcal{O}_1(t) \,. \tag{3.34}$$

In particular, if this inequality were not valid, the dipole term in (3.33) would contribute to (3.23) with a magnitude comparable to the single pole term of (3.32), and it would be inconsistent to ignore it in the derivation of the effective equation of motion.

The consistency condition (3.34) can be rewritten into a more explicit form. Substituting (3.33) and (3.9) into (3.34), we get

$$\mathcal{O}_1(T) \geq \eta \left[2\,\mathrm{Re}\left(\langle \Psi^\perp | \hat{T}_{\mu\nu} | \Psi \rangle \right) - \int_{\mathcal{C}} d\tau\, \bar{B}^{\mu\nu}(\tau) \frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}} \right] .$$

In addition, one can use (3.28) and (3.32) to eliminate the coefficient $\bar{B}^{\mu\nu}$ in favor of $T^{\mu\nu}$ and $m(\tau)$, which are arguably more observable, obtaining

$$\mathcal{O}_1(T) \geq 2\eta\,\mathrm{Re}\left(\langle \Psi^\perp | \hat{T}_{\mu\nu} | \Psi \rangle \right) + T^{\mu\nu} - \int_{\mathcal{C}} d\tau\, m(\tau) u^\mu u^\nu \frac{\delta^{(4)}(x - z(\tau))}{\sqrt{-g}} \,. \tag{3.35}$$

This inequality should be interpreted as follows. Given an explicit model of quantum gravity, and within it an explicit configuration of matter fields that make up a particle, one can estimate all three quantities on the right-hand side of (3.35), namely the off-diagonal components of the stress-energy operator, its expectation value in the dominant classical state, and the total mass of the particle, respectively. Then, the consistency condition (3.35) gives a lower bound on the scale $\mathcal{O}_1$, which represents an estimate of the error when discussing the effective equation of motion for the particle. In other words, the equation of motion can be considered to be approximately valid only across scales much larger than the $\mathcal{O}_1$ scale, bounded from below by inequality (3.35).

Finally, if one needs better precision than the scale determined by (3.35), one should take into account the dipole term in (3.33) and rederive a more precise form of the equation of motion. Still better precision would be obtained by including the dipole term in (3.32), which would amount to the equation of motion in the full pole-dipole approximation, and so on.

4 Status of the weak equivalence principle

In light of the results of section 3, it is important to discuss the status of the equivalence principle (EP). Throughout the literature, one can find various different formulations of EP, in various flavors such as weak, medium-strong, strong, and so on (see [35, 36] for a review, and [2–5, 37, 38] for various examples). Often these formulations and flavors are interpretation-dependent, and it is not always clear whether they are mutually equivalent or not, and what are the underlying assumptions and definitions used to express them.

Needless to say, such situation is less than satisfactory [35, 36], and in order to circumvent it, in this section we opt to specify one particular definition of the weak and strong equivalence principles (WEP and SEP, respectively) and to use this definition in the rest of the text. We do not aspire to claim that our definition is either equivalent to, or in any sense better than, other definitions present in the literature, and may not even correspond to the usual usage of the terminology. But for the purpose of clarity, it is prudent to fix one definition and stick to it. Therefore, in light of the results obtained in section 3, in this section we discuss the status of WEP defined as below.

4.1 Definition and flavors of the equivalence principle

The purpose of the equivalence principle is to prescribe the coupling of matter to gravity [39]. Its precise formulation therefore depends on the particular choice of the gravitational and matter degrees of freedom which one uses to describe matter and gravity. For the purpose of this paper, we assume that the classical limit of quantum gravity corresponds to general relativity, which means that in this limit the fundamental gravitational degrees of freedom give rise to a nonflat spacetime metric. Given any choice of the gravitational degrees of freedom that belong to this class, in the classical framework one can formulate the equivalence principle as a two-step recipe to couple matter to gravity (we will discuss the quantum framework in subsection 4.2).

Start from the classical equation of motion for matter degrees of freedom in flat spacetime, written symbolically as

$$\mathcal{D}_{\text{flat}}[\phi, \eta_{\mu\nu}] = 0 \,, \tag{4.1}$$

where ϕ denotes the matter degrees of freedom, $\eta_{\mu\nu}$ is the Minkowski metric, while $\mathcal{D}_{\text{flat}}$ is an appropriate functional describing the equation of motion for ϕ in flat spacetime and is assumed to be local. Given this equation of motion, couple it to gravity as follows:

1. Rewrite the equation of motion in a manifestly diffeomorphism-invariant form, typically by a change of variables to a generic curvilinear coordinate system,
$$\mathcal{D}_{\text{curvilinear}}[\phi, g^{(0)}_{\mu\nu}] = 0 \,,$$
where $g^{(0)}_{\mu\nu}$ is still the flat spacetime metric, appropriately transformed from $\eta_{\mu\nu}$, and similarly for $\mathcal{D}_{\text{curvilinear}}$.

2. Promote the curvilinear equation of motion to the equation of motion in curved spacetime by replacing the flat spacetime metric $g^{(0)}_{\mu\nu}$ with an arbitrary metric $g_{\mu\nu}$,
$$\mathcal{D}_{\text{curvilinear}}[\phi, g_{\mu\nu}] = 0 \,,$$
thereby specifying the equation of motion for matter coupled to gravity.

The first step describes the matter equation of motion from a perspective of a generic curvilinear (or "arbitrarily accelerated") coordinate system, reflecting the principle of *general relativity*. The second step simply promotes that same equation to curved spacetime as it stands, with no additional coupling of any kind. This can be loosely formulated as a statement of *local equivalence between gravity and acceleration*, which is how the EP historically got its name. Also, note that these two steps operationally correspond to the standard *minimal coupling* prescription [39].

It is important to stress the *local* nature of EP, which manifests itself in the assumption that the initial equation of motion (4.1) is local, and that the EP essentially does not change it at all, at any given point in spacetime. This has one important implication — the gravitational degrees of freedom manifest themselves only through *nonlocal measurements*, as tidal effects induced by spacetime curvature. We will return to this point and comment more on it later in the text.

Depending on the further specification of the matter degrees of freedom, one can distinguish between various flavors of the EP. For example, if one talks about the mechanics of point particles, one can start from the Newton's first law of motion, which states that in the absence of any forces, a particle has a straight-line trajectory in Minkowski spacetime. According to the step 1 above, the differential equation for a straight line in a generic curvilinear coordinate system is the geodesic equation,

$$\frac{d^2 z^\lambda}{d\tau^2} + \Gamma^\lambda_{(0)\mu\nu} \frac{dz^\mu}{d\tau} \frac{dz^\mu}{d\tau} = 0 \,,$$

where the index (0) on the Christoffel symbol indicates that it is calculated using the metric $g^{(0)}_{\mu\nu}$, which is obtained by a curvilinear coordinate transformation from the Minkowski metric $\eta_{\mu\nu}$. Then, according to step 2, one again writes the same equation, only dropping the requirement of flat spacetime metric,

$$\frac{d^2 z^\lambda}{d\tau^2} + \Gamma^\lambda{}_{\mu\nu} \frac{dz^\mu}{d\tau} \frac{dz^\mu}{d\tau} = 0 \,,$$

so that this time the Christoffel symbol is calculated using an arbitrary metric $g_{\mu\nu}$, and now encodes the interaction with the gravitational degrees of freedom. So one starts from the Newton's first law of motion for a particle in the absence of the gravitational field, and ends up with a geodesic equation in the presence of the gravitational field. We define this flavor of the EP as the *weak equivalence principle* (WEP).

Instead of mechanical particles, one can study matter degrees of freedom described by a field theory. For example, if one starts from the equation of motion for a single real scalar field,

$$(\eta^{\mu\nu} \partial_\mu \partial_\nu - m)\, \phi = 0 \,,$$

according to the step 1 of the EP, one can rewrite it in a general curvilinear coordinate system as

$$\left(g^{\mu\nu}_{(0)} \nabla_\mu \nabla_\nu - m \right) \phi = 0 \,,$$

where the Christoffel symbol inside the covariant derivative is again calculated using the flat-space metric $g^{(0)}_{\mu\nu}$. Then, according to step 2 of the EP, this equation is promoted to curved spacetime as it stands, leading to

$$(g^{\mu\nu} \nabla_\mu \nabla_\nu - m)\, \phi = 0 \,,$$

where now the covariant derivative is given with respect to an arbitrary metric $g_{\mu\nu}$ describing curved spacetime. Thus one arrives to the equation of motion for a scalar field coupled to gravity. We define this flavor of the EP as the *strong equivalence principle* (SEP).

So in short, WEP is a statement about mechanical systems such as particles and small bodies, while SEP is a statement about fields. We emphasize again that the above definitions may or may not correspond to what is known in other literature as WEP and SEP, depending on the particular source one compares our definitions to. For example, one can often find a definition of WEP as a statement about equality of inertial and gravitational masses. As another example, one can also find a definition of WEP as Galileo's statement that the acceleration of a particle due to the gravitational field is independent of the particle's internal details such as mass or chemical composition, a property also called *universality*, emphasizing the fact that gravitation interacts with all types of particles in the same way. For an excellent review of the various formulations and flavors of EP present in the literature, see [35].

In relation to these alternative formulations of WEP, one should note two comments. First, while the notion of "gravitational mass" may be useful in the context of Newtonian theory, in frameworks such as GR it is not useful, since the source in Einstein's equations is the whole stress-energy tensor, rather than any particular mass-like parameter. This renders any definition of WEP which relies on the notion of the gravitational mass unsuitable for analysis in a fundamental QG framework. Second, one can argue (see for example [35]) that the property of universality is implicitly present even without gravitational interaction, in the Newton's first law of motion. Namely, the first Newton's law can be formulated more precisely as follows: in the absence of any forces, a particle has a straight-line trajectory in Minkowski spacetime, *regardless of its internal details such as mass or chemical composition.* The Newton's first law is never spelled out in this way in textbooks, making room for a point of view that universality has something to do with gravity or the EP. However, if one accepts our definition of WEP given above, it is more natural to say that universality is a property of Newtonian mechanics, and is merely *being preserved* by the WEP when one lifts the straight-line equation of motion to curved spacetime. So from this point of view, one should arguably say that WEP is merely *compatible* with universality, rather than equivalent to it.

Given all these reasons, and despite the fact that these alternative definitions of WEP may be suitable in various other contexts, they are not quite adequate for the analysis given in this paper. We therefore choose to retain our own definition of WEP, while the principles of universality and equality between inertial and gravitational mass will be called as such. They are discussed in more detail in subsection 4.3.

4.2 Equivalence principle and quantum theory

Adopting the above definitions of WEP and SEP, it is important to discuss their relationship. From the perspective of the classical field theory (CFT), the notion of a particle can be introduced as a localized kink-like configuration of matter fields, described as a solution of the (usually quite complicated) matter field equations. One can then employ the apparatus of multipole formalism and describe the evolution of this kink configuration in the single pole approximation, as was discussed in section 2. Using this method, one can recover the equation of motion for a particle in classical mechanics (CM) as an approximation of the field theory. Moreover, all this can be done before or after the application of the EP, leading to the following diagram:

$$
\begin{array}{ccc}
\mathrm{CFT}_\eta & \xrightarrow{\text{single pole approx.}} & \mathrm{CM}_\eta \\
\Big\downarrow{\scriptstyle \text{SEP}} & & \Big\downarrow{\scriptstyle \text{WEP}} \\
\mathrm{CFT}_g & \xrightarrow{\text{single pole approx.}} & \mathrm{CM}_g
\end{array}
$$

Here the indices η and g indicate that equations of motion in a given theory are written in flat and in curved spacetime, respectively.

The question whether this diagram commutes is nontrivial. Namely, on one hand, one can start from a flat-space classical field theory, approximate it to derive the equations of motion for a particle in flat-space classical mechanics, and then invoke WEP to reach classical mechanics coupled to gravity. On the other hand, one can first invoke SEP to couple matter to gravity at the field theory level, and then approximate it to derive the equation of motion

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for a particle in curved spacetime. A priori, there is no guarantee that one will reach the same equation of motion for a particle in curved spacetime using both methods.

It is in fact the existence of the local Poincaré symmetry that leads to the commutativity of the diagram. Namely, as was discussed in section 2, in the curved spacetime local Poincaré symmetry gives rise to the covariant conservation equation for the stress-energy tensor of matter fields, and this is all one needs to reach the geodesic equation as an equation of motion for the particle, in the sense that one does not need to know the full matter field equations in curved spacetime. This establishes the ⟨SEP → single pole⟩ path of the diagram. On the other hand, in flat spacetime one can also perform the calculation of section 2, this time using the ordinary (noncovariant) conservation equation for the stress-energy tensor, which is a consequence not of the local, but rather of the global Poincaré invariance of Minkowski spacetime. Repeating the calculation of section 2 with the symbolic substitutions $g \to \eta$ and $\nabla \to \partial$, it is not hard to conclude that one will obtain the equation of motion for a straight line in flat spacetime, again without knowing all details of the full matter field equations in flat spacetime. Then, applying WEP as discussed in subsection 4.1, one reaches the geodesic equation in curved spacetime. This establishes the ⟨single pole → WEP⟩ path of the diagram, concluding that the resulting equation of motion for the particle is the same in both cases, i.e., that the diagram commutes.

Let us also note that, going beyond the single pole approximation, WEP is known to be violated, with SEP remaining valid. For example, in the pole-dipole approximation, it is well known that the analogous diagram

$$
\begin{array}{ccc}
\mathrm{CFT}_\eta & \xrightarrow{\text{pole-dipole approx.}} & \mathrm{CM}_\eta \\
\Big\downarrow{\scriptstyle \mathrm{SEP}} & & \Big\downarrow{\scriptstyle \mathrm{WEP}} \\
\mathrm{CFT}_g & \xrightarrow{\text{pole-dipole approx.}} & \mathrm{CM}_g
\end{array}
$$

fails to commute. Namely, the ⟨SEP → pole-dipole⟩ path leads to an effective equation of motion for the particle in which there is an explicit coupling of the particle's total angular momentum to the spacetime curvature [10]. On the other hand, the ⟨pole-dipole → WEP⟩ path produces the equation of motion without the curvature term. Thus, in the pole-dipole approximation, WEP fails to reproduce the correct equation of motion, since the particle is coupled to gravity in a nonminimal way, in spite of the fact that the fields which make up the particle are still minimally coupled to gravity, in line with SEP. Of course, this situation is to be expected, given that in the pole-dipole approximation the particle is no longer completely pointlike, and the coupling of the angular momentum to the curvature can be understood as a tidal effect of gravity across the "width" of the particle. On the other hand, one can instead argue that it would be wrong to apply WEP to the pole-dipole equation of motion for a particle. Namely, despite the fact that the latter is formally still local, it describes an object that is "less-than-perfectly pointlike", in the sense that its stress-energy tensor is proportional not only to a δ function but also to its derivative. From that point of view, one should not be allowed to apply the two-step prescription of EP defined above. Either way, the bottom line is that one can either declare WEP as violated or as inapplicable beyond the single pole

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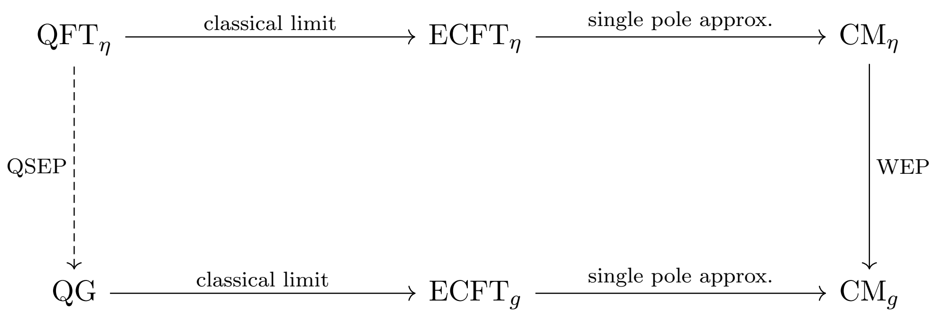
approximation, but it cannot be declared as valid. This results in the noncommutativity of the above diagram.

Let us now turn to the quantum theory. Starting first from some quantum field theory (QFT_η) which describes the fundamental matter fields in Minkowski spacetime, one can take its classical limit, giving rise to some effective classical field theory ($ECFT_\eta$). Then, assuming that the latter features kink solutions, one can describe those using the single pole approximation, leading to classical mechanics (CM_η) of the corresponding particles. Finally, applying WEP one couples those particles to gravity. The resulting equation of motion will always be a geodesic equation, assuming that the initial QFT and all subsequent approximations respect the global Poincaré invariance of Minkowski spacetime. This symmetry guarantees the conservation of the stress-energy tensor of the matter fields throughout the sequence of approximations, leading invariably to the geodesic equation of motion for the particle.

On the other hand, it is arguably more appropriate to take an alternative, more fundamental route — start from some fundamental quantum gravity (QG) model, and take the classical limit leading to some effective classical field theory ($ECFT_g$) for both matter and gravity. Then, again assuming that this theory features kink solutions, employ the single pole approximation to obtain the classical mechanics for the particle in the gravitational field (CM_g). Note that this is in fact precisely the program that was performed in section 3, leading to the non-geodesic equation of motion (3.31) for the particle. In effect, one can conclude that the following diagram fails to commute:



As a side comment, note that the dashed QSEP arrow represents some hypothetical map leading from a QFT in Minkowski spacetime to a full-blown model of QG, according to a notion that might be called a "quantum strong equivalence principle". It is unclear whether such a principle exists or not, let alone what its formulation is supposed to be, even if one is given precisely defined models of QFT and QG in question. We introduce it here simply for completeness, speculating that such a notion should exist, as a generalization of SEP from classical to quantum physics. It is also convenient to introduce it, in order to close the diagram and discuss its commutativity.

It is important to stress the reason why this diagram does not commute. Recalling the details of section 3, the local Poincaré symmetry is assumed to be respected at the fundamental level of QG and onwards, just like in the classical case. Moreover, the single pole approximation is used, avoiding any nonminimal coupling of the tidal forces that may be present. And yet, in spite of all that, the resulting equation of motion is not a geodesic. Looking at the equation of motion (3.31), the reason for this is the nontrivial interference between classical states describing two classical configurations of matter, and more importantly, of gravity. In other words, the deviation from the geodesic motion is a *pure quantum gravity effect* — it is not present in the classical case, nor in the case of quantum matter in

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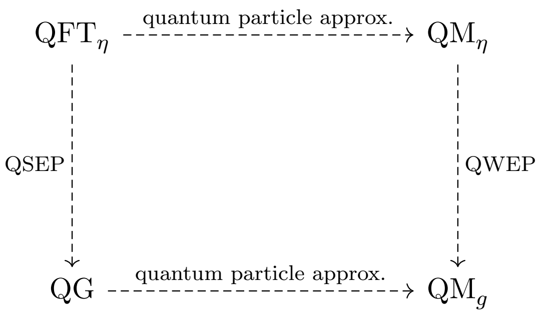
classical Minkowski spacetime. A testimony of this fact is the quantum correction term for the metric (3.8), which features off-diagonal matrix elements of the metric operator $\hat{g}_{\mu\nu}$:

$$h_{\mu\nu} = 2\,\mathrm{Re}\left(\kappa\langle\Psi^{\perp}|\hat{g}_{\mu\nu}|\Psi\rangle\right) + \mathcal{O}(\eta)\,.$$

In this sense, due to the noncommutativity of the above diagram, one can argue that (within the discussed framework) *quantum gravity violates the weak equivalence principle.* Nevertheless, we would like to stress that our discussion regarding both strong and weak equivalence principles, based on the above prescription from subsection 4.1, is inherently *classical.* Indeed, in steps 1 and 2 which define the implementation of EP, one considers classical equations of motion. In our case, such definition suffices, as our entangled state (3.2) consists of a dominant and a sub-dominant term. Thus, we could expand our entangled equations (3.10) and (3.11) around the dominant classical terms, and discuss WEP in such a scenario. In fact, according to the definition of WEP, in general one can discuss its violation only *with respect to* some (perhaps unspecified, but assumed) classical spacetime metric. In our case, this role is played by the dominant classical metric $g_{\mu\nu}$.

In the more general case of superpositions of states which are more equally weighted, $\alpha \approx \beta$, and which consist of almost orthogonal states, $\langle\Psi|\tilde{\Psi}\rangle \approx 0$, one cannot single out a preferred classical metric, and therefore the classical definitions of SEP and WEP are inapplicable in this regime. Therefore, both equivalence principles ought to be extended to their respective *quantum* domains, denoted QSEP and QWEP respectively, in the sense of the following diagram:



Note that here all arrows are dashed, indicating the speculative nature of all these maps. Also, QM_g represents a hypothetical theory of quantum particles coupled to a quantum gravitational field.

In this highly quantum regime ($\alpha \approx \beta$ and $\langle\Psi|\tilde{\Psi}\rangle \approx 0$), one could try to define the quantum weak equivalence principle (QWEP) in terms of the classical WEP, applied separately to each "branch" in the superposition. As long as the two "branches" $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$ are themselves classical states, corresponding to the respective solutions of Einstein's equations, such a definition might seem suitable. Note that this approach is compatible with the notion of a superposed observer (see recent work [40] and the references therein). However, the formulation of the quantum strong and weak equivalence principles for the case of generic non-classical quantum states is an open question, outside of the scope of the current work.

Finally, the quantum version of the single pole approximation, called "quantum particle approximation" in the diagram above, is also not well defined — neither conceptually nor technically. Essentially, the whole diagram represents merely a speculation about the prescriptions which ought to map between the respective theories. In addition, like in the

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previous cases, the commutativity of the diagram (i.e., the violation of QWEP, given the validity of QSEP) would also be an open question. In some sense, the QSEP would represent a "true" equivalence principle, while QWEP would be a particle-like approximate image of QSEP. Being approximate, QWEP could possibly be violated in some cases, giving rise to noncommutativity of the diagram.

4.3 Universality, gravitational and inertial mass

In light of the results of section 3, in addition to the discussion of WEP violation, it is also important to discuss the status of the principle of universality, and the principle of equality between inertial and gravitational masses. In order to discuss them, it is instructive to study the Newtonian limit of the effective equation of motion (3.31), as follows.

We define the Newtonian limit in the standard way [39] — by assuming small spacetime curvature, nonrelativistic motion, and ignoring the backreaction of the particle on the background spacetime geometry. These approximations are implemented in the following way. First, ignoring the backreaction of the particle allows us to choose the dominant classical metric $g_{\mu\nu}$ as specified by the Newtonian line element

$$ds^2 = -\left(1 - \frac{2GM}{r}\right) dt^2 + dx^2 + dy^2 + dz^2 \,, \tag{4.2}$$

where $x^\mu \equiv (t, x, y, z)$ are spacetime coordinates, M is the mass of the gravitational source, $r \equiv \sqrt{x^2 + y^2 + z^2}$, and $G \equiv l_p^2$ is Newton's gravitational constant. We will discuss the motion of a test-particle in this background, given by the effective equation of motion (3.31). Second, the assumption of nonrelativistic motion of the particle allows us to neglect its spacelike velocity,

$$u^k \equiv \frac{dz^k}{d\tau} \approx 0 \,,$$

leaving only the timelike component $u^0 \equiv dz^0/d\tau$ nonzero (the position of the particle $z^\mu(\tau)$ should not be confused with the label for the third spatial coordinate $z \equiv x^3$). Finally, the assumption of small spacetime curvature allows us to neglect all terms of order $\mathcal{O}(M^2)$ and higher.

Given this setup, one can easily calculate all nonzero Christoffel symbols corresponding to the dominant metric, obtaining:

$$\varGamma^0{}_{0k} = \varGamma^0{}_{k0} = \varGamma^k{}_{00} = \frac{GM}{r^3} x^k \,, \qquad k \in \{1, 2, 3\} \,.$$

One can then employ them to write the time and space components for the particle's effective equation of motion (3.31). Using (2.8) and (3.21), after some straightforward algebra, the time component of the equation of motion reduces to

$$\frac{d^2 z^0(\tau)}{d\tau^2} = 0 \,,$$

owing to the normalization condition $u^\mu u^\nu g_{\mu\nu} = -1$ and the presence of the orthogonal projector in (3.31). Using convenient initial conditions, this equation can be integrated to make an identification between the proper time τ and the time component of the particle's parametric equation of trajectory $x^\mu = z^\mu(\tau)$ as

$$t = z^0(\tau) = \tau \,,$$

reflecting the notion of global universal time of Newtonian theory. Using this result, one can show that the space components of the particle's equation of motion obtain the following form (note that the spacelike indices can be raised and lowered at will, since the spatial part of the metric (4.2) is a unit matrix):

$$\frac{d^2 z^k}{d\tau^2} + \frac{GM}{r^3} z^k + \eta \left[\partial_0 h_{0k} - \frac{1}{2} \partial_k h_{00} - \frac{GM}{r^3} z^j h_{jk} \right] = 0 \, . \tag{4.3}$$

Note that here r has been evaluated at the position of the particle, $r = \sqrt{z^k z_k}$, and similarly for the gradients of h_{0k} and h_{00}. The first two terms in the equation come from the classical geodesic part ∇u^k in (3.31), while the third term is the quantum correction, coming from the effective force term $\eta u^\nu u^\sigma F^k_{\perp\nu\sigma}$.

The most important aspect of equation (4.3) is the similarity between the second term of the classical part and the final term of the quantum correction. The spacelike components h_{jk} can be separated into the trace and traceless part,

$$h_{jk} \equiv \frac{1}{3} h^i{}_i \, \delta_{jk} + \tilde{h}_{ij} \, , \qquad \tilde{h}^k{}_k \equiv 0 \, ,$$

and the trace can be grouped together with the classical term, giving

$$\frac{d^2 z^k}{d\tau^2} + \frac{GM}{r^3} z^k \left(1 - \frac{1}{3} \eta h^i{}_i \right) + \eta \left[\partial_0 h_{0k} - \frac{1}{2} \partial_k h_{00} - \frac{GM}{r^3} z^j \tilde{h}_{jk} \right] = 0 \, . \tag{4.4}$$

Finally, multiplying the whole equation (4.4) with an arbitrary positive number, called the particle's *inertial mass* and denoted m_I, it takes the form of the Newton's second law of motion,

$$m_I \frac{d^2 z^k}{d\tau^2} = -m_I \left(1 - \frac{1}{3} \eta h^i{}_i \right) \frac{GM}{r^3} z^k - \eta m_I \left[\partial_0 h_{0k} - \frac{1}{2} \partial_k h_{00} - \frac{GM}{r^3} z^j \tilde{h}_{jk} \right] . \tag{4.5}$$

One can recognize two force terms on the right-hand side. The second term is of purely quantum origin, and represents the effective force acting on the particle ultimately due to the presence of the quantum state $|\tilde{\Psi}\rangle$ in (3.2). It has a non-Newtonian form, in the sense that none of its parts can be grouped together with the first force term, as was done with the trace part. The first force term, however, can be recognized as the classical Newton's gravitational force law, provided that one defines the ratio between the *gravitational mass* m_G and the *inertial mass* m_I of the particle as

$$\frac{m_G}{m_I} \equiv \left(1 - \frac{1}{3} \eta h^i{}_i \right) . \tag{4.6}$$

At this point we are ready to discuss the principles of universality and of the equality between gravitational and inertial masses. To begin with, it is obvious from (4.6) that the gravitational mass is equal to the inertial mass only up to a quantum correction term. This term contains the trace of spatial components of the metric interference tensor $h_{\mu\nu}$, defined by equation (3.8), from which we obtain:

$$h^i{}_i = 2\delta^{ij} \, \mathrm{Re} \left(\kappa \langle \Psi^\perp | \hat{g}_{ij} | \Psi \rangle \right) + \mathcal{O}(\eta) \, . \tag{4.7}$$

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It is crucial to notice that, in addition to the dependence of the off-diagonal matrix element of the metric operator, this expression also depends on the matter fields (which are present in $|\Psi\rangle$ and $|\Psi^{\perp}\rangle$), including the particle itself. Therefore, the term in the parentheses in (4.6) cannot be reabsorbed into the constants G and M, since these describe the external source of gravity which should remain independent of the properties of the test particle. Thus, the only possibility to cast the first force term in (4.5) into the form of the Newton's law of gravitation, is to define the ratio between the gravitational and the inertial mass as in (4.6). As a consequence, the principle of equality between gravitational and inertial masses is violated by the presence of the correction term coming from quantum gravity.

A similar argument can be made regarding the principle of universality. One may cancel away the inertial mass from the Newton's law (4.5), returning to (4.4) which describes the acceleration of the particle in the presence of an external gravitational field. Again, the presence of (4.7) in the classical gravitational acceleration term guarantees that this term depends not only on the external gravitational source, but also on the structure of the test particle itself. Moreover, the remaining quantum correction terms also depend on $h_{\mu\nu}$, and therefore they too carry information about the internal structure of the particle. In this sense, test particles described by different matter configurations may therefore display different accelerations, given the same background gravitational field. This means that the principle of universality is violated by the presence of the quantum gravity correction terms.

As a final comment, we should also note that m_I (and consequently m_G as well) is a completely free parameter in the Newtonian setup, and should be determined by the interactions of nongravitational type. In particular, the Newtonian framework does not allow us to connect m_I, m_G with the effective mass m of the particle, discussed in the context of (3.28) and (3.30). This is because the total rest-energy of a particle is an inherently relativistic concept, not defined in Newtonian mechanics. On the other hand, if one goes to the relativistic framework, the notions of inertial and gravitational masses become ill-defined, since gravitational interaction cannot be described anymore by a mere force law in the Newtonian sense. Therefore, the relationship between m on one side, and both m_I, m_G on the other side, remains undefined.

5 Conclusions

5.1 Summary of the results

In this paper, we have discussed the effective motion of a point particle within the framework of quantum gravity, in particular the case where both matter and gravity are in a quantum superposition of the Schrödinger cat type. In section 2 we gave a recapitulation of the results of the classical theory, introducing the multipole formalism framework and illustrating the derivation of the geodesic equation for the motion of a particle in GR. Section 3 was devoted to the generalization of these results to the realm of the full quantum gravity. In subsection 3.1 we introduced the abstract quantum gravity framework, discussed the model of the superposition of two classical states, and established the main assumptions for the derivation of the effective equation of motion. In subsection 3.2 we have analyzed in detail the quantum version of the equation for the covariant conservation of stress-energy tensor, which is a crucial ingredient in the derivation of the effective equation of motion. The explicit derivation of the equation of motion itself was then given in subsection 3.3, giving rise to the main results of the paper — the equation for the stress-energy kernel (3.28), the equation for the time-evolution of the particle's mass (3.30), and the effective equation of motion for the particle (3.31). Most importantly, the effective equation of motion turns out to contain a non-geodesic term, giving rise to an effective force acting on the particle, as a consequence of the interference terms between the two classical states of the gravity-matter system. The last subsection 3.4 discusses the self-consistency of the assumptions used in the above analysis, giving rise to the equation (3.35) for the error estimate of the single pole approximation scale.

In light of the nongeodesic motion established in section 3, it is important to discuss it in the context of the equivalence principle. This topic was taken up in section 4. After we have defined various flavors of the equivalence principle in subsection 4.1, the main analysis was presented in subsection 4.2, discussing a possible violation of (various forms of) the weak equivalence principle, as a consequence of the nongeodesic correction to the equation of motion (3.31). Also, given the inherently classical nature of the equivalence principle, we have also speculated on possible generalizations to the quantum realm, introducing the notions of the quantum strong and weak equivalence principles, albeit without giving explicit statements about their definitions. Finally, in subsection 4.3 we have discussed the notions of universality and equality between inertial and gravitational masses in the context of quantum gravity, by studying the Newtonian limit of the equation of motion (3.31). This analysis gave a clear interpretation that both universality and the equality between gravitational and inertial masses are violated in our context, corroborating the conclusions of the abstract analysis of the EP given in subsection 4.2.

5.2 Discussion of the results

By far the most interesting topic to discuss in the context of the equation of motion (3.31) is how to estimate the magnitude of the nongeodesic term. As far as the analysis of this paper goes, we can only say that this term is very small, given that it is proportional to η, which is in turn bounded from above by phenomenological argument that we do not observe superpositions of the gravitational field in nature. However, aside from this qualitative argument, in order to estimate the actual magnitude of the nongeodesic term one would need to go beyond the abstract quantum gravity formalism, and construct an explicit quantum gravity model coupled to matter fields, find some explicit kink solutions of the matter sector, and then calculate the overlap terms and the off-diagonal interference terms of the metric operator. Of course, any estimate obtained in such a way would be model-dependent. We consider this to be a feature of the abstract quantum gravity approach, since the magnitude of the nongeodesic term represents one way to operationally distinguish between different QG models. In other words, one could use equation (3.31) to experimentally test and compare these models, at least in principle. Probably the most obvious such test would employ equation (4.6) which relates the gravitational and inertial mass of the particle.

One result that was not discussed in detail is the nonconservation law for the effective mass of the particle, (3.30). However, it is not really surprising that the particle's total rest energy fails to be constant in the presence of gravity-matter entanglement. As (3.30) tells us, the nonconservation is actually a consequence of the additional effective force, which is itself a consequence of the quantum interference between two classical geometries and matter states. Nevertheless, it would indeed be interesting to study the mass nonconservation in more detail.

It is also important to discuss the generalization of our results from the case of the superposition of two classical states to many classical states. In particular, one could discuss the case where the state $|\tilde{\Psi}\rangle$ in (3.2) is not a single classical state, but a superposition of many classical states,

$$|\tilde{\Psi}\rangle = \sum_i \gamma_i |\Psi_i\rangle \,.$$

As long as we maintain the assumption that the fidelity $F(|\Psi\rangle, |\mathbf{\Psi}\rangle) \approx 1$, it is straightforward to see that all our results and conclusions still hold in the generic case. Therefore, there is no substantial difference in the analysis of a state which is a superposition of two classical states, compared to the analysis of a superposition of many classical states, as long as one of them is dominant while all others are sub-dominant. Note that in this case, even when β is finite and $\epsilon \to 0$, the role of the metrics generated by $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$ cannot be exchanged anymore, as the latter generically does not satisfy Einstein's equations. This fixes the choice of $|\Psi\rangle$ as the dominant state. A detailed quantitative description is technically more complicated, but qualitatively all results will hold for both types of states.

5.3 Future lines of research

One of the main lines of future work would be to perform a similar analysis as was done in this paper, but keeping the η^2 terms. This would naturally include the sub-dominant effective metric and stress-energy (3.3), giving qualitatively new insight into the notion of quantum superpositions of two classical geometries. That analysis might provide clues about the properties of quantum gravity which could arguably hold even in the equal-weight superpositions of two classical states, defined by the choice $\alpha \approx \beta \approx 1/\sqrt{2}$ in (3.2).

Alternatively, one could repeat the analysis of this paper, but in a pole-dipole approximation. This would also lead to novel effects, one of which might be a coupling of various quantum interference terms to the spacetime curvature and the angular momentum of the particle, generalizing the classical pole-dipole equation of motion [10].

Also, given that the multipole formalism is also applicable to Riemann-Cartan spacetimes [19–22], the analysis of this paper could be generalized to include coupling of quantum interference terms to spacetime torsion and the spin of the particle.

Finally, one could further discuss a more general setup in which the off-diagonal terms in the covariant conservation equation (3.14) are not ignored, in the sense of going beyond the approximations (3.15) and (3.16).

In addition to all of the above, one important line of research would be to study possible connections to experiments. First, one should study the counterpart of the so-called *geodesic deviation equation*. Namely, in GR, the geodesic motion as such is not observable, as a consequence of the equivalence principle. As we have emphasized in subsection 4.1, the EP dictates that the only way to observe gravitational degrees of freedom is via *nonlocal measurements*, which are not encoded in the geodesic equation. Therefore, what one can actually observe is the change in the relative separation of two nearby geodesic trajectories, due to the tidal effects. This is in turn described by the geodesic deviation equation, which explicitly features the Riemann curvature tensor. In our case, the equation of motion (3.31) is not a geodesic, but is still local in character, in the sense that it does contain gravitational degrees of freedom at the given point, but still it does not combine gravitational degrees of freedom of two or more points. Thus, one ought to compare the trajectories of two nearby particles, both following a trajectory determined by (3.31). The equation governing the separation between two particles in such a setup would be a counterpart to the geodesic deviation equation of GR with a corresponding quantum correction term. It should be derived and studied in detail, in order to better understand what effects could be in principle directly experimentally observable.

Second, one could also test our results by measuring the violation of the universality and of the equality of the gravitational and the inertial mass in the semiclassical Newtonian limit.

The above list of possible topics for further research is of course not exhaustive — one can probably study various additional aspects and topics related to this work, in particular giving more precise meaning to the notions of the quantum strong and weak equivalence principles.

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A Short review of the multipole formalism

In this appendix we give a short review of the multipole formalism, providing some basic motivation for its introduction and a few elementary properties. A more rigorous treatment and more details can be found in [25].

The multipole formalism revolves around the idea of expanding a function into a series of derivatives of the Dirac δ function, or δ series for short. Perhaps the easiest way to understand the δ series is to introduce it as a Fourier transform of a power series. For example, given a real-valued function $f(x)$, one can write it as a Fourier transform of $\tilde{f}(k)$ as

$$f(x) = \int_{\mathbb{R}} dk \, \tilde{f}(k) \, e^{ikx} \,. \tag{A.1}$$

In principle, we can expand $\tilde{f}(k)$ into power series as

$$\tilde{f}(k) = \sum_{n=0}^{\infty} c_n k^n \,,$$

where c_n are some coefficients, substitute the expansion back into (A.1), and integrate term by term. Using the identity

$$k^n e^{ikx} = (-i)^n \frac{\partial^n}{\partial x^n} e^{ikx}$$

and the integral representation of the Dirac δ function

$$\delta(x) = \frac{1}{2\pi} \int_{\mathbb{R}} dk\, e^{ikx} \,,$$

we obtain

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty} c_n \int_{\mathbb{R}} dk\, k^n\, e^{ikx} = \sum_{n=0}^{\infty} (-i)^n c_n \frac{d^n}{dx^n} \int_{\mathbb{R}} dk\, e^{ikx} \\ &= \sum_{n=0}^{\infty} 2\pi (-i)^n c_n \frac{d^n}{dx^n} \delta(x) \equiv \sum_{n=0}^{\infty} b_n \frac{d^n}{dx^n} \delta(x) \,. \end{aligned}$$

In the last step, we have merely renamed the coefficients in the expansion.

The above example is the most elementary construction of the δ series, providing some intuition. It is straightforward to see that one can generalize the procedure to perform the expansion around an arbitrary point z instead of zero, such that

$$f(x) = \sum_{n=0}^{\infty} b_n \frac{d^n}{dx^n} \delta(x-z) \,.$$

The coefficients b_n can be evaluated using the inverse formula,

$$b_n = \frac{(-1)^n}{n!} \int_{\mathbb{R}} dx\, (x-z)^n f(x) \,, \tag{A.2}$$

and are usually called *n-th order moments* of the function $f(x)$. From (A.2) one sees that the δ series is well defined for every function $f(x)$, which falls off to zero faster than any power of x at both infinities.

Let us study an instructive example. Let the function $f(x)$ be an ordinary Gaussian, peaked around the point x_0,

$$f(x) = \frac{1}{\sqrt{\pi}} e^{-(x-x_0)^2} \,.$$

One can evaluate the coefficients in the corresponding δ series using (A.2) to obtain:

$$b_n = \begin{cases} \displaystyle\sum_{k=0}^{n/2} \frac{(z-x_0)^{n-2k}}{4^k\, k!\, (n-2k)!} & \text{for even } n \,, \\[2ex] \displaystyle -\sum_{k=0}^{(n-1)/2} \frac{(z-x_0)^{n-2k}}{4^k\, k!\, (n-2k)!} & \text{for odd } n \,. \end{cases}$$

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It is important to note the following property — if the expansion point z does not coincide with the peak of the Gaussian, x_0, the magnitude of the coefficients b_n in general grows with n. For example, if $z - x_0 = 2$, we have

$$f(x) = \delta(x-z) - 2\frac{d}{dx}\delta(x-z) + \frac{9}{4}\frac{d^2}{dx^2}\delta(x-z) - \frac{11}{6}\frac{d^3}{dx^3}\delta(x-z) + \frac{115}{96}\frac{d^4}{dx^4}\delta(x-z) + \dots$$

However, if the expansion point coincides with the peak, $z - x_0 = 0$, the magnitude of the coefficients falls off as n grows:

$$f(x) = \delta(x-z) + \frac{1}{4}\frac{d^2}{dx^2}\delta(x-z) + \frac{1}{32}\frac{d^4}{dx^4}\delta(x-z) + \frac{1}{384}\frac{d^6}{dx^6}\delta(x-z) + \dots$$

From this simple example one can infer an important property of δ series — the coefficients b_n decrease as n grows, if the expansion point is near the peak of the function $f(x)$. Turning the argument around, if we require that the coefficients decrease with n,

$$|b_n| > |b_{n+1}|\,, \qquad \forall n \in \mathbb{N}_0\,,$$

this places *a restriction on the possible values of the expansion point* z. This is the crucial property of the δ series, and is being used to define the "position of the particle" which corresponds to a distribution of matter fields described by a localized function $f(x)$.

Also, assuming that the expansion point z has been chosen to be near the peak of the function, the decreasing nature of the coefficients b_n allows one to approximate the function $f(x)$ by a truncated series. This formalizes the intuitive idea that if one looks at some localized distribution of matter fields from "far away", it will look roughly as a point particle. The truncation point then quantifies the amount of "internal structure" that is known about $f(x)$. One can therefore study the function $f(x)$ at various approximation levels: the *single pole* approximation,

$$f(x) \sim b_0\delta(x-z)\,,$$

the *pole-dipole* approximation,

$$f(x) \sim b_0\delta(x-z) + b_1\frac{d}{dx}\delta(x-z)\,,$$

the *pole-dipole-quadrupole* approximation,

$$f(x) \sim b_0\delta(x-z) + b_1\frac{d}{dx}\delta(x-z) + b_2\frac{d^2}{dx^2}\delta(x-z)\,,$$

and so on.

It is completely straightforward to generalize the δ series to three (or more) dimensions, with the δ series of a function $f(\vec{x})$ around the point $\vec{z}$ defined as

$$f(\vec{x}) = \sum_{n=0}^{\infty} b_n^{i_1\dots i_n}\frac{\partial}{\partial x^{i_1}}\cdots\frac{\partial}{\partial x^{i_n}}\delta^{(3)}(\vec{x}-\vec{z})\,. \tag{A.3}$$

Here the indices $i_1, \dots i_n$ take values 1, 2 and 3, and the inverse formula for the coefficients is

$$b_n^{i_1\dots i_n} = \frac{(-1)^n}{n!}\int_{\mathbb{R}^3} d^3x\,(x^{i_1}-z^{i_1})\dots(x^{i_n}-z^{i_n})f(\vec{x})\,. \tag{A.4}$$

For example, in electrostatics, one can expand the charge density $\rho(\vec{x})$ localized around the point $\vec{z} = 0$ as

$$\rho(\vec{x}) = b_0 \delta^{(3)}(\vec{x}) + b_1^i \frac{\partial}{\partial x^i} \delta^{(3)}(\vec{x}) + \dots$$

According to (A.4), the coefficients are

$$b_0 = \int_{\mathbb{R}^3} d^3x \, \rho(\vec{x}) \equiv Q \,, \qquad \vec{b}_1 = - \int_{\mathbb{R}^3} d^3x \, \vec{x} \rho(\vec{x}) \equiv -\vec{p} \,,$$

where we recognize the total charge Q and the electrostatic dipole moment $\vec{p}$ of the source. Thus we have

$$\rho(\vec{x}) = Q\delta^{(3)}(\vec{x}) - \vec{p} \cdot \nabla \delta^{(3)}(\vec{x}) + \dots$$

Substituting the δ series expansion of $\rho(\vec{x})$ into the formula for the electrostatic potential,

$$\varphi(\vec{r}) = \int_{\mathbb{R}^3} d^3x \, \frac{\rho(\vec{x})}{|\vec{r} - \vec{x}|} \,,$$

and evaluating the integral, one obtains the familiar expression for the multipole expansion in electrostatics [41]:

$$\varphi(\vec{r}) = \frac{Q}{|\vec{r}|} + \frac{\vec{p} \cdot \vec{r}}{|\vec{r}|^3} + \dots$$

This example also illustrates what type of approximation is achieved with the truncation of the δ series.

Next we generalize to time-dependent functions. If the function $f(\vec{x})$ evolves in time, while remaining localized in space, one can expand it into δ series by choosing the most convenient reference point $z(t)$ at each moment of time,

$$f(\vec{x}, t) = \sum_{n=0}^{\infty} b^{i_1 \dots i_n}(t) \frac{\partial}{\partial x^{i_1}} \dots \frac{\partial}{\partial x^{i_n}} \delta^{(3)}(\vec{x} - \vec{z}(t)) \,, \tag{A.5}$$

where $t \in \mathbb{R}$ is a time variable, and the coefficients b are now time-dependent. Then one can introduce the proper time τ, and use the identity

$$\int_{\mathbb{R}} d\tau \, \delta(t - \tau) = 1$$

to rewrite (A.5) in a 4-dimensional manifestly Lorentz-invariant form

$$f(x) = \int_{\mathbb{R}} d\tau \sum_{n=0}^{\infty} b^{\mu_1 \dots \mu_n}(\tau) \partial_{\mu_1} \dots \partial_{\mu_n} \delta^{(4)}(x - z(\tau)) \,, \tag{A.6}$$

where we have relabeled $(\vec{x}, t) \equiv x$, introduced $z^0(\tau) = \tau$, used shorthand notation $\partial_\mu \equiv \partial / \partial x^\mu$, and defined $b^0 = b^{00} = b^{000} = \dots = 0$, since the time derivatives do not actually appear in (A.5). The introduction of these auxiliary timelike components of the b-coefficients, demanded by Lorentz invariance, gives rise to an additional gauge symmetry of the expansion coefficients, since only the "spatial" components carry nontrivial information about the function $f(x)$. This additional gauge symmetry is called *extra symmetry 1*, and is studied in detail in [25].

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Finally, one can make one more generalization, and introduce the notion of a δ series around a p-brane, a $(p+1)$-dimensional submanifold living in a D-dimensional spacetime manifold. Namely, we have seen that one can expand a function into a δ series around a point and around a one-dimensional line (equations (A.3) and (A.6), respectively). Generalizing in that direction, one can introduce the world-trajectory of a p-dimensional object through D-dimensional spacetime $\mathcal{M}$, with parametric equations $x^\mu = z^\mu(\xi^a)$ describing the trajectory as a $(p+1)$-dimensional submanifold $\Sigma \subset \mathcal{M}$. Here $\mu \in \{0, \dots, D-1\}$ and $a \in \{0, \dots p\}$, where x^μ are coordinates on $\mathcal{M}$ while ξ^a are intrinsic coordinates on Σ. Then, given a function $f(x)$ whose support is localized near the submanifold Σ, one can write its δ series expansion around Σ in a fully diffeomorphism- and reparametrization-invariant way as:

$$f(x) = \int_\Sigma d^{p+1}\xi \sqrt{-\gamma} \sum_{n=0}^{\infty} \nabla_{\mu_1} \dots \nabla_{\mu_n} \left[B^{\mu_1 \dots \mu_n}(\xi) \frac{\delta^{(D)}(x - z(\xi))}{\sqrt{-g}} \right] . \tag{A.7}$$

Here γ is the determinant of the induced metric $\gamma_{ab} = g_{\mu\nu} u^\mu_a u^\nu_b$ on Σ, where $g_{\mu\nu}$ is the metric on $\mathcal{M}$ and $u^\mu_a \equiv \partial z^\mu / \partial \xi^a$ are the tangent vectors of Σ. Note that, in order to ensure the correct tensorial behavior, the B-coefficients have been moved inside the action of the covariant derivatives. Namely, despite the fact that the covariant derivatives act with respect to x and B's do not depend on x, covariant derivatives still act nontrivially on B's with the connection terms. For similar reasons, the term $\sqrt{-g}$ has been introduced to combine with the δ function into a quantity which transforms as a scalar under diffeomorphisms. Its introduction amounts merely to a suitable redefinition of B's and does not modify the δ series in any nontrivial way.

The fully general δ series (A.7) has been studied in detail in [25]. For the purpose of the discussion given in the main text of this paper, we are interested in the case of a particle, i.e., a $(p=0)$-brane, moving along a 1-dimensional timelike curve $\mathcal{C}$ which is a submanifold of the $(D=4)$-dimensional spacetime $\mathcal{M}$. In this case, there is only one intrinsic coordinate on $\mathcal{C}$, denoted $\xi^0 \equiv \tau$, only one tangent vector

$$u^\mu_0 \equiv \frac{\partial z^\mu(\xi)}{\partial \xi^0} = \frac{dz^\mu(\tau)}{d\tau} = u^\mu ,$$

while the induced metric tensor is a 1×1 matrix $\gamma_{00} = g_{\mu\nu} u^\mu_0 u^\nu_0$. The parametrization of the curve $\mathcal{C}$ with the coordinate τ can be chosen to fix the reparametrization gauge symmetry via the gauge-fixing condition $\gamma_{00} = -1$, which is actually the natural normalization of the tangent vector, $g_{\mu\nu} u^\mu u^\nu = -1$. Finally, one can then apply the δ series expansion (A.7) to the stress-energy tensor $T^{\mu\nu}(x)$ of the matter fields as

$$T^{\mu\nu}(x) = \int_\mathcal{C} d\tau \sum_{n=0}^{\infty} \nabla_{\rho_1} \dots \nabla_{\rho_n} \left[B^{\mu\nu\rho_1 \dots \rho_n}(\tau) \frac{\delta^{(D)}(x - z(\tau))}{\sqrt{-g}} \right] .$$

Note that the coefficients B now carry two additional indices inherited from the stress-energy tensor. In the single pole approximation, one drops all terms in the sum except the $n=0$ term, truncating the series to the form

$$T^{\mu\nu}(x) = \int_\mathcal{C} d\tau \, B^{\mu\nu}(\tau) \frac{\delta^{(D)}(x - z(\tau))}{\sqrt{-g}} ,$$

as used in the main text.

B Separable classical states

As mentioned in the main text, a recent study suggests that physical states of gravity and matter are generically entangled [1]. In this appendix, we analyze a simple, yet possibly intriguing, consequence of the assumption that the overall classical gravity-matter state can be approximated by (or indeed is) the product of the gravity and the matter classical states, $|\Psi\rangle = |g\rangle \otimes |\phi\rangle$, where $|g\rangle \in \mathcal{H}_G$ and $|\phi\rangle \in \mathcal{H}_M$ are classical states for the gravity and the matter sector, respectively (and analogously for $|\tilde{\Psi}\rangle$).

To begin with we introduce the overlaps as follows:

$$S_G \equiv \langle g|\tilde{g}\rangle\,, \qquad S_M \equiv \langle \phi|\tilde{\phi}\rangle\,, \qquad S \equiv \langle \Psi|\tilde{\Psi}\rangle = S_G S_M\,.$$

Note that, since in (3.2) only the relative phase between $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$ is important, we can reabsorb the phases of the coefficients α and β into $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$, respectively. In this way, we have $\alpha, \beta \in \mathbb{R}$, while only the overlap S between the two coherent states carries the information about the relative phase, and is therefore complex. Moreover, since S is a product between S_G and S_M, the phase of S can be distributed between S_G and S_M in an arbitrary way. A convenient choice is to have the phase in the matter sector, so that $S_G \in \mathbb{R}$ and $S_M \in \mathbb{C}$. Next, we can decompose $|\tilde{g}\rangle$ and $|\tilde{\phi}\rangle$ into parts proportional to and orthogonal to $|g\rangle$ and $|\phi\rangle$, respectively,

$$|\tilde{g}\rangle = S_G|g\rangle + \epsilon_G|g^\perp\rangle\,, \qquad |\tilde{\phi}\rangle = S_M|\phi\rangle + \epsilon_M|\phi^\perp\rangle\,, \tag{B.1}$$

where $\langle g|g^\perp\rangle \equiv 0$, $\langle \phi|\phi^\perp\rangle \equiv 0$, and

$$\epsilon_G \equiv \sqrt{1-(S_G)^2}\,, \qquad \epsilon_M \equiv \sqrt{1-|S_M|^2}\,.$$

Note that $\epsilon_G, \epsilon_M \in \mathbb{R}$. Additionally, one can use (B.1) to rewrite $|\tilde{\Psi}\rangle$ into the form

$$|\tilde{\Psi}\rangle = S|\Psi\rangle + \epsilon|\Psi^\perp\rangle\,,$$

where

$$\epsilon = \sqrt{\epsilon_M^2 + \epsilon_G^2 - \epsilon_M^2\epsilon_G^2}\,,$$

and

$$|\Psi^\perp\rangle = \frac{\epsilon_M S_G}{\epsilon}|g\rangle \otimes |\phi^\perp\rangle + \frac{\epsilon_G S_M}{\epsilon}|g^\perp\rangle \otimes |\phi\rangle + \frac{\epsilon_G \epsilon_M}{\epsilon}|g^\perp\rangle \otimes |\phi^\perp\rangle\,. \tag{B.2}$$

Note that in the cases when S_G and S_M are large (and consequently ϵ_G and ϵ_M are small), we can neglect the final term from (B.2), obtaining the Schmidt form of the "orthogonal correction" of the state $|\tilde{\Psi}\rangle$, with respect to $|\Psi\rangle$. It is interesting to observe that such a state is always necessarily entangled, as its entanglement entropy is always bigger than zero. In other words, to obtain a nearby classical product state of gravity and matter $|\tilde{\Psi}\rangle$, one has to perturb the original (classical product) state $|\Psi\rangle$ with an entangled state $|\Psi^\perp\rangle \approx \epsilon^{-1}\epsilon_M S_G|g\rangle \otimes |\phi^\perp\rangle + \epsilon^{-1}\epsilon_G S_M|g^\perp\rangle \otimes |\phi\rangle$.

C Phase of interference terms

In this appendix, we analyze the expressions for the expectation values of the metric and the stress-energy tensors in the entangled state (3.5), given by (3.6) and (3.7), respectively. We show that their third, interference, terms are generically different from zero, and thus contain non-trivial contributions linear in η. Since the two terms have the same form, we will consider the case of the metric operator only.

By writing $\kappa = |\kappa| e^{i\varphi_\kappa} = F e^{i\varphi_\kappa}$ and $\langle\Psi^\perp|\hat{g}_{\mu\nu}|\Psi\rangle = |\langle\Psi^\perp|\hat{g}_{\mu\nu}|\Psi\rangle| e^{i\varphi_g}$, the third term of (3.6) has the form

$$2\eta\,\mathrm{Re}\left(\kappa\langle\Psi^\perp|\hat{g}_{\mu\nu}|\Psi\rangle\right) = 2\eta F|\langle\Psi^\perp|\hat{g}_{\mu\nu}|\Psi\rangle|\cos(\varphi_\kappa+\varphi_g)\,. \tag{C.1}$$

In case $\varphi_\kappa + \varphi_g = \pm\pi/2$, i.e., the interference term is zero, then for *any other generic* choice of $|\Psi'\rangle = e^{i\delta}|\Psi\rangle$, we have that $\varphi'_\kappa + \varphi'_g \neq \pm\pi/2$.

Indeed, changing $|\Psi\rangle \to |\Psi'\rangle = e^{i\delta}|\Psi\rangle$ induces the change of the other classical state

$$|\tilde{\Psi}\rangle = S|\Psi\rangle + \epsilon|\Psi^\perp\rangle \;\longrightarrow\; |\tilde{\Psi}'\rangle = S|\Psi'\rangle + \epsilon|\Psi^\perp\rangle = S'|\Psi\rangle + \epsilon|\Psi^\perp\rangle$$

with $S' = Se^{i\delta} = |S|e^{i(\varphi_s+\delta)}$ (where $S = |S|e^{i\varphi_s}$), but the orthogonal state $|\Psi^\perp\rangle$ *does not* change. Thus, the phase of the matrix element from (C.1) changes to $\varphi'_g = \varphi_g + \delta$. On the other hand, the phase of κ changes to $\varphi'_\kappa = \varphi_\kappa + \tilde{\delta}$ (note that $\tilde{\delta}$ is a function of δ, see below). Since

$$\begin{aligned}\kappa &= \alpha + \beta|S|e^{i\varphi_s} = |\kappa|e^{i\varphi_\kappa}\,,\\ \kappa' &= \alpha + \beta|S|e^{i(\varphi_s+\delta)} = |\kappa|e^{i\varphi'_\kappa}\,,\end{aligned}$$

it is obvious that for a generic choice of the parameters, i.e., in but a discrete number of points, we have $\tilde{\delta} = \varphi'_k - \varphi_k \neq -\delta$, obtaining $\varphi'_\kappa + \varphi'_g = (\varphi_s+\varphi_\kappa) + (\delta+\tilde{\delta}) = \pm\pi/2 + (\delta+\tilde{\delta}) \neq \pm\pi/2$.

Thus, the linear correction to (3.6), and to (3.7) as well, is zero only for a discrete number of the relative phases between the classical states $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$. Otherwise, it is generically non-trivial.

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Hamiltonian analysis of the *BFCG* formulation of general relativity

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Abstract

We perform the complete Hamiltonian analysis of the BFCG action for general relativity. We determine all the constraints of the theory and classify them into the first-class and the second-class constraints. We also show how the canonical formulation of BFCG general relativity reduces to the Einstein–Cartan and triad canonical formulations. The reduced phase space analysis also gives a 2-connection which is suitable for the construction of a spin-foam basis which will be a categorical generalization of the spin-network basis from loop quantum gravity.

Keywords: BFCG model, Poincaré 2-group, general relativity, Hamiltonian analysis, algebra of constraints, spin-cube model, spin-foam model

1. Introduction

Among the fundamental problems of modern theoretical physics, by far the most prominent one is the construction of the tentative theory of quantum gravity (QG). There are many approaches to QG, one of which is called loop quantum gravity (LQG), see [1–4]. As with any other physical system, the quantization of the gravitational field can be performed either canonically, using the Hamiltonian framework, or covariantly, using the Lagrangian, i.e. the path integral framework. Within the LQG approach, in the canonical framework [2] one chooses the connection variables and their momenta as fundamental fields for gravity, and uses them to construct an appropriate physical Hilbert space, giving rise to the spin-network states. In the covariant framework, one puts the connection variables onto a spacetime triangulation, see [3, 4], and uses this construction to define a path integral for gravity, giving rise to the spin-foam (SF) models.

The *BFCG* formulation of GR [5] was invented in order to find a categorical generalization of the SF models. A categorical generalization of a SF model is called a spin-cube model, since the path integral is based on a colored 3-complex where the colors are the representations of a 2-group [5, 6]. The 2-group, see [7] for a review and references, replaces the Lorentz group, and becomes the fundamental algebraic structure. The reason for introducing spin-cube models was that the SF models have two problems. One problem is that the classical limit of a SF model is described by the area-Regge action [6, 8]. The second problem is that the fermions cannot be coupled to a SF model [5]. These two problems are caused by the fact that the tetrads are absent from the Plebanski action, see [3, 9–11], which is used as the classical action to build the SF amplitudes. The *BFCG* action for GR is a categorical generalization of the Plebanski action, and the *BFCG* action contains both the B field and the tetrads [5].

The path integral quantization of *BFCG* GR reduces to the Regge path integral [6]. However, in the case of the canonical quantization, it is not known what kind of theories can be obtained. It was argued in [12] that a spin-foam basis should exist, as a categorical generalization of the spin-network basis from LQG, but in order to rigorously prove such a statement, one needs a canonical formulation of the *BFCG* GR theory. The canonical analysis of *BFCG* GR action is much more complicated than the canonical analysis of the Einstein–Hilbert action. One can see what kind of canonical analysis will be necessary from the canonical analysis of simpler but related actions given by the unconstrained *BFCG* action [13] or the Einstein–Cartan action [14].

In this paper we present the Hamiltonian analysis of the *BFCG* GR theory in full detail. Despite being straightforward, the calculations involved are quite nontrivial, so it is important to perform the full analysis in a systematic manner. Due to the amount of material presented, subsequent topics such as quantization schemes and similar have been postponed for future work, while the present paper deals only with the canonical structure of the classical theory.

The paper is organized as follows. In section 2 we give an overview of the *BFCG* GR action, discuss the Lagrange equations of motion, and prepare for the Hamiltonian analysis. The first part of the Hamiltonian analysis is done in section 3. We evaluate the conjugate momenta for the fields, obtain the primary constraints and construct the Hamiltonian of the theory. Then we impose consistency conditions on on all constraints in turn, giving rise to a full set of primary, secondary and tertiary constraints, along with some determined Lagrange multipliers. Section 4 is devoted to the second part of the Hamiltonian analysis—the separation of the constraints into first and second class, computing their algebra, and determining the number of physical degrees of freedom. Building on these results, in section 5 we discuss various avenues for the elimination of the second class constraints from the theory, gauge fixing conditions and the analysis of the first class constraints, and the resulting possible reductions of the phase space of the theory. Section 6 contains our concluding remarks, discussion of the results and future lines of research. The appendix contains four sections with a lot of technical details about the calculations performed in the main text.

Our notation and conventions are as follows. The spacetime indices are denoted with lowercase Greek alphabet letters from the middle of the alphabet $\lambda, \mu, \nu, \rho, \dots$ and take the values $0, 1, 2, 3$. When discussing the foliation of spacetime into space and time, the spacetime indices are split as $\mu = (0, i)$, where the lowercase indices from the middle of the Latin alphabet $i, j, k, \dots$ take only spacelike values $1, 2, 3$. The Poincaré group indices are denoted with lowercase letters from the beginning of the Latin alphabet, $a, b, c, \dots$ and take the values $0, 1, 2, 3$, while their spacelike counterparts are denoted by the lower-case Greek letters from the beginning of the alphabet $\alpha, \beta, \dots$, and take the values $1, 2, 3$. The group indices are raised and lowered with the Minkowski metric $\eta_{ab} = \mathrm{diag}(-1, 1, 1, 1)$. Capital Latin indices $A, B, C, \dots$ represent multi-index notation, and are used to count the second class constraints, fields and momenta, and various other objects, depending on the context. Antisymmetrization is denoted with the square brackets around the indices with the $1/2$ factor, $X_{[ab]} \equiv (X_{ab} - X_{ba})/2$. In order to simplify the notation involving Poisson brackets, we will adopt the following convention. The left quantity in every Poisson bracket is assumed to be evaluated at the point $x = (t, \vec{x})$, while the right quantity at the point $y = (t, \vec{y})$. In addition, we use the shorthand notation for the 3-dimensional Dirac delta function $\delta^{(3)} \equiv \delta^{(3)}(\vec{x} - \vec{y})$. For example, an expression

$$\{ U^{\alpha}(t,\vec{x}) \, , \, V^{\beta}(t,\vec{y}) \} = W^{\alpha\beta}(t,\vec{x})\delta^{(3)}(\vec{x}-\vec{y}) + Z^{\alpha\beta i}(t,\vec{x}) \, \partial_i \delta^{(3)}(\vec{x}-\vec{y}), \qquad (1)$$

where $\partial_i = \partial/\partial x^i$, can be written more compactly as

$$\{ U^{\alpha} \, , \, V^{\beta} \} = W^{\alpha\beta}\delta^{(3)} + Z^{\alpha\beta i} \, \partial_i \delta^{(3)}, \qquad (2)$$

usually without any ambiguity. In the rare ambiguous cases, the expressions will be written more explicitly. This notation will be used systematically unless stated otherwise.

2. *BFCG* action for GR

Given a Lie group $\mathcal{G}$ and its Lie algebra $\mathfrak{g}$, and the $\mathfrak{g}$-valued connection one-form A on a spacetime manifold $\mathcal{M}$, the *BF* action (see [15] for a review and applications to gravity)

$$S_{BF} = \int_{\mathcal{M}} \langle B \wedge F \rangle_{\mathfrak{g}}, \qquad (3)$$

describes the dynamics of flat connections, where $F = \mathrm{d}A + A \wedge A$ is the curvature two-form. B is a $\mathfrak{g}$-valued Lagrange multiplier two-form and $\langle , \rangle_{\mathfrak{g}}$ represents the invariant nondegenerate symmetric bilinear form in $\mathfrak{g}$. The *BF* theory relevant for the construction of spin-foam models is based on the Lorentz group $SO(3,1)$. A categorical generalization of the *BF* theory is based on the concept of a strict 2-group, which is a pair of groups $(\mathcal{G}, \mathcal{H})$ with certain maps between them (see [7] for details). The corresponding theory of flat 2-connections is called the *BFCG* theory [16, 17], and its dynamics is given by the action

$$S_{BFCG} = \int_{\mathcal{M}} \left[\langle B \wedge F \rangle_{\mathfrak{g}} + \langle C \wedge G \rangle_{\mathfrak{h}} \right]. \qquad (4)$$

The second term in (4) consists of a $\mathfrak{h}$-valued one-form Lagrange multiplier C, and a curvature three-form $G = \mathrm{d}\beta + A \wedge \beta$ for the $\mathfrak{h}$-valued two-form β, where $\mathfrak{h}$ is the Lie algebra of the group $\mathcal{H}$. The pair (A, β) is called the 2-connection for the 2-group, while the pair (F, G) is the corresponding 2-curvature. The $\langle , \rangle_{\mathfrak{h}}$ is the invariant nondegenerate symmetric bilinear form in $\mathfrak{h}$, which is $\mathfrak{g}$-invariant.

The Poincaré 2-group, defined by $\mathcal{G} = SO(3,1)$ and $\mathcal{H} = \mathbb{R}^4$, is relevant for GR since the Einstein equations can be obtained from a constrained *BFCG* action [5], given by

$$S_{GR} = \int_{\mathcal{M}} \left[\langle B \wedge R \rangle_{\mathfrak{g}} + \langle e \wedge G \rangle_{\mathfrak{h}} - \langle \phi \wedge (B - \star(e \wedge e)) \rangle_{\mathfrak{g}} \right]. \qquad (5)$$

Here we have relabeled $C \equiv e$ and $F \equiv R$, since in the case of the Poincaré 2-group these fields have the interpretation of the tetrad field and the curvature two-form for the spin connection $A \equiv \omega$. The $\mathfrak{g}$-valued two-form ϕ is an additional Lagrange multiplier, featuring in the simplicity constraint term. The $\star$ is the Hodge dual operator for the Minkowski space.

The action (5) can be written as

$$S_{GR} = \int_{\mathcal{M}} \left[B_{ab} \wedge R^{ab} + e^a \wedge G_a - \phi^{ab} \wedge \left(B_{ab} - \varepsilon_{abcd}\, e^c \wedge e^d \right) \right] , \tag{6}$$

where the curvatures R^{ab} and G^a are given by

$$R^{ab} = \mathrm{d}\omega^{ab} + \omega^a{}_c \wedge \omega^{cb}, \tag{7}$$

$$G^a = \nabla \beta^a \equiv \mathrm{d}\beta^a + \omega^a{}_b \wedge \beta^b. \tag{8}$$

The action (6) can even be extended to include the cosmological constant, and it is related to the MacDowell–Mansouri action [18–22], see appendix E for details.

It is convenient to introduce the torsion 2-form

$$T^a = \nabla e^a \equiv \mathrm{d}e^a + \omega^a{}_b \wedge e^b, \tag{9}$$

so that one can rewrite the action as

$$S_{PGT} = \int_{\mathcal{M}} \left[B_{ab} \wedge R^{ab} + \beta^a \wedge T_a - \phi^{ab} \wedge \left(B_{ab} - \varepsilon_{abcd}\, e^c \wedge e^d \right) \right] \tag{10}$$

by using the integration by parts. The action (10) is a constrained *BF* action for the Poincaré group, since the tetrads and the spin connection can be considered as components of a Poincaré group connection, while the curvature and the torsion are the components of the Poincaré group curvature [12]. This equivalence of a Poincaré gauge theory formulation to a 2-group gauge theory formulation is specific to 4 spacetime dimensions only.

The relationship between the topological, unconstrained versions of the actions (6) and (10) has been discussed in detail in [13]. There, a real parameter ξ was introduced to interpolate between the two actions, the full Hamiltonian analysis was performed, and the implications of the parameter ξ for the structure of the resulting phase space were studied in detail. It is noteworthy that the actions (6) and (10) differ from the actions discussed in [13] only by the presence of the simplicity constraint term, which is the same for both actions and does not contain any time derivatives. Therefore, the presence of the simplicity constraint does not change any results of [13] pertaining to the ξ parameter, and all conclusions related to ξ given in [13] carry over unmodified to the constrained actions (6) and (10) discussed in this paper. Given this situation, we opt not to introduce and discuss the ξ parameter again in this paper, and refer the reader to [13] instead.

It is clear that the actions (6) and (10) give rise to the same set of equations of motion, since these do not depend on the boundary. Taking the variation of (6) with respect to all the variables, one obtains

$$\delta B : R^{ab} - \phi^{ab} = 0, \tag{11}$$

$$\delta \beta : T^a = 0, \tag{12}$$

$$\delta e : G_a + 2\varepsilon_{abcd}\, \phi^{bc} \wedge e^d = 0, \tag{13}$$

$$\delta \omega : \nabla B^{ab} - e^{[a} \wedge \beta^{b]} = 0, \tag{14}$$

$$\delta \phi : B_{ab} - \varepsilon_{abcd}\, e^c \wedge e^d = 0, \tag{15}$$

where the covariant exterior derivative of B^{ab} is defined as

$$\nabla B^{ab} \equiv \mathrm{d}B^{ab} + \omega^a{}_c \wedge B^{cb} + \omega^b{}_c \wedge B^{ac}. \tag{16}$$

One can simplify the equations of motion in the following way. Taking the covariant exterior derivative of (15) and using (12) one obtains $\nabla B^{ab} = 0$. Substituting this into (14) one further obtains $e^{[a} \wedge \beta^{b]} = 0$. Under the assumption that $\det(e^a{}_\mu) \neq 0$, it follows that $\beta^a = 0$ (see appendix in [5] for proof), and therefore also $G^a = 0$. As a consequence, we see that the equations of motion (11)–(15) are equivalent to the following system:

- the equation that determines the multiplier ϕ^{ab} in terms of curvature,

$$\phi^{ab} = R^{ab}, \tag{17}$$

- the equation that determines the multiplier B^{ab} in terms of tetrads,

$$B_{ab} = \varepsilon_{abcd}\, e^c \wedge e^d, \tag{18}$$

- the equation that determines β^a,

$$\beta^a = 0, \tag{19}$$

- the equation for the torsion,

$$T^a = 0, \tag{20}$$

- and the Einstein field equation,

$$\varepsilon_{abcd}\, R^{bc} \wedge e^d = 0. \tag{21}$$

Finally, for the convenience of the Hamiltonian analysis, we need to rewrite both the action and the equations of motion in a local coordinate frame. Choosing $\mathrm{d}x^\mu$ as basis one-forms, we can expand the fields in the standard fashion:

$$e^a = e^a{}_\mu \mathrm{d}x^\mu, \qquad \omega^{ab} = \omega^{ab}{}_\mu \mathrm{d}x^\mu, \tag{22}$$

$$B^{ab} = \frac{1}{2} B^{ab}{}_{\mu\nu} \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu, \quad \beta^a = \frac{1}{2}\beta^a{}_{\mu\nu} \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu, \quad \phi^{ab} = \frac{1}{2}\phi^{ab}{}_{\mu\nu} \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu. \tag{23}$$

Similarly, the field strengths for ω, e and β are

$$\begin{aligned} R^{ab} &= \frac{1}{2} R^{ab}{}_{\mu\nu} \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu, \\ T^a &= \frac{1}{2} T^a{}_{\mu\nu} \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu, \\ G^a &= \frac{1}{6} G^a{}_{\mu\nu\rho} \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho. \end{aligned} \tag{24}$$

Using the relations (7)–(9), we can write the component equations

$$\begin{aligned} R^{ab}{}_{\mu\nu} &= \partial_\mu \omega^{ab}{}_\nu - \partial_\nu \omega^{ab}{}_\mu + \omega^a{}_{c\mu}\omega^{cb}{}_\nu - \omega^a{}_{c\nu}\omega^{cb}{}_\mu, \\ T^a{}_{\mu\nu} &= \partial_\mu e^a{}_\nu - \partial_\nu e^a{}_\mu + \omega^a{}_{b\mu} e^b{}_\nu - \omega^a{}_{b\nu} e^b{}_\mu, \\ G^a{}_{\mu\nu\rho} &= \partial_\mu \beta^a{}_{\nu\rho} + \partial_\nu \beta^a{}_{\rho\mu} + \partial_\rho \beta^a{}_{\mu\nu} + \omega^a{}_{b\mu}\beta^b{}_{\nu\rho} + \omega^a{}_{b\nu}\beta^b{}_{\rho\mu} + \omega^a{}_{b\rho}\beta^b{}_{\mu\nu}. \end{aligned} \tag{25}$$

Substituting expansions (22)–(24) into the action, we obtain

$$S = \int_{\mathcal{M}} \mathrm{d}^4x\, \varepsilon^{\mu\nu\rho\sigma} \left[\frac{1}{4} B_{ab\mu\nu} R^{ab}{}_{\rho\sigma} + \frac{1}{6} e_{a\mu} G^a{}_{\nu\rho\sigma} - \frac{1}{4}\phi^{ab}{}_{\mu\nu} \left(B_{ab\rho\sigma} - 2\varepsilon_{abcd}\, e^c{}_\rho e^d{}_\sigma \right) \right]. \tag{26}$$

Assuming that the spacetime manifold has the topology $\mathcal{M} = \Sigma \times \mathbb{R}$, where Σ is a 3-dimensional spacelike hypersurface, from the above action we can read off the Lagrangian, which is the integral of the Lagrangian density over the hypersurface Σ:

$$L = \int_\Sigma \mathrm{d}^3 x\, \varepsilon^{\mu\nu\rho\sigma} \left[\frac{1}{4} B_{ab\mu\nu} R^{ab}{}_{\rho\sigma} + \frac{1}{6} e_{a\mu} G^a{}_{\nu\rho\sigma} - \frac{1}{4} \phi^{ab}{}_{\mu\nu} \left(B_{ab\rho\sigma} - 2\varepsilon_{abcd}\, e^c{}_\rho e^d{}_\sigma \right) \right]. \tag{27}$$

Finally, the component form of equations of motion (17)–(21) is:

$$\begin{aligned} &\phi^{ab}{}_{\mu\nu} = R^{ab}{}_{\mu\nu}, \qquad && B_{ab\mu\nu} = 2\varepsilon_{abcd}\, e^c{}_\mu e^d{}_\nu, \\ &\beta^a{}_{\mu\nu} = 0, && T^a{}_{\mu\nu} = 0, \\ &\varepsilon^{\lambda\mu\nu\rho} \varepsilon_{abcd}\, R^{bc}{}_{\mu\nu} e^d{}_\rho = 0. && \end{aligned} \tag{28}$$

3. Hamiltonian analysis

Now we turn to the Hamiltonian analysis. A detailed review of the general formalism can be found in [14], chapter V. In addition, a good pedagogical example of the Hamiltonian analysis which is relevant for our case is the topological *BFCG* gravity [13].

3.1. Primary constraints and the Hamiltonian

As a first step, we calculate the momenta π corresponding to the field variables $B^{ab}{}_{\mu\nu}$, $\phi^{ab}{}_{\mu\nu}$, $e^a{}_\mu$, $\omega^{ab}{}_\mu$ and $\beta^a{}_{\mu\nu}$. Differentiating the action (26) with respect to the time derivative of the appropriate fields, we obtain the momenta as follows:

$$\begin{aligned} \pi(B)_{ab}{}^{\mu\nu} &= \frac{\delta S}{\delta \partial_0 B^{ab}{}_{\mu\nu}} = 0, \\ \pi(\phi)_{ab}{}^{\mu\nu} &= \frac{\delta S}{\delta \partial_0 \phi^{ab}{}_{\mu\nu}} = 0, \\ \pi(e)_a{}^\mu &= \frac{\delta S}{\delta \partial_0 e^a{}_\mu} = 0, \\ \pi(\omega)_{ab}{}^\mu &= \frac{\delta S}{\delta \partial_0 \omega^{ab}{}_\mu} = \varepsilon^{0\mu\nu\rho} B_{ab\nu\rho}, \\ \pi(\beta)_a{}^{\mu\nu} &= \frac{\delta S}{\delta \partial_0 \beta^a{}_{\mu\nu}} = -\varepsilon^{0\mu\nu\rho} e_{a\rho}. \end{aligned} \tag{29}$$

None of the momenta can be solved for the corresponding 'velocities', so they all give rise to primary constraints:

$$\begin{aligned} P(B)_{ab}{}^{\mu\nu} &\equiv \pi(B)_{ab}{}^{\mu\nu} \approx 0, \\ P(\phi)_{ab}{}^{\mu\nu} &\equiv \pi(\phi)_{ab}{}^{\mu\nu} \approx 0, \\ P(e)_a{}^\mu &\equiv \pi(e)_a{}^\mu \approx 0, \\ P(\omega)_{ab}{}^\mu &\equiv \pi(\omega)_{ab}{}^\mu - \varepsilon^{0\mu\nu\rho} B_{ab\nu\rho} \approx 0, \\ P(\beta)_a{}^{\mu\nu} &\equiv \pi(\beta)_a{}^{\mu\nu} + \varepsilon^{0\mu\nu\rho} e_{a\rho} \approx 0. \end{aligned} \tag{30}$$

The weak, on-shell equality is denoted '$\approx$', as opposed to the strong, off-shell equality which is denoted by the usual symbol '$=$'.

Next we introduce the fundamental simultaneous Poisson brackets between the fields and their conjugate momenta,

$$\begin{aligned}
\{ B^{ab}{}_{\mu\nu} \,,\, \pi(B)_{cd}{}^{\rho\sigma} \} &= 4\delta^a_{[c}\delta^b_{d]}\delta^\rho_{[\mu}\delta^\sigma_{\nu]}\delta^{(3)}, \\
\{ \phi^{ab}{}_{\mu\nu} \,,\, \pi(\phi)_{cd}{}^{\rho\sigma} \} &= 4\delta^a_{[c}\delta^b_{d]}\delta^\rho_{[\mu}\delta^\sigma_{\nu]}\delta^{(3)}, \\
\{ e^a{}_\mu \,,\, \pi(e)_b{}^\nu \} &= \delta^a_b\delta^\nu_\mu\delta^{(3)}, \\
\{ \omega^{ab}{}_\mu \,,\, \pi(\omega)_{cd}{}^\nu \} &= 2\delta^a_{[c}\delta^b_{d]}\delta^\nu_\mu\delta^{(3)}, \\
\{ \beta^a{}_{\mu\nu} \,,\, \pi(\beta)_b{}^{\rho\sigma} \} &= 2\delta^a_b\delta^\rho_{[\mu}\delta^\sigma_{\nu]}\delta^{(3)},
\end{aligned} \tag{31}$$

and we employ them to calculate the algebra of primary constraints,

$$\begin{aligned}
\{ P(B)^{abjk} \,,\, P(\omega)_{cd}{}^i \} &= 4\varepsilon^{0ijk}\delta^a_{[c}\delta^b_{d]}\delta^{(3)}, \\
\{ P(e)^{ak} \,,\, P(\beta)_b{}^{ij} \} &= -\varepsilon^{0ijk}\delta^a_b\delta^{(3)},
\end{aligned} \tag{32}$$

while all other Poisson brackets vanish.

Next we construct the canonical, on-shell Hamiltonian:

$$\begin{aligned}
H_c = \int_\Sigma \mathrm{d}^3\vec{x} \Bigg[&\frac{1}{4}\pi(B)_{ab}{}^{\mu\nu}\partial_0 B^{ab}{}_{\mu\nu} + \frac{1}{4}\pi(\phi)_{ab}{}^{\mu\nu}\partial_0\phi^{ab}{}_{\mu\nu} + \pi(e)_a{}^\mu\partial_0 e^a{}_\mu \\
&+ \frac{1}{2}\pi(\omega)_{ab}{}^\mu\partial_0\omega^{ab}{}_\mu + \frac{1}{2}\pi(\beta)_a{}^{\mu\nu}\partial_0\beta^a{}_{\mu\nu} \Bigg] - L.
\end{aligned} \tag{33}$$

The factors $1/4$ and $1/2$ are introduced to prevent overcounting of variables. Using (25) and (27), one can rearrange the expressions such that all velocities are multiplied by primary constraints, and therefore vanish from the Hamiltonian. After some algebra, the resulting expression can be written as

$$\begin{aligned}
H_c = -\int_\Sigma \mathrm{d}^3\vec{x}\,\varepsilon^{0ijk} \Bigg[&\frac{1}{2}B_{ab0i}\left(R^{ab}{}_{jk} - \phi^{ab}{}_{jk}\right) + e^a{}_0\left(\frac{1}{6}G_{aijk} + \varepsilon_{abcd}\,\phi^{bc}{}_{ij}e^d{}_k\right) \\
&+ \frac{1}{2}\beta_{a0k}T^a{}_{ij} + \frac{1}{2}\omega_{ab0}\left(\nabla_i B^{ab}{}_{jk} - e^a{}_i\beta^b{}_{jk}\right) - \frac{1}{2}\phi^{ab}{}_{0i}\left(B_{abjk} - 2\varepsilon_{abcd}\,e^c{}_j e^d{}_k\right)\Bigg],
\end{aligned} \tag{34}$$

up to a boundary term. The canonical Hamiltonian does not depend on any momenta, but only on fields and their spatial derivatives. Finally, introducing Lagrange multipliers λ for each of the primary constraints, we construct the total, off-shell Hamiltonian:

$$\begin{aligned}
H_T = H_c + \int_\Sigma \mathrm{d}^3\vec{x} \Bigg[&\frac{1}{4}\lambda(B)^{ab}{}_{\mu\nu}P(B)_{ab}{}^{\mu\nu} + \frac{1}{4}\lambda(\phi)^{ab}{}_{\mu\nu}P(\phi)_{ab}{}^{\mu\nu} \\
&+ \lambda(e)^a{}_\mu P(e)_a{}^\mu + \frac{1}{2}\lambda(\omega)^{ab}{}_\mu P(\omega)_{ab}{}^\mu + \frac{1}{2}\lambda(\beta)^a{}_{\mu\nu}P(\beta)_a{}^{\mu\nu}\Bigg].
\end{aligned} \tag{35}$$

3.2. Consistency procedure

We proceed with the calculation of the consistency requirements for the constraints. The consistency requirement is that the time derivative of each constraint (or equivalently its Poisson bracket with the total Hamiltonian (35)) must vanish on-shell. This requirement can either give rise to a new constraint, or determine some multiplier, or be satisfied identically. In our case, the consistency requirements give rise to a complicated chain structure, depicted in the following diagram:

$$
\begin{array}{lclclcl}
P(\beta)_a{}^{0i} & \xrightarrow{1} & S(T)^{ai} & \xrightarrow{15} & T(eR\phi)^{ai} & \rceil \xrightarrow{16} & T(eR\phi)^{ab}{}_k \\
P(e)_a{}^i & \xrightarrow{11} & S(eR\phi)^{ai} & \longrightarrow & \longrightarrow & \rfloor & \\
P(B)_{ab}{}^{0i} & \xrightarrow{2} & S(R\phi)^{abi} & \xrightarrow{13} & \lambda(\phi)_{abij} & & \downarrow 17 \\
P(\phi)_{ab}{}^{ij} & \xrightarrow{3} & S(Bee)^{abij} & \xrightarrow{14} & \lambda(B)_{ab0i} & & \lambda(\phi)^{ab}{}_{0i} \\
P(B)_{ab}{}^{ij} & \xrightarrow{4} & \lambda(\omega)_{abi} & & & & \\
P(\beta)_a{}^{ij} & \xrightarrow{5} & \lambda(e)_{ai} & & & & \\
P(\omega)_{ab}{}^i & \xrightarrow{6} & \lambda(B)_{abij} & & & & \\
P(\phi)_{ab}{}^{0i} & \xrightarrow{7} & S(Bee)^{abi} & \rceil \xrightarrow{8} & T(\beta)^a{}_{\mu\nu} & \xrightarrow{9} & \lambda(\beta)^a{}_{\mu\nu} \\
P(\omega)_{ab}{}^0 & \longrightarrow & \longrightarrow & \rfloor & & & \\
P(e)_a{}^0 & \xrightarrow{10} & S(eR)^a & \xrightarrow{12} & 0 & &
\end{array}
$$

Here every arrow represents one consistency requirement, and numbers on the arrows denote the order in which we will discuss them. Steps 8 and 16 involve multiple constraints simultaneously, and will require special consideration. Primary, secondary and tertiary constraints are denoted as P, S and T, respectively.

We begin by discussing consistency conditions 1–7,

$$
\begin{aligned}
&\dot{P}(\beta)_a{}^{0i} \approx 0, \quad \dot{P}(B)_{ab}{}^{0i} \approx 0, \quad \dot{P}(\phi)_{ab}{}^{ij} \approx 0, \quad \dot{P}(\phi)_{ab}{}^{0i} \approx 0, \\
&\dot{P}(B)_{ab}{}^{ij} \approx 0, \quad \dot{P}(\beta)_a{}^{ij} \approx 0, \quad \dot{P}(\omega)_{ab}{}^i \approx 0.
\end{aligned} \tag{36}
$$

Calculating the corresponding Poisson brackets with the total Hamiltonian, these give rise to the following secondary constraints,

$$
\begin{array}{lcl}
S(T)^{ai} & \equiv & \varepsilon^{0ijk} T^a{}_{jk} \approx 0, \\
S(R\phi)^{abi} & \equiv & \varepsilon^{0ijk} \left(R^{ab}{}_{jk} - \phi^{ab}{}_{jk} \right) \approx 0, \\
S(Bee)^{abij} & \equiv & \varepsilon^{0ijk} \left(B^{ab}{}_{0k} - 2\varepsilon^{abcd} \, e_{c0} e_{dk} \right) \approx 0, \\
S(Bee)^{abi} & \equiv & \varepsilon^{0ijk} \left(B^{ab}{}_{jk} - 2\varepsilon^{abcd} \, e_{cj} e_{dk} \right) \approx 0,
\end{array} \tag{37}
$$

and determine the following multipliers,

$$
\begin{array}{lcl}
\lambda(\omega)^{ab}{}_i & \approx & \nabla_i \omega^{ab}{}_0 + \phi^{ab}{}_{0i}, \\
\lambda(e)^a{}_i & \approx & \nabla_i e^a{}_0 - \omega^a{}_{b0} e^b{}_i, \\
\lambda(B)^{ab}{}_{ij} & \approx & 4\varepsilon^{abcd} \left(\nabla_{[i} e_{c0} - \omega_{cf0} e^f{}_{[i} \right) e_{dj]} + e^{[a}{}_0 \beta^{b]}{}_{ij} - 2e^{[a}{}_{[i} \beta^{b]}{}_{0j]}.
\end{array} \tag{38}
$$

In step 8 we discuss the consistency conditions

$$
\dot{S}(Bee)^{abi} \approx 0, \qquad \dot{P}(\omega)_{ab}{}^0 \approx 0, \tag{39}
$$

simultaneously. Calculating the time derivatives, we obtain

$$
\varepsilon^{0ijk} \left(e^{[a}{}_0 \beta^{b]}{}_{jk} - 2e^{[a}{}_j \beta^{b]}{}_{0k} \right) \approx 0, \qquad \varepsilon^{0ijk} \, e^{[a}{}_i \beta^{b]}{}_{jk} \approx 0, \tag{40}
$$

which can be jointly written as a covariant equation

$$
\varepsilon^{\mu\nu\rho\sigma} \, e^{[a}{}_\nu \beta^{b]}{}_{\rho\sigma} \approx 0. \tag{41}
$$

With the assumption that $\det(e^a{}_\mu) \neq 0$, this can be solved for β^a, giving a set of very simple tertiary constraints:

$$T(\beta)^a{}_{\mu\nu} \equiv \beta^a{}_{\mu\nu} \approx 0. \tag{42}$$

At this point we can immediately analyze the consistency step 9 as well. Taking the time derivative of (42), one easily determines the corresponding multipliers,

$$\lambda(\beta)^a{}_{\mu\nu} \approx 0. \tag{43}$$

Next, in steps 10 and 11, from the consistency conditions for the remaining two primary constraints,

$$\dot{P}(e)_a{}^0 \approx 0, \qquad \dot{P}(e)_a{}^i \approx 0, \tag{44}$$

we obtain two new secondary constraints,

$$\begin{array}{lcl} S(eR)_a & \equiv & \varepsilon^{0ijk}\varepsilon_{abcd}e^b{}_iR^{cd}{}_{jk} \approx 0, \\ S(eR\phi)_a{}^i & \equiv & \varepsilon^{0ijk}\varepsilon_{abcd}\left(e^b{}_0R^{cd}{}_{jk} - 2e^b{}_j\phi^{cd}{}_{0k}\right) \approx 0. \end{array} \tag{45}$$

In step 12 we need to discuss the consistency condition for the constraint $S(eR)_a$. After a straightforward but tedious calculation, one eventually ends up with the following expression:

$$\dot{S}(eR)_a = \nabla_i S(eR\phi)_a{}^i + \omega^b{}_{a0}S(eR)_b + 2\varepsilon_{abcd}\phi^{cd}{}_{0k}S(T)^{bk}, \tag{46}$$

up to terms proportional to primary constraints. Since the time derivative is already expressed as a linear combination of constraints, the consistency condition is trivially satisfied, which is denoted with a zero in the diagram above.

Moving on to steps 13–15, the consistency conditions

$$\dot{S}(R\phi)^{abi} \approx 0, \qquad \dot{S}(Bee)^{abij} \approx 0, \qquad \dot{S}(T)^{ai} \approx 0, \tag{47}$$

determine the multipliers

$$\begin{array}{lcl} \lambda(\phi)^{ab}{}_{jk} & \approx & 2\omega^{[a}{}_{c0}R^{b]c}{}_{jk} + 2\nabla_{[j}\phi^{ab}{}_{0k]}, \\ \lambda(B)_{ab0k} & \approx & 2\varepsilon_{abcd}\left[e^d{}_k\lambda(e)^c{}_0 - e^d{}_0\nabla_k e^c{}_0 + \omega^c{}_{f0}e^d{}_0e^f{}_k\right], \end{array} \tag{48}$$

and another tertiary constraint

$$T(eR\phi)^{ai} \equiv \varepsilon^{0ijk}\left(R^{ab}{}_{jk}e_{b0} + 2\phi^{ab}{}_{0j}e_{bk}\right) \approx 0. \tag{49}$$

Now we turn to step 16. At this point there are only two constraints, $T(eR\phi)^{ai}$ and $S(eR\phi)^{ai}$, whose consistency conditions have not been discussed yet. To this end, note that these two constraints can be rewritten into a very similar form,

$$\begin{array}{lcl} S(eR\phi)_a{}^i & = & \varepsilon_{abcd}\varepsilon^{0ijk}\left(e^b{}_0R^{cd}{}_{jk} - 2e^b{}_j\phi^{cd}{}_{0k}\right), \\ T(eR\phi)_a{}^i & = & \eta_{ac}\eta_{bd}\varepsilon^{0ijk}\left(e^b{}_0R^{cd}{}_{jk} - 2e^b{}_j\phi^{cd}{}_{0k}\right), \end{array} \tag{50}$$

where the identical expression in parentheses is contracted with ε_{abcd} in the first constraint and with $\eta_{ac}\eta_{bd}$ in the second. This suggests that we should discuss their consistency conditions simultaneously. As suggested in the diagram above, we will first rewrite these 24 constraints (50) into a system of $18 + 6$ constraints (to be denoted $T(eR\phi)_{abk}$ and $T(eR\phi)_{jk}$ respectively) as follows. Given that the tetrad $e^a{}_\mu$ is nondegenerate, we can freely multiply the constraints with it and split the index μ into space and time components. The $\mu = 0$ part is

$$
\begin{array}{rcl}
e^a{}_0 S(eR\phi)_a{}^i & = & -2\varepsilon_{abcd}\varepsilon^{0ijk} e^a{}_0 e^b{}_j \phi^{cd}{}_{0k}, \\
e^a{}_0 T(eR\phi)_a{}^i & = & -2\eta_{ac}\eta_{bd}\varepsilon^{0ijk} e^a{}_0 e^b{}_j \phi^{cd}{}_{0k},
\end{array} \tag{51}
$$

where the curvature terms have automatically vanished, while the $\mu = m$ part is

$$
\begin{array}{rcl}
e^a{}_m S(eR\phi)_a{}^i & = & e^a{}_m \varepsilon_{abcd}\varepsilon^{0ijk} \left(e^b{}_0 R^{cd}{}_{jk} - 2e^b{}_j \phi^{cd}{}_{0k} \right), \\
e^a{}_m T(eR\phi)_a{}^i & = & e^a{}_m \eta_{ac}\eta_{bd}\varepsilon^{0ijk} \left(e^b{}_0 R^{cd}{}_{jk} - 2e^b{}_j \phi^{cd}{}_{0k} \right).
\end{array} \tag{52}
$$

The system of 18 constraints (52) can be shown to be equivalent to the following constraint:

$$
T(eR\phi)^{ab}{}_k \equiv \phi^{ab}{}_{0k} - e^f{}_0 R^{cd}{}_{ij} F^{abij}{}_{fcdk}, \tag{53}
$$

where $F^{abij}{}_{fcdk}$ is a complicated function of $e^a{}_i$ only. The proof that the system (52) is equivalent to (53) is given in appendix C, and the explicit expression for $F^{abij}{}_{fcdk}$ is given in equation (C.27). Second, introducing the shorthand notation $K_{abcd} \in \{\varepsilon_{abcd}, \eta_{ac}\eta_{bd}\}$ and using (53), we define

$$
T(eR\phi)^i \equiv -2K_{abcd}\varepsilon^{0ijk} e^a{}_0 e^b{}_j e^f{}_0 R^{gh}{}_{mn} F^{cdmn}{}_{fghk}, \tag{54}
$$

which represents a set of $3 + 3 = 6$ constraints equivalent to (51). However, a straightforward and meticulous (albeit very long) calculation shows that the expression (54) is already a linear combination of known constraints and Bianchi identities, and is thus already weakly equal to zero. Therefore, $T(eR\phi)^i$ is not a new independent constraint, and its consistency condition is automatically satisfied.

Summing up the step 16, we have replaced the set of constraints (50) by an equivalent set (53). It thus follows that the consistency conditions for $S(eR\phi)_a{}^i$ and $T(eR\phi)_a{}^i$ are equivalent to the consistency condition for $T(eR\phi)^{ab}{}_k$. Consequently, in step 17, we find that the consistency condition

$$
\dot{T}(eR\phi)^{ab}{}_k \approx 0 \tag{55}
$$

determines the multiplier $\lambda(\phi)^{ab}{}_{0k}$ as

$$
\begin{aligned}
\lambda(\phi)^{ab}{}_{0k} \approx {} & \lambda(e)^f{}_0 R^{cd}{}_{ij} F^{abij}{}_{fcdk} + 2e^f{}_0 \left[R^c{}_{hij}\omega^{hd}{}_0 + \nabla_i \phi^{cd}{}_{0j} \right] F^{abij}{}_{fcdk} \\
& + e^f{}_0 R^{cd}{}_{ij} \frac{\partial F^{abij}{}_{fcdk}}{\partial e^h{}_m} \left(\nabla_m e^h{}_0 - \omega^h{}_{g0} e^g{}_m \right).
\end{aligned} \tag{56}
$$

This concludes the consistency procedure for all constraints.

3.3. Results

Let us sum up the results of the consistency procedure. We have determined the full set of constraints and multipliers as follows: the primary constraints are

$$
P(B)_{ab}{}^{\mu\nu}, \qquad P(\phi)_{ab}{}^{\mu\nu}, \qquad P(\beta)_a{}^{\mu\nu}, \qquad P(\omega)_{ab}{}^{\mu}, \qquad P(e)_a{}^{\mu}, \tag{57}
$$

and they have 36, 36, 24, 24 and 16 components, respectively, or 136 in total. The secondary constraints are

$$
S(T)^{ai}, \qquad S(R\phi)^{abi}, \qquad S(Bee)^{abij}, \qquad S(Bee)^{abi}, \qquad S(eR)^a, \tag{58}
$$

and they have $12 + 18 + 18 + 18 + 4 = 70$ components in total. The tertiary constraints are

$$
T(\beta)^a{}_{\mu\nu}, \qquad T(eR\phi)^{ab}{}_i \tag{59}
$$

and they have $24+18=42$ components. In addition, the determined multipliers are

$$\lambda(B)^{ab}{}_{\mu\nu}, \qquad \lambda(\phi)^{ab}{}_{\mu\nu}, \qquad \lambda(\beta)^{a}{}_{\mu\nu}, \qquad \lambda(\omega)^{ab}{}_{i}, \qquad \lambda(e)^{a}{}_{i}, \tag{60}$$

and they have $36+36+24+18+12=126$ components. Finally, there are 10 remaining undetermined multipliers,

$$\lambda(\omega)^{ab}{}_{0}, \qquad \lambda(e)^{a}{}_{0}. \tag{61}$$

In total, there are $C=136+70+42=248$ constraints, 126 determined and 10 undetermined multipliers, the latter corresponding to the 10 parameters of the local Poincaré symmetry of the action.

4. The physical degrees of freedom

Once we have found all the constraints in the theory, we need to classify each constraint as a first-class or a second-class constraint. While some of the second class constraints can be identified from (32), the classification is not easy since constraints are unique only up to linear combinations. The most efficient way to tabulate all first class constraints is to substitute all determined multipliers into the total Hamiltonian (35) and rewrite it in the form

$$H_T = \int \mathrm{d}^3\vec{x} \left[\frac{1}{2}\lambda(\omega)^{ab}{}_0\,\Phi(\omega)_{ab} + \lambda(e)^a{}_0\,\Phi(e)_a + \frac{1}{2}\omega^{ab}{}_0\,\Phi(T)_{ab} + e^a{}_0\,\Phi(R)_a \right]. \tag{62}$$

The quantities Φ are linear combinations of the constraints, and they must all be of the first class, since the total Hamiltonian weakly commutes with all constraints. Written in terms of the primary and the secondary constraints, the first-class constraints are given by

$$\begin{aligned}
\Phi(\omega)^{ab} &= P(\omega)^{ab0}, \\
\Phi(e)_a &= P(e)_a{}^0 + \frac{1}{2}R^{cd}{}_{ij}F^{fbij}{}_{acdk}P(\phi)_{fb}{}^{0k} + \varepsilon_{abcd}e^b{}_kP(B)^{cd0k}, \\
\Phi(T)^{ab} &= 4\varepsilon^{abcd}e_{ci}S(T)_d{}^i - \nabla_iS(Bee)^{abi} + \varepsilon^{0ijk}e^{[a}{}_iT(\beta)^{b]}{}_{jk} \\
&\quad +2\varepsilon^{abcd}e^f{}_ie_{cj}P(B)_{fd}{}^{ij} - \nabla_iP(\omega)^{abi} + 2e^{[a}{}_iP(e)^{b]i} \\
&\quad -R^{[ac}{}_{ij}P(\phi)_c{}^{b]ij}, \\
\Phi(R)_a &= -S(eR)_a + R^c{}_{hij}\omega^{hd}{}_0F^{fbij}{}_{acdk}P(\phi)_{fb}{}^{0k} \\
&\quad +R^{cd}{}_{ij}\frac{\partial F^{fbij}{}_{acdk}}{\partial e^h{}_m}\left(\nabla_me^h{}_0 - \omega^h{}_{g0}e^g{}_m\right)P(\phi)_{fb}{}^{0k} \\
&\quad -\varepsilon^{0ijk}\nabla_iT(\beta)_{ajk} + \varepsilon_{abcd}e^b{}_i\nabla_jP(B)^{cdij} - \nabla_iP(e)_a{}^i \\
&\quad +\varepsilon_{abcd}\left(\nabla_ke^b{}_0 - \omega^b{}_{f0}e^f{}_k\right)P(B)^{cd0k} \\
&\quad +\frac{1}{2}R^{cd}{}_{ij}F^{fbij}{}_{acdk}\left[S(Bee)_{fb}{}^k + P(\omega)_{fb}{}^k + \nabla_mP(\phi)_{fb}{}^{km}\right. \\
&\qquad \left. -2\nabla_m\left(e^e{}_0F^{ghmk}{}_{efbn}P(\phi)_{gh}{}^{0n}\right)\right].
\end{aligned} \tag{63}$$

The constraints (63) are the first-class constraints in the theory. The remaining constraints are of the second class

$$\begin{array}{lcl} \chi(T)^{ai} & = & S(T)^{ai}, \\ \chi(R\phi)^{abi} & = & S(R\phi)^{abi}, \\ \chi(Bee)^{abij} & = & S(Bee)^{abij}, \\ \chi(Bee)^{abi} & = & S(Bee)^{abi}, \\ \chi(\beta)^{a}{}_{\mu\nu} & = & T(\beta)^{a}{}_{\mu\nu}, \\ \chi(eR\phi)^{ab}{}_{i} & = & T(eR\phi)^{ab}{}_{i}. \end{array} \qquad \begin{array}{lcl} \chi(B)_{ab}{}^{\mu\nu} & = & P(B)_{ab}{}^{\mu\nu}, \\ \chi(\phi)_{ab}{}^{\mu\nu} & = & P(\phi)_{ab}{}^{\mu\nu}, \\ \chi(\beta)_{a}{}^{\mu\nu} & = & P(\beta)_{a}{}^{\mu\nu}, \\ \chi(\omega)_{ab}{}^{i} & = & P(\omega)_{ab}{}^{i}, \\ \chi(e)_{a}{}^{i} & = & P(e)_{a}{}^{i}. \end{array} \tag{64}$$

Note that $\chi(\beta)_a{}^{\mu\nu}$ and $\chi(\beta)^a{}_{\mu\nu}$ are different constraints, despite similar notation. Of course, there is no possibility of confusion since we will never raise or lower spacetime indices of these constraints in the rest of this paper. Also, note that despite the fact that there are 12 components of $\chi(T)^{ai}$, only 6 of them can be considered second class, since the other 6 are part of the first class constraint $\Phi(T)^{ab}$.

At this point we can count the physical degrees of freedom. Given a field theory with N fields whose canonical formulation possesses F first-class constraints, one can gauge fix F fields. The second-class constraints do not generate any gauge symmetries and S second-class constraints are equivalent to vanishing of $S/2$ fields and $S/2$ canonically conjugate momenta. Hence the number of independent (physical) fields is given by

$$n = N - F - \frac{S}{2}\,. \tag{65}$$

The number of field components for each of the fundamental fields is

$\omega^{ab}{}_{\mu}$	$\beta^{a}{}_{\mu\nu}$	$e^{a}{}_{\mu}$	$B^{ab}{}_{\mu\nu}$	$\phi^{ab}{}_{\mu\nu}$
24	24	16	36	36

which gives the total $N = 136$. The number of components of the first class constraints is

$\Phi(e)_a$	$\Phi(\omega)_{ab}$	$\Phi(R)^a$	$\Phi(T)^{ab}$
4	6	4	6

which gives the total of $F = 20$. Similarly, the number of components for the second class constraints is

$\chi(R\phi)^{abi}$	$\chi(Bee)^{abij}$	$\chi(Bee)^{abi}$	$\chi(\beta)^{a}{}_{\mu\nu}$	$\chi(eR\phi)^{ab}{}_{i}$
18	18	18	24	18

and

$\chi(B)_{ab}{}^{\mu\nu}$	$\chi(\phi)_{ab}{}^{\mu\nu}$	$\chi(\beta)_{a}{}^{\mu\nu}$	$\chi(\omega)_{ab}{}^{i}$	$\chi(e)_{a}{}^{i}$	$\chi(T)^{ai}$
36	36	24	18	12	$12-6$

where we have denoted that only 6 of the total 12 components of $\chi(T)^{ai}$ are independent. Thus the total number of independent second class constraints is $S = 228$. This number can also be deduced as the difference between the previously counted total number of constraints $C = 248$ and the number of first class constraints $F = 20$.

Finally, substituting N, F and S into (65), we obtain:

$$n = 136 - 20 - \frac{228}{2} = 2. \tag{66}$$

We conclude that the theory has two physical degrees of freedom, as expected for general relativity.

At this point it is convenient to rewrite the last term in (62) in the traditional ADM form. This is done by projecting the constraint $\Phi(R)_a$ onto the hypersurface Σ and its orthogonal direction. Using the inverse tetrad $e^\mu{}_a$, define the unit vector n_a orthogonal to Σ as

$$n_a \equiv \frac{e^0{}_a}{\sqrt{-g^{00}}} \tag{67}$$

where $g^{00} \equiv \eta^{ab} e^0{}_a e^0{}_b$ is the time-time component of the inverse metric $g^{\mu\nu}$. The vector n_a is thus normalized, $n_a n^a = -1$, and we can define the orthogonal and parallel projectors with respect to Σ as

$$P^a_{\perp b} \equiv -n^a n_b, \qquad P^a_{\parallel b} \equiv \delta^a_b + n^a n_b. \tag{68}$$

One can then employ these projectors to rewrite the final term in (62) as

$$\begin{aligned} e^a{}_0 \Phi(R)_a &= e^a{}_0 \left(P^b_{\perp a} + P^b_{\parallel a} \right) \Phi(R)_b \\ &= -e^a{}_0 n_a n^b \Phi(R)_b + e^a{}_0 P^b_{\parallel a} \left(e^\mu{}_b e^c{}_\mu \right) \Phi(R)_c \\ &= \left[e^a{}_0 n_a \right] \left[-n^b \Phi(R)_b \right] + \left[e^a{}_0 P^b_{\parallel a} e^i{}_b \right] \left[e^c{}_i \Phi(R)_c \right] + \left[e^a{}_0 P^b_{\parallel a} e^0{}_b \right] \left[e^c{}_0 \Phi(R)_c \right] \\ &= N \mathcal{H}_\perp + N^i \mathcal{D}_i. \end{aligned} \tag{69}$$

Note that the final term in the second-to-last equality drops out because $P^b_{\parallel a} e^0{}_b = \sqrt{-g^{00}} P^b_{\parallel a} n_b \equiv 0$. In the last equality we have introduced the well known ADM lapse and shift functions,

$$N \equiv e^a{}_0 n_a = \frac{1}{\sqrt{-g^{00}}}, \qquad N^i \equiv e^a{}_0 P^b_{\parallel a} e^i{}_b = -\frac{g^{0i}}{g^{00}}, \tag{70}$$

and we have split the constraint $\Phi(R)_a$ into the scalar constraint and 3-diffeomorphism constraint,

$$\mathcal{H}_\perp \equiv -n^b \Phi(R)_b, \qquad \mathcal{D}_i \equiv e^c{}_i \Phi(R)_c. \tag{71}$$

The constraints $\Phi(T)^{ab}$ are equivalent to the local Lorentz constraints $\mathcal{J}^{ab}$, which generate the local Lorentz transformations, and together with the 10 momentum constraints $\Phi(\omega)^{ab}$ and $\Phi(e)_a$, one can use the scalar constraint $\mathcal{H}_\perp$ and the 3-diffeomorphism constraint $\mathcal{D}_i$ to find the Poisson bracket algebra of the first-class constraints. This algebra takes the form

$$\begin{aligned} \{ \mathcal{J}^{ab}(x) \, , \, \mathcal{J}^{cd}(y) \} &= \frac{1}{2} \left[\eta^{a[c} \mathcal{J}^{d]b}(x) - \eta^{b[c} \mathcal{J}^{d]a}(x) \right] \delta^{(3)}, \\ \{ \mathcal{D}_i(x) \, , \, \mathcal{D}_j(y) \} &= \left[\mathcal{D}_i(x) + \mathcal{D}_i(y) \right] \partial_j \delta^{(3)} + R^{ab}{}_{ij}(x) \mathcal{J}_{ab}(x) \, \delta^{(3)}, \\ \{ \mathcal{D}_i(x) \, , \, \mathcal{H}_\perp(y) \} &= \left[\mathcal{H}_\perp(x) + \mathcal{H}_\perp(y) \right] \partial_i \delta^{(3)} + R^{ab}{}_{i0}(x) \mathcal{J}_{ab}(x) \, \delta^{(3)}, \\ \{ \mathcal{H}_\perp(x) \, , \, \mathcal{H}_\perp(y) \} &= \left[\tilde{g}^{ij}(x) D_j(x) + \tilde{g}^{ij}(y) D_j(y) \right] \partial_i \delta^{(3)}, \end{aligned} \tag{72}$$

while all other first-class Poisson brackets are zero, see [23]. Here it is assumed that $x \equiv (t, \vec{x})$, $y \equiv (t, \vec{y})$ and $\delta^{(3)} \equiv \delta^{(3)}(\vec{x} - \vec{y})$, while $\tilde{g}^{ij}$ is the 3D inverse metric, defined in appendix B.

The Poisson brackets between the second class constraints and the Poisson brackets between the first and the second class constraints can be calculated, but we do not give their explicit form because we do not need these Poisson brackets for the purposes of this paper. Their generic structure is given by

$$\{\,\chi_I(x)\,,\,\chi_J(y)\,\} = \Delta_{IJ}(x,y) + \tilde{\Delta}_{IJ}(x,y), \tag{73}$$

and

$$\begin{aligned}\{\,\Phi_A(x)\,,\,\chi_I(y)\,\} \;&=\; f_{AI}{}^{B}(x,y)\,\Phi_B(x) + \tilde{f}_{AI}{}^{B}(x,y)\,\Phi_B(y)\\ &\quad + f_{AI}{}^{J}(x,y)\,\chi_J(x) + \tilde{f}_{AI}{}^{J}(x,y)\,\chi_J(y).\end{aligned} \tag{74}$$

If we denote all the fields collectively as $\theta^N = (e^a{}_\mu, \omega^{ab}{}_\mu, \beta^a{}_{\mu\nu}, B^{ab}{}_{\mu\nu}, \phi^{ab}{}_{\mu\nu})$ and their corresponding momenta as $\pi_N = (\pi(e)_a{}^\mu, \pi(\omega)_{ab}{}^\mu, \pi(\beta)_a{}^{\mu\nu}, \pi(B)_{ab}{}^{\mu\nu}, \pi(\phi)_{ab}{}^{\mu\nu})$, we can denote Δ and f as generalized functions of the type

$$F(\theta(x),\pi(x))\delta^{(3)} + F^i(\theta(x),\pi(x))\,\partial_i\delta^{(3)} + \cdots$$

so that all the coefficients are evaluated at the point x, while $\tilde{\Delta}$ and $\tilde{f}$ as

$$F(\theta(y),\pi(y))\delta^{(3)} + F^i(\theta(y),\pi(y))\,\partial_i\delta^{(3)} + \cdots$$

so that all the coefficients are evaluated at the point y.

5. The phase space reductions

The results of the Hamiltonian analysis imply that the $BFCG$ GR action (6) can be written as

$$\begin{aligned}S_0 \;=\; \int_{t_1}^{t_2} \mathrm{d}t \int_\Sigma \mathrm{d}^3x \Bigg[&\pi_N\dot{\theta}^N - \lambda(e)^a{}_0\Phi(e)_a - \frac{1}{2}\lambda(\omega)^{ab}{}_0\Phi(\omega)_{ab}\\ &- e^a{}_0\Phi(R)_a - \frac{1}{2}\omega^{ab}{}_0\Phi(T)_{ab} - \mu^L\chi_L\Bigg],\end{aligned} \tag{75}$$

where χ_L counts over the set of all second-class constraints (64), while μ^L are Lagrange multipliers for the second-class constraints.

This action can be reduced to an action for a smaller number of canonical variables by partially solving some of the constraints. Solving M first-class constraints $\phi_m = 0$ requires that we make M gauge-fixing conditions $G_m = 0$, such that $\{G_m, G_{m'}\} = 0$ and $\det\{G_m, \phi_{m'}\} \neq 0$. We can then solve the equations $\phi_m = 0$ for the momenta $\pi(G_m)$. The simplest way to do this is to chose G_m to be a set of M coordinates θ_m, and then to solve the corresponding M first-class constraints $\phi_m = 0$ for the momenta π_m. As far as the second-class constraints are concerned, we can solve $2K$ of them for K coordinates and their K momenta.

It is not difficult to see that one can solve the following 192 second-class constraints

$$\begin{aligned}
\chi(B)_{ab}{}^{\mu\nu} &\equiv \pi(B)_{ab}{}^{\mu\nu} \approx 0,\\
\chi(\phi)_{ab}{}^{\mu\nu} &\equiv \pi(\phi)_{ab}{}^{\mu\nu} \approx 0,\\
\chi(\beta)^a{}_{\mu\nu} &\equiv \beta^a{}_{\mu\nu} \approx 0,\\
\chi(\beta)_a{}^{\mu\nu} &\equiv \pi(\beta)_a{}^{\mu\nu} + \varepsilon^{0\mu\nu\rho}e_{a\rho} \approx 0,\\
\chi(Bee)^{abij} &\equiv \varepsilon^{0ijk}\left(B^{ab}{}_{0k} - 2\varepsilon^{abcd}e_{c0}e_{dk}\right) \approx 0,\\
\chi(Bee)^{abi} &\equiv \varepsilon^{0ijk}\left(B^{ab}{}_{jk} - 2\varepsilon^{abcd}e_{cj}e_{dk}\right) \approx 0,\\
\chi(R\phi)^{abi} &\equiv \varepsilon^{0ijk}\left(R^{ab}{}_{jk} - \phi^{ab}{}_{jk}\right) \approx 0,\\
\chi(eR\phi)^{ab}{}_i &\equiv \phi^{ab}{}_{0i} - e^f{}_0R^{cd}{}_{jk}F^{abjk}{}_{fcdi} \approx 0,
\end{aligned} \tag{76}$$

for (B,β,ϕ) and their momenta. This will give (B,β,ϕ) and their momenta as functions of the canonical coordinates $(e,\omega,\pi(e),\pi(\omega))$ so that one obtains a reduced phase-space (RPS) theory described by the action

$$S_1 = \int \mathrm{d}^4x \left[\pi(e)_a{}^\mu \dot{e}^a{}_\mu + \frac{1}{2}\pi(\omega)_{ab}{}^\mu \dot{\omega}^{ab}{}_\mu - \lambda(e)^a{}_0\tilde{\Phi}(e)_a - \frac{1}{2}\lambda(\omega)^{ab}{}_0\tilde{\Phi}(\omega)_{ab} - e^a{}_0\tilde{\Phi}(R)_a - \frac{1}{2}\omega^{ab}{}_0\tilde{\Phi}(T)_{ab} - \mu^L\tilde{\chi}_L\right], \quad (77)$$

where $\tilde{C}$ denotes a constraint C on the RPS $(e,\omega,\pi(e),\pi(\omega))$. There are still 20 first-class constraints, namely $\tilde{\Phi}(\omega)^{ab}$, $\tilde{\Phi}(e)_a$, $\tilde{\Phi}(T)^{ab}$, $\tilde{\Phi}(R)_a$, and 36 second-class constraints $\tilde{\chi}_L = (\tilde{\chi}(e)_a{}^i, \tilde{\chi}(\omega)_{ab}{}^i, \tilde{\chi}(T)^{ai})$ on the RPS, so that S_1 is equivalent to the Hamiltonian form of the Einstein–Cartan action [14].

One would like to understand a reduction of S_1 to an action for the triads and spatial spin connections $(e^\alpha{}_i, \omega^{\alpha\beta}{}_i)$. This can be done by gauge fixing $e^a{}_0 = 0$ and solving the corresponding momenta from $\tilde{\Phi}(e)_a = 0$. One can also gauge fix $\omega^{ab}{}_0 = 0$ and eliminate the corresponding momenta from $\tilde{\Phi}(\omega)^{ab} = 0$, as well as to set $e^{\underline{0}}{}_i = 0$ and eliminate the corresponding momenta from $\tilde{\Phi}(T)^{\underline{0}\alpha} = 0$. Note that here we have split the group indices into space and time components, $a = (\underline{0}, \alpha)$ where $\alpha = 1,2,3$, see appendix B for details and the notation.

As far as the second-class constraints $\tilde{\chi}_L$ are concerned, one can eliminate $\omega^{\underline{0}\alpha}{}_i$ and the corresponding momenta from

$$\tilde{\chi}(\omega)_{\underline{0}\alpha}{}^i = 0, \qquad \tilde{\chi}(e)_a{}^i = 0, \qquad \tilde{\chi}(T)^{\underline{0}i} = 0. \quad (78)$$

Note that there are 24 constraints in (78), but there are six relations among them, so that we have only 18 independent constraints.

Solving the constraints (78) leads to a RPS based on $(e^\alpha{}_i, \omega^{\alpha\beta}{}_i) \cong (e^\alpha{}_i, \omega^\alpha{}_i)$ and their momenta. However, there are still 7 first-class constraints

$$\tilde{\Phi}(R)^a = 0, \qquad \tilde{\Phi}(T)^{\alpha\beta} = 0, \quad (79)$$

and 18 second-class constraints

$$\tilde{\chi}(T)^{\alpha i} = 0, \qquad \tilde{\chi}(\omega)_{\alpha\beta}{}^i = 0. \quad (80)$$

The corresponding action is given by

$$S_2 = \int \mathrm{d}^4x \left[\pi(e)_\alpha{}^i \dot{e}^\alpha{}_i + \pi(\omega)_\alpha{}^i \dot{\omega}^\alpha{}_i - N\tilde{\mathcal{H}}_\perp - N^i\tilde{\mathcal{D}}_i - \frac{1}{2}\omega^{\alpha\beta}{}_0\tilde{\mathcal{J}}_{\alpha\beta} - \mu^L\tilde{\chi}_L\right], \quad (81)$$

where $\tilde{\chi}_L = (\tilde{\chi}(T)^{\alpha i}, \tilde{\chi}(\omega)_{\alpha\beta}{}^i)$ and $\omega^\alpha{}_i \equiv \frac{1}{2}\varepsilon^{\alpha\beta\gamma}\omega_{\beta\gamma i}$.

We can further eliminate $\omega^\alpha{}_i$ and their momenta from the 18 second-class constraints (80) so that one obtains a RPS based on $(e,\pi(e))$ variables and the action

$$S_3 = \int \mathrm{d}^4x \left[\pi(e)_\alpha{}^i \dot{e}^\alpha{}_i - N\tilde{\mathcal{H}}_\perp - N^i\tilde{\mathcal{D}}_i - \frac{1}{2}\omega^{\alpha\beta}{}_0\tilde{\mathcal{J}}_{\alpha\beta}\right]. \quad (82)$$

This action corresponds to the triad Hamiltonian formulation of general relativity. The ADM formulation is obtained by using the $3D$ metric $g_{ij} \equiv e^a{}_i e_{aj} = e^\alpha{}_i e_{\alpha j}$ and the corresponding momenta. The ADM variables are invariant under the local rotations generated by $\tilde{\mathcal{J}}^{\alpha\beta}$, so that the corresponding action is given by

$$S_4 = \int \mathrm{d}^4x \left[\pi(g)^{ij}\,\dot{g}_{ij} - N\tilde{\mathcal{H}}_\perp - N^i\tilde{\mathcal{D}}_i\right], \tag{83}$$

where $\mathcal{H}_\perp$ and $\mathcal{D}_i$ are the ADM constraints.

6. Conclusions

We found all the constraints and determined the Lagrange multipliers for the *BFCG* GR action (6). We also determined the total Hamiltonian (62), the first-class constraints (63), the second-class constraints (64) and the algebra of the constraints (72)–(74). The obtained constraints also give the correct number of the physical DOF, see (66). We also showed how the other known canonical formulations of GR, namely Einstein–Cartan, triad and ADM, arise from the canonical formulation of *BFCG* GR by performing the RPS analysis. This analysis also gave a new canonical formulation for GR, namely the action S_2, which is based on the reduced phase space of triads and $SO(3)$ connections and their canonically conjugate momenta.

Since the main motivation for finding a canonical formulation of the *BFCG* GR theory is the construction of a spin-foam basis which will be a categorical generalization of the spin-network basis from LQG, then the results of the RPS analysis in section 5 are of great importance for this goal. Namely, in order to construct such a spin-foam basis one needs a 2-connection (A,β) for the Euclidean 2-group $(SO(3),\mathbb{R}^3)$ on the spatial manifold Σ, see [12]. This makes the RPS space $(e^\alpha{}_i, \omega^{\alpha\beta}{}_i, \pi(e)_\alpha{}^i, \pi(\omega)_{\alpha\beta}{}^i)$ and the corresponding action S_2 a natural starting point for the canonical quantization. Furthermore, this RPS provides a natural 2-connection on Σ

$$(A^{\alpha\beta}{}_i\,,\beta^\alpha{}_{ij}) = (\omega^{\alpha\beta}{}_i, \epsilon_{ijk}\tilde{e}^{k\alpha}\,), \tag{84}$$

where $\tilde{e}^k{}_\alpha$ are the inverse triads.

Hence one can use the 2-holonomy invariants for the 2-connection (84) associated to embedded 2-graphs in Σ, see [24], in order to construct the wavefunctions corresponding to the spin-foam basis. However, the existence of the second-class constraints χ_m will complicate the task of obtaining the physical Hilbert space. One can avoid the second-class constraints by using the Dirac brackets, but this may produce non-canonical commutators among the fields and their canonical momenta. If one wants to preserve the Heisenberg algebra of the canonical variables, then one can use the Gupta–Bleuler quantization approach, where the second-class constraints would be imposed weakly, as $\langle\Psi|\hat{\chi}_m|\Psi\rangle = 0$.

A simpler approach to the problem of second-class constraints in quantum theory is to solve classically the second-class constraints χ_m, which is equivalent to using the $(e^\alpha{}_i, \pi(e)_\alpha{}^i)$ RPS and the action S_3. Then the spin connection $\omega^{\alpha\beta}{}_i$ becomes a function of the triads and the components of the 2-connection (84) will still commute as operators, so that a spin-foam basis can be constructed, and the e-representation will be the most convenient for this.

Note that in the triad formulation of GR the Ashtekar variables can be defined via a series of canonical transformations,

$$(e^\alpha{}_i, \pi(e)_\alpha{}^i) \to (\tilde{e}^i{}_\alpha\,, \pi(\tilde{e})_i{}^\alpha) \to \Big(f(\zeta)E^i{}_\alpha = |e|_3\,\tilde{e}^i{}_\alpha\,, A^\alpha{}_i = \omega(e)^\alpha{}_i + \frac{\zeta}{|e|_3}\pi(\tilde{e})_i{}^\alpha\Big), \tag{85}$$

where $|e|_3 = \det(e^\alpha{}_i)$ and for $\zeta = \sqrt{-1}$, $f(\zeta) = 1$ [25] while for $\zeta \in \mathbb{R}$, $f(\zeta) = \zeta$ [26]. Then one can define the spin-network basis by using spin-network graphs and the associated holonomies for the connection A, see [1]. This suggests that the Ashtekar variables could be also a natural starting point for the construction of a spin-foam basis. However, the corresponding 2-connection components

$$A^{\alpha\beta}{}_i = \epsilon^{\alpha\beta\gamma} A_{\gamma i}, \qquad \beta^{\alpha}{}_{ij} = \epsilon_{ijk} E^{k\alpha}, \tag{86}$$

will not commute as operators and one has to use again the 2-connection (84).

Let us also note that the results obtained about the Hamiltonian structure of the theory can be important if one considers minisuperspace or midisuperspace models of quantum gravity, as is commonly done in the context of cosmology. For example, in Loop Quantum Cosmology (for a review, see [27–30] and references therein), one typically performs some type of symmetry reduction or gauge fixing prior to quantization, and then considers a resulting quantum-mechanical model of the Universe. However, in this work we have discussed only pure gravity, without matter fields. For this reason, our results are not directly applicable in the context of cosmology, since cosmological models without matter fields are not realistic. Repeating our analysis with included matter fields therefore represents an interesting avenue for further research.

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Appendix A. Bianchi identities

Recalling the definitions of the torsion and curvature 2-forms,

$$T^a = \mathrm{d}e^a + \omega^a{}_b \wedge e^b, \qquad R^{ab} = \mathrm{d}\omega^{ab} + \omega^a{}_c \wedge \omega^{cb}, \tag{A.1}$$

one can take the exterior derivative of T^a and R^a, and use the property $\mathrm{dd} \equiv 0$ to obtain the following two identities:

$$\begin{array}{lcl} \nabla T^a & \equiv & \mathrm{d}T^a + \omega^a{}_b \wedge T^b = R^a{}_b \wedge e^b, \\ \nabla R^{ab} & \equiv & \mathrm{d}R^{ab} + \omega^a{}_c \wedge R^{cb} + \omega^b{}_c \wedge R^{ac} = 0. \end{array} \tag{A.2}$$

These two identities are universally valid for torsion and curvature, and are called Bianchi identities. By expanding all quantities into components as

$$T^a = \frac{1}{2} T^a{}_{\mu\nu} \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu, \qquad R^{ab} = \frac{1}{2} R^{ab}{}_{\mu\nu} \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu, \tag{A.3}$$

$$e^a = e^a{}_\mu \mathrm{d}x^\mu, \qquad \omega^{ab} = \omega^{ab}{}_\mu \mathrm{d}x^\mu, \tag{A.4}$$

and using the formula $\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho \wedge \mathrm{d}x^\sigma = \varepsilon^{\mu\nu\rho\sigma} \mathrm{d}^4 x$, one can rewrite the Bianchi identities in component form as

$$\varepsilon^{\lambda\mu\nu\rho} \left(\nabla_\mu T^a{}_{\nu\rho} - R^a{}_{b\mu\nu} e^b{}_\rho \right) = 0, \tag{A.5}$$

and

$$\varepsilon^{\lambda\mu\nu\rho}\nabla_{\mu}R^{ab}{}_{\nu\rho}=0. \tag{A.6}$$

For the purpose of Hamiltonian analysis, one can split the Bianchi identities into those which do not feature a time derivative and those that do. The time-independent pieces are obtained by taking $\lambda=0$ components:

$$\varepsilon^{0ijk}\left(\nabla_{i}T^{a}{}_{jk}-R^{a}{}_{bij}e^{b}{}_{k}\right)=0, \tag{A.7}$$

$$\varepsilon^{0ijk}\nabla_{i}R^{ab}{}_{jk}=0. \tag{A.8}$$

These identities are valid as off-shell, strong equalities for every spacelike slice in spacetime, and can be enforced in all calculations involving the Hamiltonian analysis. The time-dependent pieces are obtained by taking $\lambda=i$ components:

$$\varepsilon^{0ijk}\left(\nabla_{0}T^{a}{}_{jk}-2\nabla_{j}T^{a}{}_{0k}-2R^{a}{}_{b0j}e^{b}{}_{k}-R^{a}{}_{bjk}e^{b}{}_{0}\right)=0, \tag{A.9}$$

and

$$\varepsilon^{0ijk}\left(\nabla_{0}R^{ab}{}_{jk}-2\nabla_{j}R^{ab}{}_{0k}\right)=0. \tag{A.10}$$

Due to the fact that they connect geometries of different spacelike slices in spacetime, they cannot be enforced off-shell. Instead, they can be derived from the Hamiltonian equations of motion of the theory.

In light of the Bianchi identities, we should note that the action (6) features three more fields, β^{a}, B^{ab} and ϕ^{ab}, which also have field strengths G^{a}, ∇B^{ab}, $\nabla\phi^{ab}$, and for which one can similarly derive Bianchi-like identities,

$$\begin{aligned}\nabla G^{a}&=R^{a}{}_{b}\wedge\beta^{b},\\ \nabla^{2}B^{ab}&=R^{a}{}_{c}\wedge B^{cb}+R^{b}{}_{c}\wedge B^{ac},\\ \nabla^{2}\phi^{ab}&=R^{a}{}_{c}\wedge\phi^{cb}+R^{b}{}_{c}\wedge\phi^{ac}.\end{aligned} \tag{A.11}$$

However, due to the fact that all three fields are two-forms, in 4-dimensional spacetime these identities will be single-component equations, with no free spacetime indices,

$$\varepsilon^{\lambda\mu\nu\rho}\left(\frac{2}{3}\nabla_{\lambda}G^{a}{}_{\mu\nu\rho}-R^{a}{}_{b\mu\nu}\beta^{b}{}_{\nu\rho}\right)=0, \tag{A.12}$$

and similarly for $\nabla^{2}B^{ab}$ and $\nabla^{2}\phi^{ab}$. Therefore, these equations necessarily feature time derivatives of the fields, and do not have a purely spatial counterpart to (A.7) and (A.8). In this sense, like the time-dependent pieces of the Bianchi identities, they do not enforce any restrictions in the sense of the Hamiltonian analysis, but can instead be derived from the equations of motion and expressions for the Lagrange multipliers.

Appendix B. Inverse tetrad and metric

We perform the split of the group indices into space and time components as $a=(\underline{0},\alpha)$ where $\alpha=1,2,3$, and write the tetrad $e^{a}{}_{\mu}$ as a $1+3$ matrix

$$e^a{}_\mu = \left[\begin{array}{c|c} e^0{}_0 & e^0{}_m \\ \hline e^\alpha{}_0 & e^\alpha{}_m \end{array}\right]. \tag{B.1}$$

Then the inverse tetrad $e^\mu{}_b$ can be expressed in terms of the $3D$ inverse tetrad $\tilde{e}^m{}_\beta$ as

$$e^\mu{}_b = \left[\begin{array}{c|c} \frac{1}{\sigma} & -\frac{1}{\sigma}\tilde{e}^m{}_\beta\, e^0{}_m \\ \hline -\frac{1}{\sigma}\tilde{e}^m{}_\alpha\, e^\alpha{}_0 & \tilde{e}^m{}_\beta + \frac{1}{\sigma}\left(\tilde{e}^m{}_\alpha\, e^\alpha{}_0\right)\left(\tilde{e}^k{}_\beta\, e^0{}_k\right) \end{array}\right], \tag{B.2}$$

where

$$\sigma \equiv e^0{}_0 - e^0{}_k \tilde{e}^k{}_\alpha\, e^\alpha{}_0 \tag{B.3}$$

is the 1×1 Schur complement [31] of the 4×4 matrix $e^a{}_\mu$. By definition, the $3D$ tetrad satisfies the identities

$$e^\alpha{}_m \tilde{e}^m{}_\beta = \delta^\alpha_\beta, \qquad e^\alpha{}_m \tilde{e}^n{}_\alpha = \delta^n_m. \tag{B.4}$$

In addition, if we denote $e \equiv \det e^a{}_\mu$ and $e_3 \equiv \det e^\alpha{}_m$, the Schur complement σ satisfies the Schur determinant formula

$$e = \sigma e_3, \tag{B.5}$$

which can be proved as follows.

Given any square matrix divided into blocks as

$$\Delta = \left[\begin{array}{c|c} A & B \\ \hline C & M \end{array}\right] \tag{B.6}$$

such that A and M are square matrices and M has an inverse, we can use the Aitken block diagonalization formula [31]

$$\left[\begin{array}{c|c} I & -BM^{-1} \\ \hline 0 & I \end{array}\right] \left[\begin{array}{c|c} A & B \\ \hline C & M \end{array}\right] \left[\begin{array}{c|c} I & 0 \\ \hline -M^{-1}C & I \end{array}\right] = \left[\begin{array}{c|c} S & 0 \\ \hline 0 & M \end{array}\right], \tag{B.7}$$

where

$$S = A - BM^{-1}C \tag{B.8}$$

is called the Schur complement of the matrix Δ. The Aitken formula can be written in the compact form

$$P\Delta Q = S \oplus M, \tag{B.9}$$

where P and Q are the above triangular matrices. Taking the determinant, we obtain

$$\det P \det \Delta \det Q = \det S \det M. \tag{B.10}$$

Since the determinant of a triangular matrix is the product of its diagonal elements, we have $\det P = \det Q = 1$, which then gives the famous Schur determinant formula:

$$\det \Delta = \det S \det M. \tag{B.11}$$

Now, performing the $1+3$ block splitting of the tetrad matrix $\Delta = [e^a{}_\mu]_{4\times4}$, we obtain the Schur complement $S = [\sigma]_{1\times1}$, while $M = [e^\alpha{}_m]_{3\times3}$. The Schur determinant formula then gives

$$e = \sigma e_3, \tag{B.12}$$

which completes the proof.

Similarly to the tetrad, one can perform a $1+3$ split of the metric $g_{\mu\nu}$,

$$g_{\mu\nu} = \left[\begin{array}{c|c} g_{00} & g_{0j} \\ \hline g_{i0} & g_{ij} \end{array}\right]. \tag{B.13}$$

The inverse metric $g^{\mu\nu}$ can be expressed in terms of the $3D$ inverse metric $\tilde{g}^{ij}$ as

$$g^{\mu\nu} = \left[\begin{array}{c|c} \dfrac{1}{\rho} & -\dfrac{1}{\rho}\tilde{g}^{in}g_{0i} \\ \hline -\dfrac{1}{\rho}\tilde{g}^{mj}g_{0j} & \tilde{g}^{mn} + \dfrac{1}{\rho}\left(\tilde{g}^{mj}g_{0j}\right)\left(\tilde{g}^{in}g_{0i}\right) \end{array}\right], \tag{B.14}$$

where

$$\rho \equiv g_{00} - g_{0i}\tilde{g}^{ij}g_{0j} \tag{B.15}$$

is the 1×1 Schur complement of $g_{\mu\nu}$. By definition, the $3D$ metric satisfies the identity

$$g_{ij}\tilde{g}^{jk} = \delta_i^k. \tag{B.16}$$

In addition, if we denote $g \equiv \det g_{\mu\nu}$ and $g_3 \equiv \det g_{ij}$, the Schur complement ρ satisfies the Schur determinant formula

$$g = \rho g_3. \tag{B.17}$$

The components of the metric can of course be written in terms of the components of the tetrad,

$$g_{\mu\nu} = \eta_{ab}e^a{}_\mu e^b{}_\nu. \tag{B.18}$$

Regarding the inverse metric, the only nontrivial identity is between $\tilde{g}^{ij}$ and $\tilde{e}^i{}_\alpha$. Introducing the convenient notation $e_\alpha \equiv \tilde{e}^i{}_\alpha\, e^0{}_i$, it reads:

$$\tilde{g}^{ij} = \tilde{e}^i{}_\alpha\, \tilde{e}^j{}_\beta \left[\eta^{\alpha\beta} + \frac{e^\alpha e^\beta}{1 - e_\gamma e^\gamma}\right]. \tag{B.19}$$

The relationship between determinants and Schur complements is:

$$g = -e^2, \qquad g_3 = (e_3)^2\left(1 - e_\alpha e^\alpha\right), \qquad \rho = \frac{\sigma^2}{e_\alpha e^\alpha - 1}. \tag{B.20}$$

Finally, there is one more useful identity,

$$g_{0j}\tilde{g}^{ij} = \tilde{e}^i{}_\alpha\, e^\alpha{}_0 - \frac{\sigma}{1 - e_\beta e^\beta}\tilde{e}^i{}_\alpha\, e^\alpha, \tag{B.21}$$

which can be easily proved with some patient calculation and the other identities above.

Appendix C. Solving the system of equations

In order to show that the constraints (52) are equivalent to the constraint (53), we proceed as follows. Introducing the shorthand notation $K_{abcd} \in \{\varepsilon_{abcd}, \eta_{ac}\eta_{bd}\}$, we can rewrite (52) in a convenient form

$$e^a{}_m K_{abcd} \varepsilon^{0ijk} \left(e^b{}_0 R^{cd}{}_{jk} - 2e^b{}_j \phi^{cd}{}_{0k} \right) \approx 0. \tag{C.1}$$

Next we multiply it with the Levi-Civita symbol ε_{0iln} in order to cancel the ε^{0ijk}, relabel the index $m \to i$ and obtain

$$K_{abcd} \left(e^a{}_i e^b{}_j \phi^{cd}{}_{0k} - e^a{}_i e^b{}_k \phi^{cd}{}_{0j} \right) \approx K_{abcd} e^a{}_i e^b{}_0 R^{cd}{}_{jk}. \tag{C.2}$$

The antisymmetrization in jk indices can be eliminated by writing each equation three times with cyclic permutations of indices ijk, then adding the first two permutations and subtracting the third. This gives:

$$K_{abcd} e^a{}_i e^b{}_j \phi^{cd}{}_{0k} \approx K_{abcd} e^a{}_0 \left[\frac{1}{2} e^b{}_k R^{cd}{}_{ij} - e^b{}_{[i} R^{cd}{}_{j]k} \right]. \tag{C.3}$$

Introducing the shorthand notation P_{ijk} and Q_{ijk} for the expression on the right-hand side as

$$\begin{aligned} P_{ijk} &\equiv \eta_{ac}\eta_{bd} e^a{}_0 \left[\frac{1}{2} e^b{}_k R^{cd}{}_{ij} - e^b{}_{[i} R^{cd}{}_{j]k} \right], \\ Q_{ijk} &\equiv \varepsilon_{abcd} e^a{}_0 \left[\frac{1}{2} e^b{}_k R^{cd}{}_{ij} - e^b{}_{[i} R^{cd}{}_{j]k} \right], \end{aligned} \tag{C.4}$$

our system can be rewritten as

$$\eta_{ac}\eta_{bd} e^a{}_i e^b{}_j \phi^{cd}{}_{0k} \approx P_{ijk}, \qquad \varepsilon_{abcd} e^a{}_i e^b{}_j \phi^{cd}{}_{0k} \approx Q_{ijk}. \tag{C.5}$$

This system consists of 18 equations for the 18 variables $\phi^{ab}{}_{0k}$. We look for a solution in the form

$$\phi^{cd}{}_{0k} = A^{cdmn} P_{mnk} + B^{cdmn} Q_{mnk}, \tag{C.6}$$

where the coefficients A^{cdmn} and B^{cdmn} are to be determined, for arbitrarily given values of P_{ijk} and Q_{ijk}. Substituting (C.6) into (C.5) we obtain

$$\begin{aligned} \left[\eta_{ac}\eta_{bd} e^a{}_i e^b{}_j A^{cdmn} - \delta_i^{[m}\delta_j^{n]} \right] P_{mnk} + \left[\eta_{ac}\eta_{bd} e^a{}_i e^b{}_j B^{cdmn} \right] Q_{mnk} &\approx 0, \\ \left[\varepsilon_{abcd} e^a{}_i e^b{}_j A^{cdmn} \right] P_{mnk} + \left[\varepsilon_{abcd} e^a{}_i e^b{}_j B^{cdmn} - \delta_i^{[m}\delta_j^{n]} \right] Q_{mnk} &\approx 0. \end{aligned} \tag{C.7}$$

Since P_{mnk} and Q_{mnk} are considered arbitrary, the expressions in the brackets must vanish, giving the following equations for A^{cdmn},

$$\eta_{ac}\eta_{bd} e^a{}_i e^b{}_j A^{cdmn} \approx \delta_i^{[m}\delta_j^{n]}, \qquad \varepsilon_{abcd} e^a{}_i e^b{}_j A^{cdmn} \approx 0, \tag{C.8}$$

and for B^{cdmn},

$$\eta_{ac}\eta_{bd} e^a{}_i e^b{}_j B^{cdmn} \approx 0, \qquad \varepsilon_{abcd} e^a{}_i e^b{}_j B^{cdmn} \approx \delta_i^{[m}\delta_j^{n]}. \tag{C.9}$$

Focus first on (C.8). The first equation can be rewritten in the form

$$e_{ci} e_{dj} A^{cdmn} \approx \delta_i^{[m}\delta_j^{n]}, \tag{C.10}$$

and we want to rewrite the second equation in a similar form as well. In order to do that, we need to get rid of the Levi-Civita symbol on the left-hand side, by virtue of the identity

$$\det(e_{a\mu})\varepsilon_{abcd} = \varepsilon^{\mu\nu\rho\sigma} e_{a\mu} e_{b\nu} e_{c\rho} e_{d\sigma}. \tag{C.11}$$

Noting that $\det(e_{a\mu}) = \det(\eta_{ab} e^b{}_\mu) = -\det(e^a{}_\mu) = -e$ and introducing the metric $g_{\mu\nu} \equiv e^a{}_\mu e_{a\nu}$, we can multiply this identity with $e^a{}_i e^b{}_j$ to obtain:

$$\varepsilon_{abcd} e^a{}_i e^b{}_j = -\frac{1}{e}\varepsilon^{\mu\nu\rho\sigma} g_{\mu i} g_{\nu j} e_{c\rho} e_{d\sigma}. \tag{C.12}$$

Substituting this into the second equation in (C.8) gives

$$\varepsilon^{\mu\nu\rho\sigma} g_{\mu i} g_{\nu j} e_{c\rho} e_{d\sigma} A^{cdmn} \approx 0. \tag{C.13}$$

Next we expand the ρ and σ indices into space and time components as $\rho = (0, k)$ and $\sigma = (0, l)$ to obtain

$$2\varepsilon^{\mu\nu 0 l} g_{\mu i} g_{\nu j} e_{c0} e_{dl} A^{cdmn} + \varepsilon^{\mu\nu kl} g_{\mu i} g_{\nu j} e_{ck} e_{dl} A^{cdmn} \approx 0. \tag{C.14}$$

The second term on the left can be evaluated using (C.10), which gives:

$$2\varepsilon^{\mu\nu 0 l} g_{\mu i} g_{\nu j} e_{c0} e_{dl} A^{cdmn} + \varepsilon^{\mu\nu mn} g_{\mu i} g_{\nu j} \approx 0. \tag{C.15}$$

The Levi-Civita symbol in the first term is nonzero only if $\mu\nu$ are spatial indices, so we can write

$$2\varepsilon^{rs0l} g_{ri} g_{sj} e_{c0} e_{dl} A^{cdmn} + \varepsilon^{\mu\nu mn} g_{\mu i} g_{\nu j} \approx 0. \tag{C.16}$$

At this point we need to introduce $3D$ inverse metric, $\tilde{g}^{ij}$, and to split the group indices into $3+1$ form $a = (\underline{0}, \alpha)$ where $\alpha = 1, 2, 3$, see appendix B. Multiplying (C.16) with two inverse spatial metrics and another Levi-Civita symbol, we can finally rewrite it as:

$$e_{c0} e_{di} A^{cdmn} \approx g_{0j} \tilde{g}^{j[m} \delta_i^{n]}. \tag{C.17}$$

The goal of all these transformations was to rewrite the system (C.8) into the form

$$e_{ci} e_{dj} A^{cdmn} \approx \delta_i^{[m} \delta_j^{n]}, \qquad e_{c0} e_{di} A^{cdmn} \approx g_{0j} \tilde{g}^{j[m} \delta_i^{n]}. \tag{C.18}$$

At this point we can expand the group indices on the left-hand side into $3+1$ form, to obtain:

$$e_{\gamma i} e_{\delta j} A^{\gamma\delta mn} + \left(e^{\underline{0}}{}_j e_{\delta i} - e^{\underline{0}}{}_i e_{\delta j}\right) A^{\underline{0}\delta mn} \approx \delta_i^{[m} \delta_j^{n]}, \tag{C.19}$$

$$e_{\gamma 0} e_{\delta j} A^{\gamma\delta mn} + \left(e^{\underline{0}}{}_j e_{\delta 0} - e^{\underline{0}}{}_0 e_{\delta j}\right) A^{\underline{0}\delta mn} \approx g_{0k} \tilde{g}^{k[m} \delta_j^{n]}. \tag{C.20}$$

Now we multiply (C.19) with $\tilde{e}^i{}_\alpha\, e^\alpha{}_0$ and subtract it from (C.20). The first terms on the left cancel, and (C.20) becomes

$$-\sigma e_{\delta j} A^{\underline{0}\delta mn} \approx g_{0k} \tilde{g}^{k[m} \delta_j^{n]} - \tilde{e}^{[m}{}_\alpha\, \delta_j^{n]} e^\alpha{}_0, \tag{C.21}$$

where σ is the 1×1 Schur complement matrix of the tetrad $e^a{}_\mu$ (see appendix B). Multiplying with another inverse $3D$ tetrad and using the identity (B.21), we finally obtain the first half of the coefficients A:

$$A^{\underline{0}\alpha mn} \approx \frac{1}{1 - e^\gamma e_\gamma} \tilde{e}^{[m}{}_\delta\, \tilde{e}^{n]\alpha}\, e^\delta. \tag{C.22}$$

Finally, substituting this back into (C.19) and multiplying with two more inverse 3D tetrads we obtain the second half of the coefficients A:

$$A^{\alpha\beta mn} \approx \tilde{e}^{[m\alpha}\,\tilde{e}^{n]\beta} + \frac{e^{\delta}}{1-e_{\gamma}e^{\gamma}}\left[e^{\alpha}\tilde{e}^{[m}{}_{\delta}\,\tilde{e}^{n]\beta} - e^{\beta}\tilde{e}^{[m}{}_{\delta}\,\tilde{e}^{n]\alpha}\right]. \tag{C.23}$$

Next we turn to the system (C.9) for coefficients B. The method to solve it is completely analogous to the above method of solving (C.8), and we will not repeat all the steps, but rather only quote the final result:

$$B^{0\beta mn} \approx \frac{1}{4}\varepsilon^{0\beta\gamma\delta}\left[\tilde{e}^{m}{}_{\gamma}\,\tilde{e}^{n}{}_{\delta} + 2\tilde{e}^{[m}{}_{\alpha}\,\tilde{e}^{n]}{}_{\delta}\,\frac{e^{\alpha}e_{\gamma}}{1-e_{\epsilon}e^{\epsilon}}\right], \tag{C.24}$$

and

$$B^{\alpha\beta mn} \approx \frac{1}{2}\,\frac{1}{1-e_{\epsilon}e^{\epsilon}}\,\varepsilon^{0\alpha\beta\gamma}\tilde{e}^{[m}{}_{\gamma}\,\tilde{e}^{n]}{}_{\delta}\,e^{\delta}. \tag{C.25}$$

To conclude, by determining the A and B coefficients in (C.6) we have managed to solve the original system of equations (C.1) for $\phi^{ab}{}_{0k}$. Substituting (C.4) into (C.6) the expression for $\phi^{ab}{}_{0k}$ can be arranged into the form

$$\phi^{ab}{}_{0k} \approx e^{f}{}_{0}R^{cd}{}_{mn}F^{abmn}{}_{fcdk}, \tag{C.26}$$

where

$$\begin{aligned} F^{abmn}{}_{fcdk} \;\equiv\; & \frac{1}{2}\Big[A^{abmn}\eta_{fc}e_{dk} - 2A^{abim}\eta_{fc}e_{di}\delta^{n}_{k} \\ & + B^{abmn}\varepsilon_{fhcd}e^{h}{}_{k} - 2B^{abim}\varepsilon_{fhcd}e^{h}{}_{i}\delta^{n}_{k}\Big], \end{aligned} \tag{C.27}$$

and coefficients A and B are specified by (C.22)–(C.25). Note that (C.27) depends only on $e^{a}{}_{i}$ components of the metric (in a very complicated way), while the dependence of $\phi^{ab}{}_{0k}$ on $e^{a}{}_{0}$ and $\omega^{ab}{}_{i}$ is factored out in (C.26).

Appendix D. Levi-Civita identity

The identity for the Levi-Civita symbol in 4 dimensions used in the main text is:

$$A_{[a}\varepsilon_{b]cdf}C^{c}D^{d}F^{f} = -\frac{1}{2}\varepsilon_{abcd}A_{f}\left[C^{d}D^{f}F^{c} + C^{c}D^{d}F^{f} + C^{f}D^{c}F^{d}\right]. \tag{D.1}$$

The proof goes as follows. Denote the left-hand side of the identity as

$$K_{ab} \equiv A_{[a}\varepsilon_{b]cdf}C^{c}D^{d}F^{f} \tag{D.2}$$

and take the dual to obtain:

$$\varepsilon^{aba'b'}K_{ab} = \varepsilon^{aba'b'}\varepsilon_{bcdf}A_{a}C^{c}D^{d}F^{f}. \tag{D.3}$$

Next expand the product of two Levi-Civita symbols into Kronecker deltas and use them to contract the vectors A, C, D and F:

$$\varepsilon^{aba'b'}K_{ab} = 2\left[(A\cdot D)F^{[a'}C^{b']} + (A\cdot F)C^{[a'}D^{b']} + (A\cdot C)D^{[a'}F^{b']}\right]. \tag{D.4}$$

Now take the dual again, i.e. contract with $\varepsilon_{a'b'cd}$ to obtain

$$\begin{aligned} -4K_{cd} &= \varepsilon_{a'b'cd}\varepsilon^{aba'b'}K_{ab} \\ &= 2\varepsilon_{a'b'cd}\left[(A\cdot D)F^{[a'}C^{b']} + (A\cdot F)C^{[a'}D^{b']} + (A\cdot C)D^{[a'}F^{b']}\right]. \end{aligned} \tag{D.5}$$

Finally, multiply by $-1/4$ and relabel the indices to obtain

$$K_{ab} = -\frac{1}{2}\varepsilon_{abcd}A_f\left[C^dD^fF^c + C^cD^dF^f + C^fD^cF^d\right], \tag{D.6}$$

which proves the identity.

Appendix E. Relation between the *BFCG* and the MacDowell–Mansouri models

Given that the constrained *BFCG* action (6) is equivalent to GR, it is a straightforward exercise to include a cosmological constant term:

$$\begin{aligned} S_{GR\Lambda} &= \int_{\mathcal{M}}\Big[B_{ab}\wedge R^{ab} + e^a\wedge G_a - \phi^{ab}\wedge\left(B_{ab} - \varepsilon_{abcd}\,e^c\wedge e^d\right) \\ &\qquad -\frac{\Lambda}{6}\,\varepsilon_{abcd}\,e^a\wedge e^b\wedge e^c\wedge e^d\Big], \end{aligned} \tag{E.1}$$

Working out the corresponding equations of motion, one obtains the same set (17)–(20) as for the action (6), except for the Einstein field equation (21) which is modified into

$$\varepsilon_{abcd}\left(R^{bc} - \frac{\Lambda}{3}\,e^b\wedge e^c\right)\wedge e^d = 0, \tag{E.2}$$

which can in turn be rewritten into the standard component form

$$R_{\mu\nu} - \frac{1}{2}R\,g_{\mu\nu} + \Lambda\,g_{\mu\nu} = 0. \tag{E.3}$$

Here the parameter $\Lambda\in\mathbb{R}$ is the cosmological constant.

It is interesting to note that one can obtain the MacDowell–Mansouri action for GR [18–22] from the action (E.1). In particular, the relationship between (E.1) and the MacDowell–Mansouri action is analogous to the relationship between the Palatini and Einstein–Hilbert actions, respectively, as we shall now demonstrate. To this end, first add and subtract a term $\zeta B_{ab}\wedge e^a\wedge e^b$ to (E.1), where $\zeta=\pm 1$, and rewrite it in the form

$$\begin{aligned} S_{GR\Lambda} = \int_{\mathcal{M}}\Big[&B_{ab}\wedge\left(R^{ab} - \zeta e_a\wedge e_b\right) + e^a\wedge G_a - \phi^{ab}\wedge\left(B_{ab} - \varepsilon_{abcd}\,e^c\wedge e^d\right) \\ &+ e^a\wedge e^b\wedge\left(\zeta B_{ab} - \frac{\Lambda}{6}\varepsilon_{abcd}\,e^c\wedge e^d\right)\Big]. \end{aligned} \tag{E.4}$$

Next we perform the partial integration over the $e^a\wedge G_a$ term, and rewrite the action as

$$\begin{aligned} S_{GR\Lambda} = \int_{\mathcal{M}}\Big[&B_{ab}\wedge\left(R^{ab} - \zeta e_a\wedge e_b\right) + \beta^a\wedge\nabla e_a - \phi^{ab}\wedge\left(B_{ab} - \varepsilon_{abcd}\,e^c\wedge e^d\right) \\ &+ e^a\wedge e^b\wedge\left(\zeta B_{ab} - \frac{\Lambda}{6}\varepsilon_{abcd}\,e^c\wedge e^d\right)\Big]. \end{aligned} \tag{E.5}$$

Now we want to eliminate the Lagrange multiplier ϕ^{ab} from the action. This is performed in analogy with the way the Palatini action is transformed into the Einstein–Hilbert action—we take the variation of the action with respect to ϕ^{ab} to obtain the corresponding equation of motion, and then substitute this equation back into the action. The equation of motion is algebraic rather than differential,

$$B_{ab} = \varepsilon_{abcd} e^c \wedge e^d, \tag{E.6}$$

which suggests that no propagating degrees of freedom will be lost upon substituting it back into the action. So we solve it for the product of two tetrads,

$$e^a \wedge e^b = -\frac{1}{4}\varepsilon^{abcd} B_{cd}, \tag{E.7}$$

and substitute it back into (E.5), eliminating the product of the tetrads from all terms except the first one, to obtain:

$$S = \int_{\mathcal{M}} \left[B_{ab} \wedge \left(R^{ab} - \zeta e_a \wedge e_b \right) + \beta^a \wedge \nabla e_a + \frac{\Lambda - 6\zeta}{24} \varepsilon_{abcd} B^{ab} \wedge B^{cd} \right]. \tag{E.8}$$

Note that the term containing ϕ^{ab} has vanished from the action, while the final term has been transformed into the $B \wedge B$ term.

Finally, to see that (E.8) is actually the MacDowell–Mansouri action, introduce the following change of variables:

$$B^{AB} \equiv \left[\begin{array}{c|c} B^{ab} & \frac{\beta^a}{2} \\ \hline -\frac{\beta^b}{2} & 0 \end{array} \right], \qquad A^{AB} \equiv \left[\begin{array}{c|c} \omega^{ab} & e^a \\ \hline -e^b & 0 \end{array} \right], \tag{E.9}$$

and

$$F^{AB} \equiv \mathrm{d}A^{AB} + A^A{}_C \wedge A^{CB} = \left[\begin{array}{c|c} R^{ab} - \zeta e^a \wedge e^b & \nabla e^a \\ \hline -\nabla e^b & 0 \end{array} \right], \qquad V^A \equiv \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \hline 1 \end{bmatrix}. \tag{E.10}$$

These represent the 5-dimensional 2-form B^{AB}, connection 1-form A^A, its field strength 2-form F^{AB} and a 0-form V^A. The capital Latin indices take values $0, 1, 2, 3, 5$, and we can also introduce the 5-dimensional Levi-Civita symbol ε_{ABCDE}, which is related to the ordinary 4-dimensional one as $\varepsilon_{abcd5} \equiv \varepsilon_{abcd}$. Using all this, the action (E.8) can be rewritten into the form

$$S = \int_{\mathcal{M}} \left[B_{AB} \wedge F^{AB} + \frac{\Lambda - 6\zeta}{24} B^{ab} \wedge B^{cd} \, \varepsilon_{ABCDE} \, V^E \right], \tag{E.11}$$

which is manifestly covariant with respect to the action of the groups $SO(4,1)$ or $SO(3,2)$, depending on the choice of $\zeta = \pm 1$, which enters the 5-dimensional metric

$$\eta_{AB} \equiv \left[\begin{array}{cccc|c} -1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ \hline & & & & \zeta \end{array} \right], \tag{E.12}$$

where the off-diagonal values are assumed to be zero. The action (E.11) is precisely the *BF*-formulation of the MacDowell–Mansouri action [18–22], as we have set out to demonstrate.

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Gauge protected entanglement between gravity and matter

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Abstract

We show that, as a consequence of the local Poincaré symmetry, gravity and matter fields have to be entangled, unless the overall action is carefully fine-tuned. First, we present a general argument, applicable to any particular theory of quantum gravity with matter, by performing the analysis in the abstract nonperturbative canonical framework, demonstrating the nonseparability of the scalar constraint, thus promoting the entangled states as the physical ones. Also, within the covariant framework, using a particular toy model, we show explicitly that the Hartle–Hawking state in the Regge model of quantum gravity is entangled. Our result is potentially relevant for the quantum-to-classical transition, taken within the framework of the decoherence programme: due to the gauge symmetry requirements, the matter does not decohere, it is by default decohered by gravity. Generically, entanglement is a consequence of interaction. This new entanglement could potentially, in form of an 'effective interaction', bring about corrections to the weak equivalence principle, further confirming that spacetime as a smooth four-dimensional manifold is an emergent phenomenon. Finally, the existence of the gauge-protected entanglement between gravity and matter could be seen as a criterion for a plausible theory of quantum gravity, and in the case of perturbative quantisation approaches, a confirmation of the persistence of the manifestly broken gauge symmetry.

Keywords: quantum entanglement, quantum gravity, diffeomorphism invariance, scalar constraint

1. Introduction

The unsolved problems of formulating quantum theory of gravity (QG) and interpreting quantum mechanics (QM) are arguably the two most prominent ones of the modern theoretical physics. So far, most of the approaches to solve the two were studied independently. Indeed, the majority of the interpretations of QM do not involve explicit dynamical effects (with notable exceptions of the spontaneous collapse and the de Broglie–Bohm theories), while the researchers from the QG community often just adopt some particular interpretation of QM, assuming that it contains no unresolved issues. Nevertheless, the two problems share a number of similar unsolved questions and counter-intuitive features. A prominent example is nonlocality: entanglement-based nonlocality in QM, as well as the anticipated explicit dynamical nonlocality in QG (a consequence of quantum superpositions of different gravitational fields, i.e. different spacetimes and their respective causal orders). Another prominent issue relevant for both standard QM and QG is the quantum-to-classical transition and the related measurement problem.

In relation to the latter, decoherence is in QM the standard approach to the emergence of classicality: due to huge complexity of macroscopic ('classical') systems and the surrounding environment (bath), the (*for all practical purposes*) inevitable interaction between the two leads to the entanglement and the loss of coherence. While technically this is completely within the standard QM, when coupled with additional assumptions, such as the many-world interpretation (likely to be the predominant within the community working on decoherence and quantum-to-classical transition), the decoherence offers a possible solution to the measurement problem. In an alternative approach, problems with quantising gravity led to the half century old idea of gravitationally induced objective collapse of the wave function [1] (for an overview, see for example [2], chapter III.B): roughly speaking, due to the position uncertainty of massive bodies, which are the sources of gravitational field, the latter exhibits quantum fluctuations that decohere the matter, forcing it (or, rather both the matter and gravity) to collapse in a well defined (classical) state. Without invoking objective collapse, decoherence of quantum matter by purely classical gravity was studied in [3, 4]. In the context of perturbative quantum gravity, the topic of gravitationally induced decoherence of matter, taken purely within the scope of standard QM (i.e. in the same fashion in which macroscopic bodies decohere due to inevitable interaction with surrounding photons, neutrinos, microwave background radiation, etc), became recently an intensive field of research [5], see also [6] and the references therein for decoherence in the context of cosmological inflation. In addition, a lot of research focuses on entanglement induced by the presence of horizons in curved spacetime, in approaches based on the holography conjecture and in the studies of the black hole information problem [7] (for a review, see recent lecture notes [8]). In particular, these approaches study the entanglement between the degrees of freedom (*both* gravitational and matter) on the two sides of the horizon.

In this paper we study the entanglement between gravitational and matter fields, in the context of an abstract nonperturbative theory of quantum gravity, as well as on the example of the Hartle–Hawking state in the Regge quantum gravity model, and show that the two fields should *always* be entangled. Our approach is different from the standard one, studied in the perturbative framework: instead of 'for all practical purposes' inevitable fast interaction-induced decoherence from initially product states between two sub-systems [5, 9–13], we show that the gauge symmetry requirements (coming in particular from the local Poincaré symmetry) secure the entangled states between matter and gravity as physical states. We call the latter the *gauge-protected* decoherence, in contrast to the *dynamical* decoherence of the former. In addition, unlike the horizon-based studies, we discuss the entanglement between the gravitational and the matter degrees of freedom, rather than between the two specially chosen regions of spacetime.

Our analysis rests on two main assumptions. First, we assume the validity of the local Poincaré symmetry at the quantum level. In the classical field theory, the local Poincaré symmetry is a formalisation of the principle of general relativity, which is one of the foundational principles of Einstein's theory of gravity. It is therefore natural to assume that this gauge symmetry exists at the quantum level as well. Second, at the classical level we assume the validity of the equivalence principle, which is also the main ingredient of Einstein's general relativity. In particular, we assume its 'strong' version, namely that the equivalence principle applies to all matter fields (i.e. all non-gravitational fields) present in nature.

Given these two assumptions, we focus on the general nonperturbative abstract canonical quantisation of the gravitational and matter fields, thus giving a generic model-independent argument for a theory of quantum gravity with matter. We analyse the consequences of the local Poincaré symmetry-enforced scalar, 3-diffeomorphism and local Lorentz constraints on the structure of the total Hilbert space of the theory. Namely, since the physical states must be invariant with respect to the gauge symmetry, the constraints induce the Gupta–Bleuler-like conditions on the state vectors. Based on the equivalence principle, we then show that the particular non-separable form of the scalar constraint renders typical product states non-invariant. Thus, it eliminates the product states from the physical Hilbert space of the quantum theory, unless the interaction between gravity and matter is specifically designed to circumvent the non-invariance of product states. In this way, the local Poincaré symmetry protects the existence of entanglement between the gravitational and matter fields.

In order to verify our results obtained within the abstract canonical framework, we also study the covariant (i.e. path integral) quantisation. In particular, knowing that the Hartle–Hawking state [14] satisfies the scalar constraint, and is therefore an element of the physical Hilbert space, we explicitly test whether the matter and gravitational fields are entangled for this state vector. We perform the calculation in the Regge quantum gravity model, since it is one of the simplest models which provide an explicit definition of the gravitational path integral with matter, and show that the gravitational and matter fields are indeed entangled for the Hartle–Hawking state constructed on a simple toy example triangulation.

Therefore, our analysis shows that either gravity and matter fields are indeed entangled, or there exists an additional, unknown property of the action, implementing the fine tuning needed to allow for the invariance of separable states.

The paper is organised as follows. Section 2 is divided into three subsections. The first is devoted to the recapitulation of the Hamiltonian structure of Poincaré gauge theories. The second outlines the procedure of nonperturbative canonical quantisation of constrained systems and its application to the case of gravity with matter fields. In the third subsection we use those results to show that the scalar constraint suppresses the existence of separable states of a matter-gravity system. In section 3, we present a standard entanglement criterion for pure bipartite quantum states and discuss it, within the framework of the path integral quantisation, for the case of the Hartle–Hawking state of quantum fields of gravity and matter. In section 4, we first introduce the Regge model of quantum gravity, and then apply it to evaluate the entanglement criterion for the Hartle–Hawking state, demonstrating that gravity and matter are indeed entangled in this state. Finally, in section 5 we present the summary of the results, their discussion, and possible future lines of research.

It is important to stress that the gauge-protected entanglement is not an automatic consequence of the universal coupling between gravity and matter, or the fact that matter fields are always defined over some background spacetime geometry. For example, in perturbative gravity approach, it is quite possible to write the separable state between gravity and matter as

$$|\Psi\rangle = |g\rangle \otimes |\phi\rangle,$$

where $|g\rangle$ is the graviton state vector, while $|\phi\rangle$ is the state vector of a scalar particle (both vectors obtained by acting with graviton and scalar creation operators on the Minkowski vacuum state $|0\rangle \equiv |0\rangle_G \otimes |0\rangle_M$). The reason why such a state can be considered legitimate is that local Poincaré symmetry is explicitly broken in the perturbative gravity approach, with both matter and gravity being treated as spin-zero and spin-two fields, respectively, living on a Minkowski spacetime manifold. A similar situation arises in perturbative string theory, where local Poincaré symmetry is also manifestly broken. However, in quantum gravity models where the local Poincaré symmetry is not violated, our analysis shows that a generic product state between gravity and matter would fail to be gauge invariant. Thus, the gauge-protected entanglement between gravity and matter is a nontrivial statement and a consequence of local Poincaré symmetry, rather than an automatic property of matter fields living on a spacetime manifold.

Our notation and conventions are as follows. We will work in the natural system of units in which $c = \hbar = 1$ and $G = l_p^2$, where l_p is the Planck length. By convention, the metric of spacetime will have the spacelike Lorentz signature $(-,+,+,+)$. The spacetime indices are denoted with lowercase Greek letters $\mu, \nu, \dots$ and take the values $0, 1, 2, 3$. The spatial part of these, taking values $1, 2, 3$, will be denoted with lowercase Latin letters $i, j, \dots$ from the middle of the alphabet. The $SO(3,1)$ group indices will be denoted with the lowercase Latin letters $a, b, \dots$ from the beginning of the alphabet, and take the values $0, 1, 2, 3$. The Lorentz-invariant metric tensor is denoted as η_{ab}. The capital Latin indices $A, B, \dots$ count the field components in a particular representation of the $SO(3,1)$ group, and take the values from 1 up to the dimension of that representation. Quantum operators will always carry a hat, $\hat{\phi}(x)$, $\hat{g}(x)$, etc. Finally, we will systematically denote the values of functions with parentheses, $f(x)$, while functionals will be denoted with brackets, $F[\phi]$.

2. Entanglement from the scalar constraint

This section is dedicated to the analysis of the constraints imposed by the relativity and equivalence principles. In section 2.1 we briefly recapitulate the classical Hamiltonian structure of gravitational interaction, followed by a short review of canonical quantisation, presented in section 2.2. After that, in section 2.3 we present the main result of our paper: we show that the scalar constraint, and possibly the 3-diffeomorphism constraint, bring about the generic entanglement between gravity and matter.

2.1. Hamiltonian structure of Poincaré gauge theories

We begin with a short review of the Hamiltonian structure of gravitational interaction, based on the local Poincaré symmetry. This subsection is aimed to be only a review of the main results, so we will skip all proofs and derivations. The details of the Hamiltonian structure for Poincaré gauge theories (PGT) can be found in many textbooks, see for example [15], chapter V, and the references therein.

We will assume a foliation of spacetime into space and time, with the spacetime topology $\mathcal{M}_4 = \Sigma_3 \times \mathbb{R}$, where Σ_3 is the $3D$ hypersurface. For the purpose of generality, we will describe the gravitational field as $g(x)$ and matter fields as $\phi(x)$, without specifying their exact field content, except in examples. A typical example would be the Einstein–Cartan gravity coupled to a Dirac matter field, so that the choice of fundamental gravitational fields g would be the tetrads $e^a{}_\mu(x)$ and the spin connection $\omega^{ab}{}_\mu(x)$, while the choice for the fundamental matter field ϕ would be a Dirac fermion field $\psi(x)$. However, other choices for g and ϕ are also possible, for example the metric tensor $g_{\mu\nu}$ for gravity and the electromagnetic potential A^μ for matter, etc. Since our analysis is largely independent of such choices, we will stick to the abstract notation g and ϕ, assuming that one can apply our analysis to each particular concrete choice of fundamental fields.

Given the above notation, we will assume that the action of the theory can be written as

$$S[g,\phi] = S_G[g] + S_M[g,\phi], \tag{1}$$

where $S_G[g]$ is the action of the pure gravitational field, while $S_M[g,\phi]$ is the action of the matter fields coupled to gravity. Since the spacetime metric must both be a function of the gravitational field g and is always present in the definition of the dynamics of matter fields, the action for the matter fields cannot contain terms independent of g. This elementary fact is the crux of our main argument below, and is justified by the equivalence principle, which dictates how matter couples to gravity.

To a large extent, we also do not need to specify the details of the actions $S_G[g]$ and $S_M[g,\phi]$. We will only assume that the action (1) belongs to the PGT class of theories, i.e. that it is invariant with respect to local Poincaré group $P(4) = \mathbb{R}^4 \ltimes SO(3,1)$. Every theory belonging to the PGT class has the Hamiltonian with the following general structure [15]:

$$H = \int_{\Sigma_3} \mathrm{d}^3\vec{x}\, \left[N\mathcal{C} + N^i\mathcal{C}_i + N^{ab}\mathcal{C}_{ab} \right], \tag{2}$$

up to a 3-divergence. Here N, N^i and N^{ab} are Lagrange multipliers, the first two of which are commonly known as lapse and shift functions. The quantities $\mathcal{C}$, $\mathcal{C}_i$ and $\mathcal{C}_{ab}$ are usually known as the scalar constraint, 3-diffeomorphism constraint, and the local Lorentz constraint (sometimes also called the Gauss constraint), respectively. They are a (g,ϕ)-field representation of the 10 generators of the Poincaré group $P(4)$, in particular the time translation generator, the three space translation generators, and six local Lorentz generators (rotations and boosts). Note that the Hamiltonian (2) is always a linear combination of these constraints.

The constraints in (2) have the structure similar to the structure of the gravity-matter action (1), namely

$$\begin{aligned} \mathcal{C} &= \mathcal{C}^G(g,\pi_g) + \mathcal{C}^M(g,\pi_g,\phi,\pi_\phi), \\ \mathcal{C}_i &= \mathcal{C}_i^G(g,\pi_g) + \mathcal{C}_i^M(g,\pi_g,\phi,\pi_\phi), \\ \mathcal{C}_{ab} &= \mathcal{C}_{ab}^G(g,\pi_g) + \mathcal{C}_{ab}^M(g,\pi_g,\phi,\pi_\phi), \end{aligned} \tag{3}$$

where π_g and π_ϕ are the momenta canonically conjugated to the fields g and ϕ, respectively, defined as functional derivatives of the action with respect to the time-derivatives of the fields,

$$\pi_g(x) = \frac{\delta S}{\delta \partial_0 g(x)}, \qquad \pi_\phi(x) = \frac{\delta S}{\delta \partial_0 \phi(x)}.$$

The general dependence (3) on the fields and momenta reflects the corresponding dependence in (1).

The exact forms of the gravitational terms of the constraints, namely $\mathcal{C}^G$, $\mathcal{C}_i^G$ and $\mathcal{C}_{ab}^G$, will be immaterial for our main argument presented in the section 2.3 below. In contrast, the structure of the matter terms $\mathcal{C}^M$, $\mathcal{C}_i^M$ and $\mathcal{C}_{ab}^M$ will be crucial, so we discuss it here in more detail. Choose a matter field such that it transforms according to some specific irreducible transformation of the Poincaré group, and denote it as $\phi^A(x)$, where the capital index A counts the field components in that representation. Then the 3-diffeo constraint $\mathcal{C}_i^M$ and the Gauss constraint $\mathcal{C}_{ab}^M$ are given as

$$\begin{array}{rcl} \mathcal{C}_i^M(g,\pi_g,\phi,\pi_\phi) & = & \pi_{\phi A}\nabla_i{}^A{}_B\phi^B, \\ \mathcal{C}_{ab}^M(g,\pi_g,\phi,\pi_\phi) & = & \pi_{\phi A}(M_{ab})^A{}_B\phi^B, \end{array} \tag{4}$$

where $\nabla_i{}^A{}_B$ is a covariant derivative for the irreducible representation according to which the field ϕ transforms, while $(M_{ab})^A{}_B$ is the representation of the generator M_{ab} of the Lorentz group $SO(3,1)$ in the same representation. In general, the covariant derivative depends on the spacetime metric or connection, which is a function of the fundamental gravitational fields g, and possibly their momenta π_g. The Lorentz group generators, on the other hand, do not depend on the spacetime geometry, so the Gauss constraint is actually independent of g and π_g, and we can write $\mathcal{C}_{ab}^M(g,\pi_g,\phi,\pi_\phi) = \mathcal{C}_{ab}^M(\phi,\pi_\phi)$.

In order to illustrate the two constraints, we will write (4) for the scalar and Dirac fields, as the most elementary examples. In the case of the scalar field, we write $\phi^A(x) = \varphi(x)$, where the index A takes only a single value. The covariant derivative acts on the scalar field as an ordinary derivative, while the representation of the Lorentz generators is trivial, so we can write

$$\mathcal{C}_i^M(\varphi,\pi_\varphi) = \pi_\varphi\partial_i\varphi, \qquad \mathcal{C}_{ab}^M(\varphi,\pi_\varphi) = \pi_\varphi\varphi. \tag{5}$$

We see that in the case of the scalar field, both constraints are independent of the gravitational fields and their momenta. In the case of the Dirac fields, we write $\phi^A(x) = (\psi^A(x),\bar\psi^A(x))$, where the index A now represents the spinorial index, and we will omit writing it. The covariant derivative acts on the Dirac field in the standard way,

$$\begin{array}{rcl} \overrightarrow{\nabla}_\mu\psi & \equiv & \partial_\mu\psi + \dfrac{1}{2}\omega^{ab}{}_\mu\sigma_{ab}\psi, \\ \bar\psi\overleftarrow{\nabla}_\mu & \equiv & \partial_\mu\bar\psi - \dfrac{1}{2}\omega^{ab}{}_\mu\bar\psi\sigma_{ab}, \end{array} \tag{6}$$

where $\omega^{ab}{}_\mu$ is the spin connection, $\sigma_{ab} = \frac{1}{4}[\gamma_a,\gamma_b]$, and γ_a are the standard Dirac gamma-matrices satisfying the anticommutation relation $\{\gamma_a,\gamma_b\} = -2\eta_{ab}$. The representation of the Lorentz generators for the case of the Dirac field is $M_{ab} = \sigma_{ab}$. Denoting the conjugate momentum for ψ as $\bar\pi$ and conjugate momentum for $\bar\psi$ as π, we can write the constraints (4) as:

$$\begin{array}{rcl} \mathcal{C}_i^M(\omega,\psi,\bar\pi,\bar\psi,\pi) & = & \bar\pi\overrightarrow{\nabla}_i\psi + (\bar\psi\overleftarrow{\nabla}_i)\pi, \\ \mathcal{C}_{ab}^M(\psi,\bar\pi,\bar\psi,\pi) & = & \bar\pi\sigma_{ab}\psi - \bar\psi\sigma_{ab}\pi. \end{array} \tag{7}$$

Note that here, unlike in the scalar field example, the 3-diffeo constraint contains the spin connection $\omega^{ab}{}_\mu$, which is a part of the gravitational field $g = (e^a{}_\mu,\omega^{ab}{}_\mu)$ for the Einstein–Cartan gravity.

In contrast to the 3-diffeo and Gauss constraints (4), the scalar constraint $\mathcal{C}^M$ has a more complicated form,

$$\mathcal{C}^M(g,\pi_g,\phi,\pi_\phi) = \pi_{\phi A}\nabla_\perp{}^A{}_B\phi^B - \frac{1}{N}\mathcal{L}_M(g,\pi_g,\phi,\pi_\phi), \tag{8}$$

where the matter Lagrangian density is defined via

$$S_M[g,\phi] = \int \mathrm{d}^4x\,\mathcal{L}_M(g,\partial g,\phi,\partial\phi),$$

and $\nabla_\perp \equiv n^\mu \nabla_\mu$ is the covariant derivative in the direction of the timelike vector n^μ orthogonal to the spacelike hypersurface Σ_3. The vector n^μ obviously depends on the spacetime metric $g_{\mu\nu}$, and is thus a function of the fundamental gravitational fields g.

There are several things to note regarding the scalar constraint (8). First, it is clear that $N\mathcal{C}^M$ is the Legendre transformation of the Lagrangian density $\mathcal{L}_M$ with respect to the 'velocity' $N\nabla_\perp \phi$. Second, in contrast to the constraints (4), which depend only on the symmetry transformation properties of the fields, the form of the scalar constraint (8) depends also on the choice of the matter Lagrangian density $\mathcal{L}_M$, and is therefore described by the dynamics of the matter fields coupled to gravity. And third, the scalar constraint $\mathcal{C}^M$ always necessarily depends on the gravitational fields g, in contrast to the 3-diffeo constraint which may or may not depend on g, and the Gauss constraint which never depends on g. As we already suggested above, this is because the Lagrangian of the matter fields coupled to gravity always contains the gravitational degrees of freedom, courtesy of the equivalence principle.

Let us illustrate this dependence of $\mathcal{C}^M$ on the gravitational fields g in the case of the Dirac field. The action for the Dirac field $\phi = (\psi, \bar\psi)$ coupled to the gravitational fields $g = (e^a{}_\mu, \omega^{ab}{}_\mu)$ is given as

$$S_M[e,\omega,\psi,\bar\psi] = \int \mathrm{d}^4x\, e \left(\frac{\mathrm{i}}{2} \bar\psi \gamma^a e^\mu{}_a \overleftrightarrow{\nabla}_\mu \psi - m\bar\psi\psi \right), \tag{9}$$

where e is the determinant of the tetrad $e^a{}_\mu$, while $e^\mu{}_a$ is the inverse tetrad. In addition, $\overleftrightarrow{\nabla}_\mu \equiv \overrightarrow{\nabla}_\mu - \overleftarrow{\nabla}_\mu$, and the covariant derivatives $\overrightarrow{\nabla}_\mu$ and $\overleftarrow{\nabla}_\mu$ act to the right and to the left as defined in (6), from which one can see that the action also explicitly depends on the connection $\omega^{ab}{}_\mu$. From the action one can read off the Lagrangian density, and calculate the scalar constraint (8) as

$$\mathcal{C}^M(e,\omega,\psi,\bar\psi) = -\frac{e}{N} \left(\frac{\mathrm{i}}{2} \bar\psi \gamma^a e^\mu{}_a \left(\delta^\mu_\nu + n^\mu n_\nu\right) \overleftrightarrow{\nabla}_\nu \psi - m\bar\psi\psi \right).$$

Note that the quantity $\delta^\mu_\nu + n^\mu n_\nu$ is a projector to the hypersurface Σ_3.

2.2. Canonical quantisation

Having discussed the Hamiltonian structure of the action (1), we now pass on to a short description of the canonical quantisation of the theory. The quantisation of an arbitrary physical system with constraints is performed in the standard way, using the Dirac's procedure [16, 17] (see [15] for a review). One begins by classifying all constraints of the theory into the first and the second class. The second class constraints are then eliminated by passing from the Poisson brackets to the Dirac brackets. The first class constraints remain and represent the generators of the gauge symmetry. In general, the Hamiltonian of the theory can be written as

$$H = H_0 + \lambda^A \mathcal{C}_A, \tag{10}$$

where λ^A are Lagrange multipliers, $\mathcal{C}_A$ are first class constraints, and H_0 is the part of the Hamiltonian which describes the evolution of the physical degrees of freedom. Given all this, the quantisation is performed in the Heisenberg picture, promoting fundamental fields $\phi(x)$ to quantum mechanical operators $\hat\phi(x)$, and introducing the state vectors $|\Psi\rangle \in \mathcal{H}_{\mathrm{kin}}$, where $\mathcal{H}_{\mathrm{kin}}$ is the kinematical Hilbert space of the theory. The Dirac brackets between the fields and their momenta are then promoted to the commutators of the corresponding operators. The Hamiltonian, being a functional of the fields and momenta, also becomes an operator, providing the usual Heisenberg equations of motion for the field operators,

$$\mathrm{i}\frac{\partial\hat{\phi}(x)}{\partial t} = [\hat{\phi}(x), \hat{H}].$$

Finally, the kinematical Hilbert space $\mathcal{H}_{\text{kin}}$ is projected onto its gauge invariant subspace $\mathcal{H}_{\text{phys}}$, by requiring that every state vector $|\Psi\rangle \in \mathcal{H}_{\text{phys}}$ is annihilated by the generators of the gauge symmetry group,

$$\hat{\mathcal{C}}_A|\Psi\rangle = 0.$$

In quantum electrodynamics these conditions are known as Gupta–Bleuler quantisation conditions [18, 19]. This requirement ensures that the gauge symmetry of the classical theory remains to be a symmetry of the quantum theory as well.

Of course, one cannot hope to implement the above quantisation programme in full detail for the general action (1), especially without the detailed specification of the fundamental degrees of freedom that define the theory. Instead, we assume that the quantisation programme has been carried out in detail, and that all quantities we will write are well defined. This approach has one important feature and one important drawback. The feature is generality—our main argument for the inevitable entanglement between gravity and matter, to be presented in section 2.3, should hold for every particular quantum theory constructed in the above way, as it does not actually depend on the details of the quantisation. The drawback is abstractness—in using such a general formalism and making a flat assumption that all details are well defined, we lose the capability to provide any concrete examples. That said, in section 4 we discuss one rigorously defined example of a theory of quantum gravity with matter (Regge quantum gravity), and demonstrate the entanglement between gravity and matter fields. Unlike the canonical quantisation discussed in this section, that example will be done in the framework of the path integral quantisation.

Keeping this disclaimer in mind, we proceed along the lines outlined above and perform the canonical quantisation. The most prominent property of our model is the structure of the Hilbert space of the theory. The initial kinematical Hilbert space $\mathcal{H}_{\text{kin}} = \mathcal{H}_G \otimes \mathcal{H}_M$ has a natural product structure between the gravitational and matter Hilbert spaces, since we have two sets of fields, $\hat{g}$ and $\hat{\phi}$, corresponding to gravity and matter, respectively. Thus, we have a naturally preferred bipartite physical system, because gravitational and matter degrees of freedom can be fully distinguished from each other. Second, in order to preserve the Poincaré gauge symmetry of the theory at the quantum level, we have to pass from the kinematical Hilbert space to the gauge invariant, physical Hilbert space $\mathcal{H}_{\text{phys}}$. By definition, a state $|\Psi\rangle \in \mathcal{H}_{\text{kin}}$ is an element of $\mathcal{H}_{\text{phys}}$ iff it satisfies

$$\begin{aligned}
\hat{\mathcal{C}}_{ab}|\Psi\rangle &\equiv \left[\mathcal{C}^G_{ab}(\hat{g}, \hat{\pi}_g) + \mathcal{C}^M_{ab}(\hat{\phi}, \hat{\pi}_\phi)\right]|\Psi\rangle = 0, \\
\hat{\mathcal{C}}_i|\Psi\rangle &\equiv \left[\mathcal{C}^G_i(\hat{g}, \hat{\pi}_g) + \mathcal{C}^M_i(\hat{g}, \hat{\pi}_g, \hat{\phi}, \hat{\pi}_\phi)\right]|\Psi\rangle = 0,
\end{aligned} \tag{11}$$

and

$$\hat{\mathcal{C}}|\Psi\rangle \equiv \left[\mathcal{C}^G(\hat{g}, \hat{\pi}_g) + \mathcal{C}^M(\hat{g}, \hat{\pi}_g, \hat{\phi}, \hat{\pi}_\phi)\right]|\Psi\rangle = 0. \tag{12}$$

As stated above, we assume that the operators $\hat{\mathcal{C}}_{ab}$, $\hat{\mathcal{C}}_i$ and $\hat{\mathcal{C}}$ are well defined, that operator ordering choice has been fixed, as well as all other necessary technical choices, in order for the expressions above to make sense mathematically.

We argue that, due to these constraint equations, there are no states in $\mathcal{H}_{\text{phys}}$ which can be written as product states of the form $|\Psi_G\rangle \otimes |\Psi_M\rangle$, where $|\Psi_G\rangle \in \mathcal{H}_G$ and $|\Psi_M\rangle \in \mathcal{H}_M$, i.e. the states in $\mathcal{H}_{\text{phys}}$ are entangled. We focus on the scalar constraint (12), while the constraints

(11) are either irrelevant or redundant for our analysis. This main argument of our paper is presented in the next subsection.

2.3. Entanglement

Given a state vector $|\Psi\rangle \in \mathcal{H}_{\text{kin}} = \mathcal{H}_G \otimes \mathcal{H}_M$, it is an element of the physical Hilbert space $\mathcal{H}_{\text{phys}}$ if it satisfies the Gauss and 3-diffeo constraints (11) and the scalar constraint (12). Choosing the eigenbases $\{|g\rangle\}$ and $\{|\phi\rangle\}$ of the quantum field operators $\hat{g}$ and $\hat{\phi}$, respectively, we can work in the so-called field representation, defined as

$$
\begin{aligned}
\langle g|\hat{g} &= g\langle g|, & \langle g|\hat{\pi}_g &= -\mathrm{i}\frac{\delta}{\delta g}\langle g|, \\
\langle \phi|\hat{\phi} &= \phi\langle \phi|, & \langle \phi|\hat{\pi}_\phi &= -\mathrm{i}\frac{\delta}{\delta \phi}\langle \phi|.
\end{aligned} \tag{13}
$$

Acting on (12) with $\langle g,\phi| \equiv \langle g| \otimes \langle \phi|$ from the left, the scalar constraint becomes a functional partial differential equation of Wheeler–DeWitt type:

$$
\left[\mathcal{C}_G\left(g, -\mathrm{i}\tfrac{\delta}{\delta g}\right) + \mathcal{C}_M\left(g, -\mathrm{i}\tfrac{\delta}{\delta g}, \phi, -\mathrm{i}\tfrac{\delta}{\delta \phi}\right)\right] \Psi[g,\phi] = 0, \tag{14}
$$

where $\Psi[g,\phi] \equiv \langle g,\phi|\Psi\rangle$ is the wavefunctional of the combined gravity-matter system. We now try to look for a separable state, in the form $|\Psi\rangle = |\Psi_G\rangle \otimes |\Psi_M\rangle$, where $|\Psi_G\rangle \in \mathcal{H}_G$ and $|\Psi_M\rangle \in \mathcal{H}_M$, as a solution of this equation. Using the field representation (13), we write the wavefunctional $\Psi[g,\phi]$ as

$$
\begin{aligned}
\Psi[g,\phi] &\equiv \langle g,\phi|\Psi\rangle \\
&= (\langle g| \otimes \langle \phi|)\,(|\Psi_G\rangle \otimes |\Psi_M\rangle) \\
&= \langle g|\Psi_G\rangle\langle \phi|\Psi_M\rangle \\
&\equiv \Psi_G[g]\Psi_M[\phi].
\end{aligned} \tag{15}
$$

Equation (14) can have separable solutions $\Psi[g,\phi] = \Psi_G[g]\Psi_M[\phi]$ if the functional differential operator $\mathcal{C}_M$ can be written as a product of two operators, denoted $\mathcal{K}_G$ and $\mathcal{K}_M$, depending only on $(g, \frac{\delta}{\delta g})$ and on $(\phi, \frac{\delta}{\delta \phi})$, respectively,

$$
\mathcal{C}_M\left(g, -\mathrm{i}\tfrac{\delta}{\delta g}, \phi, -\mathrm{i}\tfrac{\delta}{\delta \phi}\right) = \mathcal{K}_G\left(g, \tfrac{\delta}{\delta g}\right)\mathcal{K}_M\left(\phi, \tfrac{\delta}{\delta \phi}\right). \tag{16}
$$

If such operators $\mathcal{K}_G$ and $\mathcal{K}_M$ exist so that (16) holds, the scalar constraint equation (14) can be rewritten as

$$
\Psi_M[\phi]\,\mathcal{C}_G\left(g, -\mathrm{i}\tfrac{\delta}{\delta g}\right)\Psi_G[g] = -\left[\mathcal{K}_G\left(g, \tfrac{\delta}{\delta g}\right)\Psi_G[g]\right]\left[\mathcal{K}_M\left(\phi, \tfrac{\delta}{\delta \phi}\right)\Psi_M[\phi]\right].
$$

Dividing this with $\Psi_M[\phi]\,\mathcal{K}_G\left(g, \frac{\delta}{\delta g}\right)\Psi_G[g]$, assuming it is well-defined, we obtain

$$
\frac{1}{\mathcal{K}_G\left(g, \frac{\delta}{\delta g}\right)\Psi_G[g]}\,\mathcal{C}_G\left(g, -\mathrm{i}\tfrac{\delta}{\delta g}\right)\Psi_G[g] = -\frac{1}{\Psi_M[\phi]}\,\mathcal{K}_M\left(\phi, \tfrac{\delta}{\delta \phi}\right)\Psi_M[\phi] = A,
$$

where A is a constant, since the terms on the left and the right of the first equality depend on different sets of variables. Therefore, the above equation splits into two independent equations,

$$
\begin{aligned}
\left[\mathcal{C}_G\left(g, -\mathrm{i}\tfrac{\delta}{\delta g}\right) - A\,\mathcal{K}_G\left(g, \tfrac{\delta}{\delta g}\right)\right]\Psi_G[g] &= 0, \\
\left[\mathcal{K}_M\left(\phi, \tfrac{\delta}{\delta \phi}\right) + A\right]\Psi_M[\phi] &= 0,
\end{aligned} \tag{17}
$$

which are to be solved independently for $\Psi_G[g]$ and $\Psi_M[\phi]$, thus providing a separable solution of (14).

The whole procedure above rests on the assumption (16) that the matter part $\mathcal{C}_M$ of the scalar constraint operator can be written as a product of two operators $\mathcal{K}_G$ and $\mathcal{K}_M$. Our main argument is to demonstrate that the assumption (16) is never satisfied for the usual matter fields, due to the universal nature of the coupling of gravity to matter, ultimately dictated by the equivalence principle. Namely, given the structure of the classical scalar constraint for matter (8), the corresponding operator can be written as

$$\mathcal{C}^M(\hat{g},\hat{\pi}_g,\hat{\phi},\hat{\pi}_\phi) = \hat{\pi}_{\phi A}\hat{\nabla}_\perp{}^A{}_B\hat{\phi}^B - \frac{1}{N}\mathcal{L}_M(\hat{g},\hat{\pi}_g,\hat{\phi},\hat{\pi}_\phi), \qquad (18)$$

where a certain ordering of the operators is assumed. The constraint (18) features the operator-valued matter Lagrangian $\mathcal{L}_M$. Therefore, in order to demonstrate that $\mathcal{C}_M$ does not satisfy the separability criterion (16) it is enough to demonstrate that the matter Lagrangian does not satisfy it. This can be done on a case-by-case basis, for each particular matter field. Invoking the equivalence principle, we can write the operator-valued Lagrangian for the scalar field coupled to gravity as

$$\mathcal{L}_M(\hat{g},\hat{\varphi},\partial\hat{\varphi}) = \frac{1}{2}\hat{e}\left[\hat{g}^{\mu\nu}(\partial_\mu\hat{\varphi})(\partial_\nu\hat{\varphi}) - m^2\hat{\varphi}^2 + U(\hat{\varphi})\right],$$

where $\hat{e}$ is the square-root of the minus determinant operator of the metric tensor,

$$\hat{e} \equiv \left[\frac{1}{4!}\varepsilon^{\alpha\beta\gamma\delta}\varepsilon^{\mu\nu\rho\sigma}\hat{g}_{\alpha\mu}\hat{g}_{\beta\nu}\hat{g}_{\gamma\rho}\hat{g}_{\delta\sigma}\right]^{\frac{1}{2}},$$

and U is some interaction potential of the scalar field. Ignoring the multiplicative factor $\hat{e}$ that acts only on $\mathcal{H}_G$, the Lagrangian is a sum of two types of terms: the kinetic term, containing the inverse metric $\hat{g}^{\mu\nu}$, and the mass and potential terms not featuring the gravitational field in any form. The sum cannot therefore be factored into the form $\mathcal{K}_G(\hat{g})\mathcal{K}_M(\hat{\phi},\partial\hat{\phi})$, since the Lagrangian is not a homogeneous function of the gravitational degrees of freedom. Even in the case of the massless free scalar field, i.e. when $m=0$ and $U=0$, the kinetic term is a sum of several different components of the metric and the derivatives of the scalar field,

$$\hat{g}^{00}(\partial_0\hat{\varphi})(\partial_0\hat{\varphi}) + \hat{g}^{01}(\partial_0\hat{\varphi})(\partial_1\hat{\varphi}) + \hat{g}^{12}(\partial_1\hat{\varphi})(\partial_2\hat{\varphi}) + \ldots$$

and this still cannot be factored into a product of two operators $\mathcal{K}_G$ and $\mathcal{K}_M$.

In the case of the Dirac field, again invoking the equivalence principle, the operator-valued Lagrangian is given by (9),

$$\mathcal{L}_M(\hat{e},\hat{\omega},\hat{\psi},\hat{\bar{\psi}}) = \hat{e}\left(\frac{\mathrm{i}}{2}\hat{\bar{\psi}}\gamma^a\hat{e}^\mu{}_a\overset{\leftrightarrow}{\hat{\nabla}}_\mu\hat{\psi} - m\hat{\bar{\psi}}\hat{\psi}\right).$$

Like in the case of the scalar field, the kinetic and mass terms in the Lagrangian depend differently on the gravitational fields $\hat{e}^a{}_\mu$ and $\hat{\omega}^{ab}{}_\mu$, and $\mathcal{L}_M$ cannot be factored. Moreover, the kinetic term itself cannot be factored, since it is a sum of two terms (see equations (6)), only one of which contains the spin connection $\hat{\omega}^{ab}{}_\mu$.

Next, the operator-valued Lagrangian for the electromagnetic field coupled to gravity has the form

$$\mathcal{L}_M(\hat{g},\hat{A},\partial\hat{A}) = -\frac{1}{4}\hat{e}\,\hat{g}^{\mu\rho}\hat{g}^{\nu\sigma}\hat{F}_{\mu\nu}\hat{F}_{\rho\sigma},$$

where $\hat{F}_{\mu\nu} \equiv \partial_\mu \hat{A}_\nu - \partial_\nu \hat{A}_\mu$. Applying the same argument as in the case of the free massless scalar field, this Lagrangian also cannot be factored into the form $\mathcal{K}_G \mathcal{K}_M$. The same argument also applies to the case of the non-Abelian Yang–Mills Lagrangians.

Summing up, given the ways the matter fields are coupled to gravity, based on the equivalence principle, we conclude that the separability criterion (16) is never satisfied for the physically relevant cases of scalar, spinor and vector fields. Therefore, according to the discussion above, the scalar constraint (12) should not admit separable state vectors into $\mathcal{H}_{\rm phys}$.

Regarding the above analysis, it is important to emphasize the following. Namely, one should note that it is in principle possible for equation (14) to have product state solutions (15) despite the fact that it does not satisfy the separability criterion (16). In other words, the criterion (16) is a sufficient condition for the existence of product state solutions of (14), but it is not necessary, so its violation does not strictly imply the absence of product state solutions. Nevertheless, given the arguably highly complex structure of equation (14)—meaning that it represents a nonlinear functional partial differential equation of at least second order in g and ϕ—it is natural to regard any potential product state solutions as completely accidental. Moreover, it is questionable if the boundary conditions required for such solutions correspond to any realistic physical situation in nature, i.e. they could be irrelevant for realistic physics. Due to all these arguments, the existence of product state solutions, in spite of the violation of the separability criterion (16), is in our opinion an extraordinary claim, and as such requires extraordinary evidence. In other words, the burden of proof is in fact with the statement that any product state solution exists, rather than the opposite. Consequently, product states (15) are generically not elements of $\mathcal{H}_{\rm phys}$, and even if one can prove that there exist some product states which do happen to belong to $\mathcal{H}_{\rm phys}$, such states would arguably be completely accidental, with questionable relevance for physics. Otherwise, if there exists a whole class of separable states which solve (14) despite the violation of the criterion (16), there must be some deep eluding property of the scalar constraint equation, which is both completely unknown and very interesting to study.

Finally, while it turns out that the analysis of the scalar constraint equation (12) is sufficient for our conclusions, let us briefly mention the status of the remaining two constraint equations (11). First, the Gauss constraint $\hat{\mathcal{C}}_{ab}$ obviously admits separable state vectors. On the other hand, the situation with the 3-diffeo constraint $\hat{\mathcal{C}}_i$ is more complicated, and the conclusion depends on the type of the field. For example, in the case of the scalar field, from (5) we read that $\hat{\mathcal{C}}_i^M$ depends only on the scalar field and its momentum, which means that the constraint equation does admit separable state vectors. However, in the case of the Dirac field, from (7) we read that $\hat{\mathcal{C}}_i^M$ depends on the spin connection in addition to the Dirac field, and this dependence is not homogeneous in the spin connection, see (6). Thus, the 3-diffeo constraint equation does not admit separable state vectors. However, the behaviour of the Gauss and 3-diffeo constraint equations is redundant for our argument, since the scalar constraint equation (12) already suppresses separable state vectors for all fields, due to the dynamical form of the coupling of matter to gravity. Therefore, our initial assumption of local Poincaré symmetry can be weakened to the localisation of its translational subgroup, while the generators of the local Lorentz subgroup are irrelevant for our argument.

3. Entanglement in the path integral framework

In the previous section we have discussed the gauge-protected entanglement within the framework of the canonical quantisation of the gravitational field with matter. In this section, we focus instead on the path integral framework of quantisation. We analyse the entanglement on the example of the Hartle–Hawking state, which is known to satisfy all constraints of the theory. In the next section, we are going to apply the results of this section to the concrete case of Regge quantum gravity.

First, we discuss an entanglement criterion for the case of pure overall state of the gravity and matter fields. We begin with a brief recapitulation of basic results from the standard QM and quantum information theory. A pure bipartite state $|\Psi\rangle_{12} \in \mathcal{H}_1 \otimes \mathcal{H}_2$ of systems 1 and 2 can be written in the Schmidt bi-orthogonal form (see, for example [20]):

$$|\Psi\rangle_{12} = \sum_i \sqrt{r_i}|\alpha_i\rangle_1 \otimes |\beta_i\rangle_2, \tag{19}$$

where $\{|\alpha_i\rangle_1\}$ and $\{|\beta_i\rangle_2\}$ are two sets of mutually orthogonal states from $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. The partial sub-system states are then given as

$$\hat{\rho}_1 = \sum_i r_i|\alpha_i\rangle_1 \otimes \langle\alpha_i|_1, \tag{20}$$

for the system 1, and analogously for the system 2. Squaring $\hat{\rho}_1$, we have

$$\hat{\rho}_1^2 = \sum_i r_i^2|\alpha_i\rangle_1 \otimes \langle\alpha_i|_1. \tag{21}$$

If the overall state $|\Psi\rangle_{12}$ is separable (i.e. a simple product state), the above sum in (20) will be trivial, consisting of a single projector onto the ray $|\alpha_1\rangle_1 \otimes \langle\alpha_1|_1$, with $r_1 = 1$. Thus, we have that $\hat{\rho}_1^2 = \hat{\rho}_1$, or simply, $\mathrm{Tr}\,\hat{\rho}_1^2 = \mathrm{Tr}\,\hat{\rho}_1 = 1$. In case the state $|\Psi\rangle_{12}$ is entangled, the sum (20) will consist of more than just one term, resulting in $(\forall\ i)\ r_i < 1$. Therefore, $(\forall\ i)\ r_i^2 < r_i$, and we finally have

$$\mathrm{Tr}\,\hat{\rho}_1^2 = \sum_i r_i^2 < \sum_i r_i = \mathrm{Tr}\,\hat{\rho}_1 = 1. \tag{22}$$

Due to the symmetry of the Schmidt form (19), the same is valid for the system 2 (for the formal proof of the above entanglement criterion (22), see for example [20]).

After this recapitulation of the standard results from QM, we proceed with the analysis of the bipartite system of the gravity (G) and matter (M) fields, applying the above entanglement criterion (22) to the case of quantum fields. For simplicity, we omit the subscripts G and M for pure states of gravity and matter, respectively.

Let $\mathcal{H}_{\mathrm{kin}} = \mathcal{H}_G \otimes \mathcal{H}_M$ be the combined kinematical gravity-matter Hilbert space. Denote the bases in $\mathcal{H}_G$ and $\mathcal{H}_M$ as $\{|g\rangle\}$ and $\{|\phi\rangle\}$, respectively. These are the eigenbases of the corresponding quantum field operators $\hat{g}$ and $\hat{\phi}$, evaluated on the 3D boundary $\Sigma_3 = \partial\mathcal{M}_4$ of the 4D spacetime manifold $\mathcal{M}_4$. The general state vector $|\Psi\rangle \in \mathcal{H}_{\mathrm{kin}}$ of the gravity-matter system can then be written as

$$|\Psi\rangle = \int \mathcal{D}g \int \mathcal{D}\phi\, \Psi[g,\phi]\, |g\rangle \otimes |\phi\rangle, \tag{23}$$

where $\Psi[g,\phi] = \langle g,\phi|\Psi\rangle$ is called the wavefunctional (in analogy to wavefunction from quantum mechanics), and the functional integrals over gravitational degrees of freedom g and matter degrees of freedom ϕ are assumed to be well defined in some way (in section 4 we present an explicit example of this). The bases $\{|g\rangle\}$ and $\{|\phi\rangle\}$ are assumed to be orthonormal, satisfying

$$\langle g|g'\rangle = \delta[g-g'], \qquad \langle\phi|\phi'\rangle = \delta[\phi-\phi'], \tag{24}$$

where the Dirac delta functional is assumed to satisfy the formal functional integral identities

$$\int \mathcal{D}g\, F[g]\, \delta[g-g'] = F[g'],$$
$$\int \mathcal{D}\phi\, F[\phi]\, \delta[\phi-\phi'] = F[\phi'], \tag{25}$$

for any functionals $F[g]$ and $F[\phi]$ belonging to some suitable relevant class.

From the state (23) one can construct a reduced density matrix $\hat\rho_M$ for matter fields, by taking the partial trace over gravitational degrees of freedom of the full density matrix $\hat\rho \equiv |\Psi\rangle \otimes \langle\Psi|$, as

$$\hat\rho_M = \mathrm{Tr}_G\, \hat\rho = \int \mathcal{D}g\, \langle g| \Big(|\Psi\rangle \otimes \langle\Psi| \Big) |g\rangle.$$

Substituting (23) we get

$$\hat\rho_M = \int \mathcal{D}g \int \mathcal{D}g' \int \mathcal{D}\phi' \int \mathcal{D}g'' \int \mathcal{D}\phi'' \; \Psi^*[g',\phi']\, \Psi[g'',\phi'']\, \langle g| \Big(|g''\rangle \otimes |\phi''\rangle \otimes \langle g'| \otimes \langle\phi'| \Big) |g\rangle.$$

Using (24) and (25), the expression for the reduced density matrix can be evaluated to

$$\hat\rho_M = \int \mathcal{D}g \int \mathcal{D}\phi' \int \mathcal{D}\phi''\, \Psi^*[g,\phi'] \Psi[g,\phi'']\, |\phi''\rangle \otimes \langle\phi'|. \tag{26}$$

Taking the square and using (24) and (25) again, one obtains

$$\hat\rho_M^2 = \int \mathcal{D}g \int \mathcal{D}g' \int \mathcal{D}\phi' \int \mathcal{D}\phi'' \int \mathcal{D}\phi''' \; \Psi^*[g,\phi']\, \Psi[g,\phi'']\, \Psi^*[g',\phi''']\, \Psi[g',\phi']\, |\phi''\rangle \otimes \langle\phi'''|.$$

Finally, taking the trace over matter fields,

$$\mathrm{Tr}_M\, \hat\rho_M^2 = \int \mathcal{D}\phi\, \langle\phi|\hat\rho_M^2|\phi\rangle,$$

we get

$$\mathrm{Tr}_M\, \hat\rho_M^2 = \int \mathcal{D}g \int \mathcal{D}g' \int \mathcal{D}\phi \int \mathcal{D}\phi' \; \Psi^*[g,\phi']\, \Psi[g,\phi]\, \Psi^*[g',\phi]\, \Psi[g',\phi']. \tag{27}$$

Now we want to evaluate (27) for one specific state, namely the Hartle–Hawking state, denoted $|\Psi_{\mathrm{HH}}\rangle$. This state is known to satisfy the scalar constraint equation (12), see [14], and thus belongs to the physical Hilbert space $\mathcal{H}_{\mathrm{phys}}$. Our aim is to demonstrate that the Hartle–Hawking state is nonseparable, and the strategy is to argue that $\mathrm{Tr}_M\, \hat\rho_M^2 < 1$ for $\hat\rho = |\Psi_{\mathrm{HH}}\rangle \otimes \langle\Psi_{\mathrm{HH}}|$. The Hartle–Hawking state is defined by specifying the wavefunctional $\Psi[g,\phi]$ in (23) as

$$\Psi_{\mathrm{HH}}[g,\phi] = \mathcal{N} \int \mathcal{D}G \int \mathcal{D}\Phi\, \mathrm{e}^{\mathrm{i}S_{\mathrm{tot}}[g,\phi,G,\Phi]}. \tag{28}$$

Here $\mathcal{N}$ is a normalisation constant, the variables G and Φ (denoted with the capital letters) live in the bulk spacetime $\mathcal{M}_4$, while g and ϕ (denoted with lowercase letters) live on the boundary $\Sigma_3 = \partial\mathcal{M}_4$, as before. The path integrals are taken over the bulk while keeping the boundary fields constant. Finally, the total action functional S_{tot} has the following structure

$$S_{\rm tot}[g,\phi,G,\Phi] = S_G[g,G] + S_M[g,\phi,G,\Phi], \tag{29}$$

where S_G is the action for the gravitational field (for example the Einstein–Hilbert action with a cosmological constant), while S_M is the action for the matter fields coupled to gravity—hence its dependence on both the gravitational and matter fields. See [14] for details on the construction of the expression (28).

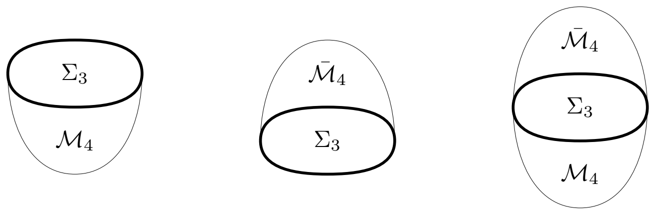
In order to analyse the expression (27) more efficiently, it is convenient to introduce the following quantity,

$$Z[\phi,\phi'] \equiv \int \mathcal{D}g\, \Psi_{\rm HH}[g,\phi]\Psi^*_{\rm HH}[g,\phi'], \tag{30}$$

which represents the matrix element of the reduced density matrix $\hat{\rho}_M$. Namely, by evaluating (26) for the Hartle–Hawking state, one obtains

$$\hat{\rho}_M = \int \mathcal{D}\phi \int \mathcal{D}\phi'\, Z[\phi,\phi']\, |\phi\rangle \otimes \langle\phi'|. \tag{31}$$

In addition, $Z[\phi,\phi']$ has an important geometric structure. Namely, one can consider two copies of the spacetime manifold $\mathcal{M}_4$, where the boundary Σ_3 of the first copy features the fields g,ϕ, while the boundary of the second copy features the fields g,ϕ', i.e. such that the gravitational field g is the same, while matter fields ϕ and ϕ' are different on the boundaries. Then one takes the second copy of $\mathcal{M}_4$, inverts it with respect to the boundary Σ_3 (the result is denoted as $\bar{\mathcal{M}}_4$), and glues it to the first copy along the common boundary, to obtain a manifold $\mathcal{M}_4 \cup \bar{\mathcal{M}}_4$, which has no boundary. This can be illustrated by the following diagrams:



The quantity $Z[\phi,\phi']$ is then obtained by integrating over all gravitational degrees of freedom, and all bulk matter degrees of freedom, weighted by the kernel $e^{iS_{\rm tot}}$ of the Hartle–Hawking wavefunction (28). This construction is important because the trace of $Z[\phi,\phi']$ is the state sum of the gravitational and matter fields over the manifold $\mathcal{M}_4 \cup \bar{\mathcal{M}}_4$:

$$\int \mathcal{D}\phi\, Z[\phi,\phi] = Z \equiv \int \mathcal{D}G \int \mathcal{D}\Phi\, e^{iS[G,\Phi]}. \tag{32}$$

Here, $S[G,\Phi]$ is the total gravity-matter action similar to (29), defined over the manifold $\mathcal{M}_4 \cup \bar{\mathcal{M}}_4$, and thus features no boundary fields. From (30)–(32) it is then easy to see that the normalization of the state sum, $Z = 1$, and simultaneously the normalization of the reduced density matrix, $\mathrm{Tr}\,\hat{\rho}_M = 1$, i.e.

$$\int \mathcal{D}\phi\, Z[\phi,\phi] = 1, \tag{33}$$

are equivalent to the normalisation of the Hartle–Hawking state, $\langle\Psi_{\rm HH}|\Psi_{\rm HH}\rangle = 1$. Finally, from the definition (30) it is easy to see that $Z[\phi,\phi']$ is self-adjoint,

$$Z[\phi,\phi'] = Z^*[\phi',\phi],$$

as the matrix elements of the density matrix $\hat{\rho}_M$ are supposed to be.

Returning to the evaluation of (27) for the Hartle–Hawking state, one can use (30) to rewrite it into the compact form

$$\mathrm{Tr}_M \, \hat{\rho}_M^2 = \int \mathcal{D}\phi \int \mathcal{D}\phi' \, \left| Z[\phi, \phi'] \right|^2 . \tag{34}$$

At this point the general analysis cannot proceed any further, since the right-hand side cannot be evaluated explicitly without specifying the details of the theory. The calculation will therefore proceed further in the next section, where we consider one detailed model of quantum gravity with matter.

Despite the inability to evaluate the integral (34) in the general case, one can give a qualitative argument that the result is not equal to one, leading to the nonseparability of the Hartle–Hawking state. Namely, given the definition (28) of the Hartle–Hawking state, it is easy to see that it essentially depends on two quantities—the normalisation constant $\mathcal{N}$, and the choice of the action S_{tot}. The normalisation constant is fixed by the requirement that (33) holds. This leaves the value of the integral (34) depending solely on the choice of the classical action of the theory. It is qualitatively straightforward to see that different choices of the action will lead to different values of $\mathrm{Tr}_M \, \hat{\rho}_M^2$, so any generic choice of S_{tot} is likely to give $\mathrm{Tr}_M \, \hat{\rho}_M^2 < 1$. A tentative choice for (29) would be the Einstein–Hilbert action for S_G and the Standard Model of elementary particle physics for S_M, based on the gauge group $SU(3) \times SU(2) \times U(1)$. However, we know that the Standard Model action is incomplete, for example due to the fact that dark matter is not included in the description. Therefore, the choice of the classical action is a sort of a moving target, and it is unlikely that any candidate action we choose will give $\mathrm{Tr}_M \, \hat{\rho}_M^2 = 1$. In this sense, one can only conclude that in a generic case the Hartle–Hawking state is nonseparable, supporting the abstract argument from section 2.

Finally, let us note that our assumption of local Poincaré gauge symmetry implies that we are discussing the Lorentzian path integral formulation of the theory. In contrast, within the Euclidean approach, the Hartle–Hawking state has some problematic characteristics, see for example [21] and references therein.

4. Regge quantum gravity example

In this section we will present a short review of the Regge quantum gravity model coupled to scalar matter, and then use this model to evaluate (34) for the Hartle–Hawking state. The Regge quantum gravity model is intimately connected to the covariant loop quantum gravity research framework [22, 23], its generalisations [24–26], and various related research areas [27, 28] (see also [29] for an interesting connection to the noncommutative geometry approach in the $3D$ case). Nevertheless, it can be introduced and studied as a simple standalone model of quantum gravity independent of any other context, as was done in [30], where some preliminary results regarding the entanglement in the Hartle–Hawking state have been announced.

4.1. Formalism of Regge quantum gravity

The Regge quantum gravity model is arguably the simplest toy-model of quantum gravity constructed by providing a rigorous definition for the gravitational path integral, generically denoted as

$$Z_G = \mathcal{N} \int \mathcal{D}g \, \mathrm{e}^{\mathrm{i}S_{\mathrm{EH}}[g]}, \tag{35}$$

where $S_{\mathrm{EH}}[g]$ is the Einstein–Hilbert action for general relativity. The construction of the path integral follows Feynman's original idea of path integral definition-by-discretisation. We begin by passing from a smooth $4D$ spacetime manifold $\mathcal{M}_4$ to a piecewise-linear $4D$ manifold, most commonly a triangulation $T(\mathcal{M}_4)$. This structure naturally features 4-simplices σ as basic building blocks, which themselves consist of tetrahedra τ, triangles Δ, edges ϵ and vertices v. The invariant quantities associated to these objects are the 4-volume of the 4-simplex ${}^{(4)}V_\sigma$, the 3-volume of the tetrahedron ${}^{(3)}V_\tau$, the area of the triangle A_Δ and the length of the edge l_ϵ, respectively, while the vertices do not have nontrivial quantities assigned to them.

It is important to emphasise that the edge lengths are most fundamental of all these quantities, since one can always uniquely express ${}^{(4)}V_\sigma$, ${}^{(3)}V_\tau$ and A_Δ as functions of l_ϵ. For example, the most well-known is the Heron formula for the area of a triangle in terms of its three edge lengths,

$$A_\Delta(l) = \sqrt{s(s-l_1)(s-l_2)(s-l_3)}, \qquad s \equiv \frac{l_1+l_2+l_3}{2},$$

where the three edges $\epsilon = 1, 2, 3$ belong to the triangle Δ.

Given a spacetime triangulation, the Einstein–Hilbert action of general relativity,

$$S_{\mathrm{EH}}[g] = -\frac{1}{16\pi l_p^2}\int_{\mathcal{M}_4} \mathrm{d}^4x\sqrt{-g}\,R(g),$$

can be reformulated in terms of edge lengths of the triangulation as the Regge action

$$S_R[l] = -\frac{1}{8\pi l_p^2}\sum_{\Delta\in T(\mathcal{M}_4)} A_\Delta(l)\delta_\Delta(l),$$

where δ_Δ is the so-called deficit angle at triangle Δ, measuring the amount of spacetime curvature around Δ. See [31] and [27] for details and a review.

Once the classical action for general relativity has been adapted to a piecewise-linear manifold structure, we can take the edge lengths of the edges in the triangulation as the fundamental degrees of freedom of the theory, and define the gravitational path integral (35) as:

$$Z_G = \mathcal{N}\int_D \prod_{\epsilon\in T(\mathcal{M}_4)} \mathrm{d}l_\epsilon\,\mu(l)\mathrm{e}^{\mathrm{i}S_R[l]}. \tag{36}$$

Here $\mathcal{N}$ is a normalisation constant, while $\mu(l)$ is the measure term which ensures the convergence of the state sum Z_G. For the purpose of this paper, we choose the exponential measure

$$\mu(l) = \exp\left(-\frac{1}{L_\mu^4}\sum_{\sigma\in T(\mathcal{M}_4)} {}^{(4)}V_\sigma(l)\right), \tag{37}$$

where $L_\mu > 0$ is a constant and a free parameter of the model (see [32–34] for motivation and analysis). Note that the sum of the 4-volumes of all 4-simplices gives the total 4-volume of the triangulation $T(\mathcal{M}_4)$, and will sometimes be denoted simply as V_4.

The choice of edge lengths as the fundamental gravitational degrees of freedom in (36) determines the integration domain D as a subset of the Cartesian product $(\mathbb{R}_0^+)^E$, where E is the total number of edges in $T(\mathcal{M}_4)$, while $\mathbb{R}_0^+$ is the maximum integration domain of each individual edge length. We should note that D is a strict subset of $(\mathbb{R}_0^+)^E$ due to the presence of triangle inequalities which must be satisfied for all triangles, tetrahedra and 4-simplices in a given triangulation.

Once we have defined the gravitational path integral (35) via the state sum (36), it is straightforward to generalise this definition to the situation which includes matter fields. For simplicity, we will discuss only a single real scalar field φ, although it is not a problem to include other fields as well. The path integral we are interested in can be denoted as

$$Z_{G+M} = \mathcal{N} \int \mathcal{D}g \int \mathcal{D}\varphi \, e^{iS_{\text{tot}}[g,\varphi]}, \tag{38}$$

where $S_{\text{tot}}[g,\varphi]$ is the sum of the Einstein–Hilbert action and the action for the scalar field in curved spacetime,

$$\begin{aligned} S_{\text{tot}}[g,\varphi] &= -\frac{1}{16\pi l_p^2} \int_{\mathcal{M}_4} d^4x \sqrt{-g}\, R(g) \\ &\quad + \frac{1}{2} \int_{\mathcal{M}_4} d^4x \sqrt{-g} \left[g^{\mu\nu} (\partial_\mu \varphi)(\partial_\nu \varphi) + m^2 \varphi^2 + U(\varphi) \right], \end{aligned}$$

where $U(\varphi)$ is a self-interaction potential of the scalar field. The corresponding lattice version of this action is given as

$$\begin{aligned} S_{\text{tot}}[l,\varphi] &= -\frac{1}{8\pi l_p^2} \sum_{\Delta \in T(\mathcal{M}_4)} A_\Delta(l) \delta_\Delta(l) + \\ &\quad + \frac{1}{2} \sum_{\sigma \in T(\mathcal{M}_4)} {}^{(4)}V_\sigma(l) g^{\mu\nu}_{(\sigma)}(l) \partial\varphi_\mu \partial\varphi_\nu \\ &\quad + \frac{1}{2} \sum_{v \in T(\mathcal{M}_4)} {}^{(4)}V^*_v(l) \left[m^2 \varphi_v^2 + U(\varphi_v) \right]. \end{aligned} \tag{39}$$

Here, a value of the scalar field $\varphi_v \in \mathbb{R}$ is assigned to each vertex $v \in T(\mathcal{M}_4)$. Given any 4-simplex $\sigma \in T(\mathcal{M}_4)$, one can label its five vertices as $0, 1, 2, 3, 4$, and then define a skew-coordinate system taking the vertex 4 as the origin and edges $4-0$, $4-1$, $4-2$, $4-3$, respectively as coordinate lines for coordinates x^μ, $\mu \in \{0, 1, 2, 3\}$. In these coordinates, the derivative $\partial_\mu \varphi$ is replaced by the finite difference between the values of the field at the vertex $v = \mu$ and at the coordinate origin of the 4-simplex σ (divided by the distance between them),

$$\partial\varphi_\mu \equiv \frac{\varphi_\mu - \varphi_4}{l_{\mu 4}}.$$

In addition, the metric tensor between vertices μ and ν is given in terms of edge lengths as

$$g^{(\sigma)}_{\mu\nu}(l) \equiv \frac{l_{\mu 4}^2 + l_{\nu 4}^2 - l_{\mu\nu}^2}{2 l_{\mu 4} l_{\nu 4}},$$

while $g^{\mu\nu}_{(\sigma)}(l)$ is its inverse matrix. Finally, ${}^{(4)}V^*_v(l)$ is the 4-volume of the 4-cell surrounding the vertex v in the Poincaré dual lattice of the triangulation $T(\mathcal{M}_4)$.

After we have defined the classical action on $T(\mathcal{M}_4)$, we finally proceed to define the path integral (38) as the state sum:

$$Z_{G+M} = \mathcal{N} \int \prod_{\epsilon \in T(\mathcal{M}_4)} dl_\epsilon \, \mu(l) \int \prod_{v \in T(\mathcal{M}_4)} d\varphi_v \, e^{iS_{\text{tot}}[l,\varphi]}. \tag{40}$$

Here, the domain of integration for the scalar field is the Cartesian product $\mathbb{R}^V$, where V is the total number of vertices in the triangulation.

The state sum (40) defines one concrete QG model, called the Regge quantum gravity model. While it goes without saying that this is just a toy model, it is nevertheless a realistic one, since it is finite and has a correct semiclassical continuum limit (see [32] for proofs). Therefore it can be used to study various aspects of quantum gravity, including the entanglement between gravity and matter fields, as we discuss next.

4.2. Calculation of the trace formula

Having formulated the Regge quantum gravity model and having the state sum (40) in hand, we can proceed to study the entanglement between gravity and matter, in particular by evaluating the expression for the trace of $\hat{\rho}_M^2$ given by equation (34). In order to evaluate it, we first need to formulate the Hartle–Hawking state (28) in the framework of Regge quantum gravity model, then work out the matrix elements of the reduced density matrix (30), and finally plug them into (34) to obtain a number. If this number is different from 1, we can conclude that the Hartle–Hawking state features entanglement between the gravitational and matter fields.

We begin by formulating the Hartle–Hawking state (28). Consider a 4-manifold $\mathcal{M}_4$ with a nontrivial boundary $\Sigma_3 = \partial\mathcal{M}_4$, such that the triangulation $T(\mathcal{M}_4)$ induces a triangulation $T(\Sigma_3)$ on the boundary. In this sense we can distinguish the vertices, edges, areas, and tetrahedra which belong to the boundary triangulation $T(\Sigma_3)$ (from now on shortly called 'boundary', and denoted as ∂T), from the vertices, edges, areas, tetrahedra and 4-simplices belonging to $T(\mathcal{M}_4)$ but not to $T(\Sigma_3)$ (from now on shortly called 'bulk', and denoted as T). Since the Regge quantum gravity model encodes gravitational degrees of freedom as lengths of the edges, and matter degrees of freedom as real numbers attached to vertices, we can easily split them into boundary variables l_ϵ, φ_v and bulk variables L_ϵ, Φ_v, where we maintain our previous convention to denote the bulk variables with capital letters and boundary variables with lowercase letters.

Given the bulk and the boundary, we use the formulation of the Regge quantum gravity state sum (40) to write down the Hartle–Hawking wavefunction as

$$\Psi_{\rm HH}[l,\varphi] = \mathcal{N} \int \prod_{\epsilon\in T} \mathrm{d}L_\epsilon \, \mu(l,L) \int \prod_{v\in T} \mathrm{d}\Phi_v \, \mathrm{e}^{\mathrm{i}S_{\rm tot}[l,\varphi,L,\Phi]}. \tag{41}$$

Next we want to construct the matrix elements of the reduced density matrix (30). To this end, we need two copies of the Hartle–Hawking state: one with matter fields φ_v on the boundary ∂T of the bulk T, and the other with matter fields φ'_v on the boundary ∂T of the bulk $\bar{T}$ defined as the mirror-reflection of T with respect to the boundary ∂T. This mirror-reflection gives rise to an additional overall minus sign in the action (39) which is then cancelled by the complex conjugation of the imaginary unit in the exponent of the second Hartle–Hawking wavefunction in (30). Integrating over the boundary edge lengths, we end up with:

$$Z[\varphi,\varphi'] = |\mathcal{N}|^2 \int \prod_{\epsilon\in T\cup\bar{T}\cup\partial T} \mathrm{d}L_\epsilon \, \mu(L) \int \prod_{v\in T\cup\bar{T}} \mathrm{d}\Phi_v \, \mathrm{e}^{\mathrm{i}S_{\rm tot}[\varphi,\varphi',L,\Phi]}. \tag{42}$$

Note that all edge lengths are being integrated over in the 'total' triangulation $T\cup\bar{T}\cup\partial T$ (and we have thus denoted them all with a capital letter L for simplicity). In contrast, the scalar field is being integrated only over the two bulks $T\cup\bar{T}$, while the boundary scalar field values φ, φ' remain fixed on two identical copies of the boundary ∂T. Also, note that

$$S_{\rm tot}[\varphi,\varphi',L,\Phi] \equiv S_{\rm tot}[\varphi,L,\Phi]\Big|_{T\cup\partial T} + S_{\rm tot}[\varphi',L,\Phi]\Big|_{\bar{T}\cup\partial T},$$

where the boundary edge lengths l have been relabelled as L and reabsorbed into the set of bulk edge lengths.

The next step one should perform is to take the trace of (42) and equate it to 1 as in (33), in order to make sure that the Hartle–Hawking wavefunction (41) is properly normalised. This leads to the equation

$$|\mathcal{N}|^2 \int \prod_{\epsilon\in T\cup\bar{T}\cup\partial T} \mathrm{d}L_\epsilon\, \mu(L) \int \prod_{v\in T\cup\bar{T}\cup\partial T} \mathrm{d}\Phi_v\, \mathrm{e}^{\mathrm{i}S_{\mathrm{tot}}[L,\Phi]} = 1,$$

which determines the normalisation constant $\mathcal{N}$ up to an overall phase factor. Note that the boundary scalar fields φ have been integrated over and consequently reabsorbed into the bulk variables Φ, similarly to edge lengths L. Both the integration over L and the integration over Φ is now being performed over the 'total' triangulation $T\cup\bar{T}\cup\partial T$ which has no boundary.

As the final step of the construction of the trace formula (34), we substitute (42) and $\mathcal{N}$ into it, to obtain:

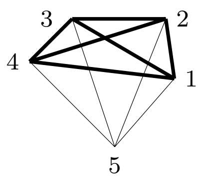
$$\mathrm{Tr}_M\, \hat{\rho}_M^2 = \frac{\displaystyle\int \prod_{v\in\partial T} \mathrm{d}\varphi_v \int \prod_{v\in\partial T} \mathrm{d}\varphi'_v \left| \int \prod_{\epsilon\in T\cup\bar{T}\cup\partial T} \mathrm{d}L_\epsilon\, \mu(L) \int \prod_{v\in T\cup\bar{T}} \mathrm{d}\Phi_v\, \mathrm{e}^{\mathrm{i}S_{\mathrm{tot}}[\varphi,\varphi',L,\Phi]} \right|^2}{\left(\displaystyle\int \prod_{\epsilon\in T\cup\bar{T}\cup\partial T} \mathrm{d}L_\epsilon\, \mu(L) \int \prod_{v\in T\cup\bar{T}\cup\partial T} \mathrm{d}\Phi_v\, \mathrm{e}^{\mathrm{i}S_{\mathrm{tot}}[L,\Phi]} \right)^2}. \tag{43}$$

This is the final expression we set out to derive. It represents a concrete realisation of the trace formula (34), it is completely well defined, and can in principle be evaluated. In practice, though, for a generic choice of the triangulation, this expression is very hard to evaluate even numerically. Therefore, in what follows we shall enforce some very hard approximations in order to make it more manageable for study. Nevertheless, by looking at the structure of the numerator and the denominator, one can already see that the two expressions can be equal to each other only in some very special cases, if at all. However, the dependence of the action S_{tot} on the boundary and bulk variables is such that one cannot rely on any special mathematical properties of the action which could help make the final result be 1, for a generic choice of the spacetime triangulation. In this sense, we can conjecture already at this level that in generic cases we have

$$\mathrm{Tr}_M\, \hat{\rho}_M^2 < 1,$$

as we wanted to demonstrate.

But in order to give a more convincing argument, let us study a special case and try to evaluate this trace to the very end. The simplest possible example of a triangulation T is a single 4-simplex. Labelling its vertices as $1, 2, 3, 4, 5$, we can depict it with a following diagram:



The 4-simplex has five boundary tetrahedra, namely

$$\tau_{1234}, \qquad \tau_{1235}, \qquad \tau_{1245}, \qquad \tau_{1345}, \qquad \tau_{2345}.$$

The first tetrahedron, τ_{1234}, is depicted with thick edges, and we will choose it to be the boundary ∂T. Since we do not want the four remaining tetrahedra to belong to the boundary, we will glue them onto each other in pairs, as

$$\tau_{1235} \equiv \tau_{1245}, \qquad \tau_{1345} \equiv \tau_{2345}.$$

This means that every point in τ_{1235} is identified with the corresponding point in τ_{1245}, and similarly with the other pair of tetrahedra. In this way we obtain a manifold with a nontrivial topology, but described with only five vertices and one boundary tetrahedron. In order for this gluing to be consistent, the gravitational and matter degrees of freedom living on $T \cup \partial T$ must satisfy the following constraints:

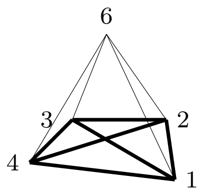
$$\begin{gathered} l_{14} = l_{23} = l_{24} = l_{13}, \qquad L_{25} = L_{15}, \qquad L_{45} = L_{35}, \\ \varphi_2 = \varphi_1, \qquad \varphi_4 = \varphi_3. \end{gathered} \tag{44}$$

This leaves us with the following independent degrees of freedom living on the 4-simplex:

$$l_{12}, \qquad l_{13}, \qquad L_{15}, \qquad l_{34}, \qquad L_{35}, \qquad \varphi_1, \qquad \varphi_3, \qquad \Phi_5,$$

where we have denoted the bulk degrees of freedom with capital letters and boundary degrees of freedom with lowercase letters. The 4-simplex diagram above is the graphical representation of the Hartle–Hawking wavefunction $\Psi_{\mathrm{HH}}[l, \varphi]$ (41).

Next we construct $\bar{T}$. Since the boundary tetrahedron ∂T defines a single 3-dimensional hypersurface, there is precisely one axis in 4-dimensional space which is orthogonal to ∂T. Performing the reflection of T with respect to ∂T is therefore identical to reversing the orientation of this orthogonal axis. In this way we construct another 4-simplex, with vertices labeled $1, 2, 3, 4, 6$ and depicted as



One can see that the main difference between the 4-simplex σ_{12346} and the previously constructed 4-simplex σ_{12345} is that the vertex 6 is on the 'opposite side' of the tetrahedron τ_{1234} as compared to the vertex 5 of σ_{12345}.

Like we did for σ_{12345}, we again want to glue the boundary tetrahedra pairwise, so that only the tetrahedron τ_{1234} remains as the boundary $\partial\bar{T}$. The pairwise gluing of tetrahedra

$$\tau_{1236} \equiv \tau_{1246}, \qquad \tau_{1346} \equiv \tau_{2346}$$

gives rise to the constraints

$$\begin{gathered} l_{14} = l_{23} = l_{24} = l_{13}, \qquad L_{26} = L_{16}, \qquad L_{46} = L_{36}, \\ \varphi'_2 = \varphi'_1, \qquad \varphi'_4 = \varphi'_3, \end{gathered}$$

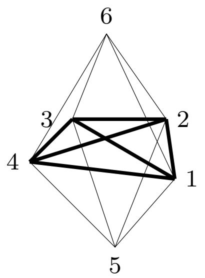
where only the constraints containing the vertex 6 are additional to (44). This leaves us with the following independent degrees of freedom living on σ_{12346}:

$$l_{12}, \qquad l_{13}, \qquad L_{16}, \qquad l_{34}, \qquad L_{36}, \qquad \varphi'_1, \qquad \varphi'_3, \qquad \Phi_6.$$

As noted in the general discussion leading to equation (43), the matter degrees of freedom on the boundary of T are different than the corresponding degrees of freedom living on the boundary of $\bar{T}$, despite the fact that the boundary is identical, $\partial\bar{T} \equiv \partial T$. To that end, we have added a prime to φ in the above equations. Like for the 4-simplex σ_{12345}, the diagram of the

4-simplex σ_{12346} above is the graphical representation of the (complex-conjugate) Hartle–Hawking wavefunction $\Psi^*_{\rm HH}[l,\varphi']$.

At this point we are ready to glue T and $\bar{T}$ along the common boundary ∂T, to obtain the manifold $T \cup \bar{T} \cup \partial T$ which has no boundary. It is depicted on the diagram below.



It consists of two 4-simplices σ_{12345} and σ_{12346} constructed above and glued along the common tetrahedron τ_{1234}. The full set of independent gravitational degrees of freedom is

$$l_{12}, \qquad l_{13}, \qquad l_{34}, \qquad L_{15}, \qquad L_{16}, \qquad L_{35}, \qquad L_{36},$$

while the independent matter degrees of freedom are

$$\varphi_1, \qquad \varphi_3, \qquad \varphi'_1, \qquad \varphi'_3, \qquad \Phi_5, \qquad \Phi_6.$$

This diagram is the graphical representation for the matrix element $Z[\varphi,\varphi']$ of the reduced density matrix $\hat{\rho}_M$ (see equations (42) and (30)).

Applying the general trace formula (43) to our case then gives

$$\mathrm{Tr}_M\, \hat{\rho}_M^2 = \frac{\displaystyle\int \mathrm{d}\varphi_1 \mathrm{d}\varphi_3 \mathrm{d}\varphi'_1 \mathrm{d}\varphi'_3 \left| \int \mathrm{d}^7 L\, \mu(L) \int \mathrm{d}\Phi_5 \mathrm{d}\Phi_6\, \mathrm{e}^{\mathrm{i}S_{\rm tot}[\varphi,\varphi',L,\Phi]} \right|^2}{\displaystyle\left(\int \mathrm{d}^7 L\, \mu(L) \int \mathrm{d}^4\Phi\, \mathrm{e}^{\mathrm{i}S_{\rm tot}[L,\Phi]} \right)^2}, \tag{45}$$

where

$$\mathrm{d}^7 L \equiv \mathrm{d}l_{12}\mathrm{d}l_{13}\mathrm{d}l_{34}\mathrm{d}L_{15}\mathrm{d}L_{16}\mathrm{d}L_{35}\mathrm{d}L_{36},$$

and

$$\mathrm{d}^4\Phi \equiv \mathrm{d}\varphi_1 \mathrm{d}\varphi_3 \mathrm{d}\Phi_5 \mathrm{d}\Phi_6.$$

Note that the action in the denominator is evaluated using $\varphi'_1 = \varphi_1$ and $\varphi'_3 = \varphi_3$, as explained in the general discussion above. In order to make the equation (45) fully explicit, we need to choose the values of the free parameters in the classical action (39) and the measure (37). The parameters of the action are the Planck length l_p, the mass m of the scalar field, and the self-interaction potential $U(\varphi)$. For the purpose of this example, the simplest possible choice is the free massless scalar field, so that we have

$$l_p = 10^{-35}\ \mathrm{m}, \qquad m = 0, \qquad U(\varphi) = 0.$$

Second, the measure (37) contains a single free parameter L_μ. This parameter can be connected to the value of the effective cosmological constant Λ, via the relation

$$\Lambda = \frac{l_p^2}{2L_\mu^4},$$

see [32–34] for details. Taking the observed value $\Lambda = 10^{-52}$ m^{-2} (also often quoted as a dimensionless product $\Lambda l_p^2 = 10^{-122}$), we obtain

$$L_\mu = 10^{-5} \text{ m}.$$

Using these numeric values of the parameters, the right-hand side of (45) is fully specified, and can be evaluated using a computer. However, in order to render the calculation more manageable, for the purpose of this paper we instead choose to evaluate (45) with $L_\mu = 10^{-33}$ m, which corresponds to a larger cosmological constant, $\Lambda l_p^2 = 10^{-8}$, to speed up the convergence of the Monte-Carlo integration method. The result is strictly less than one,

$$\mathrm{Tr}_M \, \hat{\rho}_M^2 = 0.977 \pm 0.002,$$

as we had set out to demonstrate. Note that, although close to one, the above result is: (i) strictly smaller than one (within the computational error); (ii) obtained within extremely simplified toy model whose system consists of only two 4-simplices of spacetime. Thus, our result can serve as a proof of principle that gravity-matter entanglement is always present. The total amount of such entanglement in realistic models, as well as its spatial distribution, remains to be further explored. Namely, note that even though the approximation of product gravity-matter states has been up to now successfully applied, the *overall* entanglement between the two systems, considered within complex realistic situations/models, does not at all have to be small, nor its effects negligible. Indeed, the standard entanglement that is considered to cause the decoherence of matter by the environment and the quantum-to-classical transition has profoundly striking effects, despite the fact of being difficult to characterise, evaluate and manipulate.

5. Conclusions

5.1. Summary of the results

We analyse the quantum gravity coupled to the most common matter fields (namely, scalar, spinor and vector fields), and show that the gravity and matter are generically entangled, as a consequence of the nonseparability of the scalar constraint $\mathcal{C}$, and in some cases the 3-diffeo constraint $\mathcal{C}_i^M$. Thus, simple separable gravity-matter product states are excluded from the physical Hilbert space, unless the constraint equations feature some deep unknown property which allows for the invariance of a whole class of product states. We demonstrate this in two different ways: (i) within the general abstract nonperturbative canonical formalism, by directly analysing the mathematical structure of the constraints, and (ii) within the path integral formalism, by directly checking for entanglement of the Hartle–Hawking state in the Regge model of quantum gravity.

5.2. Discussion of the results

This *gauge-protected* decoherence due to the entanglement (in contrast to the standard *'for all practical purposes'* dynamical one) offers a possibly deeper fundamental explanation of the long-standing problem of the quantum-to-classical transition: the matter does not *decohere*, it is by default *decohered*.

Any potential entanglement, either dynamical or gauge-protected one, depends on the details of the coupling between matter and gravity. For the purpose of this paper, the coupling is prescribed by the strong equivalence principle, which states that the equations of motion for all matter fields must locally be identical to the equations of motion for those fields in flat spacetime. This is implemented by choosing the action for matter fields with minimal coupling prescription, and employed in both the canonical and the path integral frameworks. We should stress that the validity of the strong equivalence principle is a sufficient, but potentially not a necessary assumption for our main result. Namely, it is plausible that nonminimal coupling choices, involving explicit spacetime curvature terms in the matter Lagrangian, could also lead to the conclusion that entanglement between gravity and matter is unavoidable. However, it is also possible that one could come up with some particular complicated choice of nonminimal coupling which does admit some nonentagled states. In order to avoid complicating the analysis with such cases, given that nonminimal coupling between gravity and matter has absolutely no experimental evidence in its favor so far, we have chosen to assume the validity of the strong equivalence principle throughout the paper.

In standard QM entanglement is a generic consequence of the interaction. Nevertheless, there exist alternative mechanisms for creating it, such as the indistinguishability of identical particles, leading to effective 'exchange interactions'. This new gauge-protected gravity-matter entanglement can thus introduce additional 'effective interaction', which can possibly result in corrections to Einstein's weak equivalence principle (see for example [35]).

It is interesting to note that a possible peculiar impact of the quantised gravity to the whole decoherence programme was already inferred in Zurek's seminal paper [36], where on page 1520 the author writes: (the assumption of pairwise interactions) 'is customary and clear, even though it may prevent one from even an approximate treatment of the gravitational interaction beyond its Newtonian pairwise form'. Our result confirms Zurek's disclaimer—gravity (environment $\mathcal{E}$) is generically entangled with the *whole* matter (both the system $\mathcal{S}$ and the apparatus $\mathcal{A}$), that way allowing for non-trivial tripartite system-apparatus-environment *effective* interaction of the form $\mathcal{H}_{\mathcal{SAE}}$, explicitly excluded in [36]. In other words, the environment (spacetime) interaction with the matter could potentially disturb the system-apparatus correlations, thus violating the stability criterion of a faithful measurement (see [37], p 1271).

As a consequence of generic gravity-matter entanglement, the effective interaction between gravity and matter forbids the existence of a single background spacetime. Thus, when concerning quantum effects of gravity, one cannot talk of 'matter in a point of space', confirming the conjecture that spacetime is an 'emergent phenomenon'. In contrast to this, Penrose argues that spacetime, seen as a (four-dimensional) differentiable manifold, does not support superpositions of massive bodies and the corresponding (relative) states of gravity (i.e. the gravity-matter entanglement), leading to the objective collapse onto the product states of matter and (classical) spacetime [38]. Our result can therefore be treated as a possible criterion for a plausible candidate theory of quantum gravity.

Finally, not allowing product states between the matter and gravity is in tune with the relational approach to physics [22], in particular to quantum gravity (note that the original name for the many-world interpretation of QM was the *'Relative State' Formulation of Quantum Mechanics* [39]). See also [40] for an interesting treatment of relative state and decoherence approaches.

5.3. Relation to common quantum gravity research programs

In order to discuss our results in the context of various quantum gravity research programs, note that the gauge-protected entanglement between gravity and matter should exist in any model of quantum gravity with matter which respects local Poincaré symmetry. In this sense, various approaches to quantum gravity can be classified into four distinct categories.

(i) The first category represents models which explicitly respect (or at least aim to respect) local Poincaré symmetry. These include nonperturbative string theory/M-theory [41–43], loop quantum gravity [22, 23], Wheeler–DeWitt quantization [44, 45], and similar approaches.
(ii) The second category represents models in which local Poincaré symmetry is explicitly broken. These include perturbative quantum gravity [46], petrurbative string theory [43], causal dynamical triangulations approach [28], doubly-special relativity models [47], Hořava–Lifshitz gravity [48], various nonrelativistic quantization proposals, and so on.
(iii) The third category represents models in which it is not clear whether local Poincaré symmetry is broken or not. For example, in the asymptotic safety approach [49] this may depend on the properties of the fixed point. In noncommutative geometry [50, 51] it depends on the particular choice of the algebra. In higher-derivative theories and theories with propagating torsion [52] it may depend on various details of the model, etc.
(iv) Finally, the fourth category represents models which have not been developed enough to allow for coupling of matter fields. In models like entropic gravity [53, 54] and causal set theory [55, 56], it is not obvious how to couple matter fields to gravity, and whether this coupling would violate local Poincaré invariance or not.

It should be clear that our results apply to the first category of quantum gravity models, while for other three categories it either does not apply, or it is an open question. We should also state that the validity of local Poincaré symmetry is ultimately an experimental question, one over which various quantum gravity proposals may disagree.

In relation to the previous comment, it is worthwhile to also discuss the impact of possible anomalies to the gauge protected entanglement. As we have discussed in the final paragraph of section 2, the entanglement is a consequence of the scalar constraint $\hat{\mathcal{C}}$, see (12), and for certain types of matter fields also of the 3-diffeo constraint $\hat{\mathcal{C}}_i$ in (11), while the local Lorentz constraint $\hat{\mathcal{C}}_{ab}$ in (11) does not require entanglement. From this one can see that if the theory features anomalies due to the breaking of the 4D diffeomorphism symmetry, one cannot impose $\hat{\mathcal{C}}$ and $\hat{\mathcal{C}}_i$ as the Gupta–Bleuler-like conditions on the Hilbert space of the theory, and thus all subsequent results regarding the entanglement are void. In short, there cannot be any gauge protected entanglement if there is no relevant gauge symmetry to begin with. Nevertheless, if the theory features anomalies due to the breaking of the local Lorentz or any internal symmetries, while maintaining diffeomoprhism symmetry at the quantum level, the gauge protected entanglement will not be influenced by the anomaly.

5.4. Future lines of research

One of the main lines of future work would be to perform a detailed numerical analysis of $\mathrm{Tr}\,\hat{\rho}_M^2$ and the von Neumann entropy $S(\hat{\rho}_M)$ for the Hartle–Hawking state (either within the Regge, or some other QG model). The latter quantity, called the *entropy of entanglement*, represents the measure of the entanglement in *pure* and *bipartite* states [57], in our case between gravity and matter in the Hartle–Hawking state. The precise numerical deviation of the $\mathrm{Tr}\,\hat{\rho}_M^2$ from its maximal value 1 could indicate in which cases this new entanglement has relevant physical consequences. This way, it would be possible to determine the boundaries of validity of the assumption of the product gravity-matter states of the form $|G\rangle|M\rangle$, which has been up to now used in numerous studies (analogously to the case of determining the regimes in which two coherent states become effectively orthogonal). In connection to this, one could analyse in more detail quantitatively to what extent the gauge-protected gravity-matter entanglement constrains the existence of macroscopic superpositions, and its effect to the quantum-to-classical transition (see the related work [3, 4, 9, 58–60]).

Further, studying the structure of the gauge-imposed entanglement for a tripartite system of gravity-matter-EM fields might bring qualitatively new effects. Unlike the case of pure bipartite states, where any two entangled states could be obtained from each other by local operations and classical communication (LOCC), thus forming a single class of entangled states and providing a unique measure of entanglement, the multipartite entanglement has a more complex structure. Indeed, in the tripartite case, in addition to the trivial classes of purely bipartite entanglement, say, $|a\rangle(|b_1c_1\rangle + |b_2c_2\rangle)$, genuine tripartite entanglement consists of a number of inequivalent classes of entangled states: in the simplest case of three qubits we have two classes of tripartite entanglement, represented by the states $|GHZ\rangle = (|0\,0\,0\rangle + |1\,1\,1\rangle)/\sqrt{2}$ and $|W\rangle = (|0\,0\,1\rangle + |0\,1\,0\rangle + |100\rangle)/\sqrt{3}$, which cannot be obtained from each other by the means of LOCC, but as soon as neither of the subsystems is a qubit, there exist infinitely many inequivalent classes [61].

It would also be interesting to see how other QG candidates incorporate the general gravity constraints regarding the entanglement with matter, in particular the string theory. Namely, perturbative string theory is formulated by manifestly breaking the gauge symmetry (a consequence of perturbative expansion of the gravitational field). The existence of the gravity-matter entanglement in, say Hartle–Hawking state, would then present a strong argument that the gauge symmetry can be restored in a tentative nonperturbative formulation of string theory. In connection to this, one could analyse the entanglement between different spacetime regions induced by the gauge-protected gravity-matter entanglement, and compare it to that present in theories based on the AdS/CFT correspondence and the holographic principle [7, 8]. Namely, entanglement is a property of a quantum state *with respect* to a particular factorisation of a composite system into its factor sub-systems. To illustrate this, consider a particle in a two-dimensional plane. Given orthogonal axes x and y of a 2D plane, the Hilbert space of the system is given by $\mathcal{H} = \mathcal{H}_x \otimes \mathcal{H}_y$, and the equal spatial superposition (for simplicity, we omit the overall normalisation constant) $|\varphi\rangle \sim (|a\rangle_x + |b\rangle_x)|0\rangle_y$, with $a, b \in \mathbb{R}$, is clearly separable, with respect to the given factorisation of $\mathcal{H}$. Nevertheless, with respect to *any other* factorisation of $\mathcal{H}$, defined by any other axes X and Y inducing the Hilbert-space factorisation $\mathcal{H} = \mathcal{H}_X \otimes \mathcal{H}_Y$, the system is entangled. As an example, for axes X and Y obtained by rotating x and y by $-\pi/4$, the same state of the system is maximally entangled, $|\varphi\rangle \sim (|a/\sqrt{2}\rangle_X |a/\sqrt{2}\rangle_Y + |b/\sqrt{2}\rangle_X |b/\sqrt{2}\rangle_Y)$ (for the entanglement in the second quantisation formalism, and its dependence on the choice of fundamental modes, see for example [62]). Following the above example, one might expect that the existence of the entanglement between gravity and matter would induce the entanglement between two generic spacetime regions (each containing a portion of both gravitational and matter degrees of freedom). Possible relationship between this, gauge-protected entanglement, and that present as a consequence of assumptions that do not explicitly rely on the existence of local Poincaré symmetry (holography and the AdS/CFT correspondence) would indicate interesting fundamental connections that could help breaching the long-standing gap between quantum mechanics and general relativity.

Finally, detecting gravity-matter entanglement in the experiment might not be that far from the reach of the current or the near-future technology, see [63] for a recent proposal of testing gravitational decoherence. Proposing, and possibly performing, experiments to distinguish different contributions of the gravitational interaction to the decoherence of matter, in particular the generic one based on the gauge symmetry constraints, presents a relevant direction of further research.

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Henneaux–Teitelboim Gauge Symmetry and Its Applications to Higher Gauge Theories

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Abstract: When discussing the gauge symmetries of any theory, the Henneaux–Teitelboim transformations are often underappreciated or even completely ignored, due to their on-shell triviality. Nevertheless, these gauge transformations play an important role in understanding the structure of the full gauge symmetry group of any theory, especially regarding the subgroup of diffeomorphisms. We give a review of the Henneaux–Teitelboim transformations and the resulting gauge group in the general case and then discuss its role in the applications to the class of topological theories called *nBF* models, relevant for the constructions of higher gauge theories and quantum gravity.

Keywords: gauge symmetry; trivial gauge transformations; *nBF* theory; Chern–Simons theory; diffeomorphism symmetry

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1. Introduction

In modern theoretical physics, gauge symmetries play a very prominent role. The two most-fundamental theories we have, which describe almost all observed phenomena in nature—namely Einstein's theory of general relativity and the Standard Model of elementary particle physics—are gauge theories. From Maxwell's electrodynamics to various approaches to quantum gravity, gauge theories play a central role, and gauge symmetry represents one of their most-important aspects. In light of this, there is one class of gauge transformations that is often slightly neglected in the literature, due to their specific nature and properties.

In order to introduce this particular gauge symmetry in the most-elementary way possible, let us look at the following simple example. Every action $S[\phi_1, \phi_2]$, which depends on the fields $\phi_1(x)$ and $\phi_2(x)$, is invariant under the following gauge transformation:

$$\delta_0\phi_1(x) = \epsilon(x)\frac{\delta S}{\delta\phi_2(x)}\,, \qquad \delta_0\phi_2(x) = -\epsilon(x)\frac{\delta S}{\delta\phi_1(x)}\,, \tag{1}$$

as one can see by calculating the variation of the action:

$$\delta S[\phi_1, \phi_2] = \frac{\delta S}{\delta\phi_1}\delta_0\phi_1 + \frac{\delta S}{\delta\phi_2}\delta_0\phi_2 = 0\,. \tag{2}$$

This gauge symmetry exists for every action that is a functional of at least two fields, irrespective of any other gauge symmetry that the action may or may not have. In the literature, this symmetry is often called *trivial* gauge symmetry, since the form variations of the fields are identically zero on-shell. This is in contrast to all other gauge symmetries, which perform some nontrivial change of the fields on-shell.

It should be noted that, being trivial on-shell, the above transformations cannot play a role in obtaining any predictions about observables in a given theory, due to the intrinsic on-shell nature of the physical observables. For example, in practical situations of scattering experiments and measurements of cross-sections, this trivial symmetry is irrelevant. Nevertheless, when constructing a new theory, in general, the off-shell properties of the theory are important. As a typical example, path integral quantization prescription depends not only on the classical equations of motion, but on the whole action of the theory. In this sense, while these trivial transformations are not relevant for making predictions, they do have methodological relevance and value in theory construction, despite their on-shell triviality.

For example, these transformations in fact represent a very important part of the gauge symmetry for any theory and play a crucial role in various contexts, such as in the Batalin–Vilkovisky formalism (see [1] for a review and also the original papers [2–6]), or when discussing the diffeomorphism symmetry of the BF-like class of theories [7–11]. Furthermore, in general, a commutator of two ordinary gauge transformations will remain an ordinary gauge transformation only up to the above trivial transformations, meaning that the latter are important for the algebraic closure of all gauge transformations into a group.

To the best of our knowledge, the most-complete treatment and discussion of the above gauge transformations can be found in the book [12] by Marc Henneaux and Claudio Teitelboim. Therefore, in this paper, we opted to call them Henneaux–Teitelboim (HT) transformations. This naming can also be justified with the paper [7] by Gary Horowitz (published two years before the book [12]), where the author attributes these transformations to Henneaux and Teitelboim in a footnote and thanks them "for explaining this to me".

Regarding terminology, we should also note that we use the terms "gauge symmetry" and "gauge transformations" with a certain level of charity. Namely, one could argue that there are two distinct types of local symmetries—those that are obtained by a localization procedure from a corresponding global symmetry group (the procedure of "gauging" a global symmetry) and those that are intrinsically local, not obtained by any such localization procedure. It is not known whether HT symmetry belongs to the former or the latter class, since a global symmetry whose localization would give rise to HT transformations has not yet been shown to exist. Either way, in the literature, there is no established terminology that distinguishes the two classes of symmetries, and most often, both are called "gauge symmetries". Therefore, in what follows, for a lack of better terminology, we will adhere to this practice and describe HT transformations as a gauge symmetry.

In some of the modern approaches to the problem of quantum gravity based on the spinfoam formalism of loop quantum gravity [13,14], as well as in other applications of the so-called higher gauge theory (see [15] for a review and [16] for an application to quantum gravity), the description of gauge symmetry is being extended from the notion of a Lie group to different algebraic structures, called 2-groups, 3-groups, and in general, n-groups [17–27]. In this context, it is important to revisit and study the specific class of HT gauge symmetries, since they provide a nontrivial insight into the properties of these more general algebraic structures, as well as the physics behind the symmetries they describe.

The purpose of this paper is to provide a review of HT transformations in general and then discuss their properties and applications in two concrete models—the Chern–Simons theory and the $3BF$ theory. The Chern–Simons case is simple enough to serve as an illustrative toy example, while the $3BF$ theory represents a basis for the construction of a realistic theory of quantum gravity with matter within the context of the spinfoam formalism (see also [16,28–32]), discussing that its HT symmetry represents an important stepping stone towards the goal of a more realistic theory. The main result of this work represents a clarification of the structure of the gauge symmetry of a pure topological $3BF$ action, as well as the corresponding symmetry for the constrained $2BF$ action, which is classically equivalent to Einstein's general relativity. We also discuss in detail the relationship between diffeomorphism symmetry and the HT symmetry for the Chern–Simons and $3BF$ theories and offer some conceptual suggestions regarding the notion of gauge symmetry as it is being used in the literature.

The layout of the paper is as follows. In Section 2, we give a review of the general theory of HT transformations and their main properties. Section 3 is devoted to the example of HT symmetry in Chern–Simons theory, which is convenient due to its simplicity. In Section 4, we discuss the main case of HT symmetry in the $3BF$ and $2BF$ theories, which are important for applications in quantum gravity models. Finally, Section 5 contains an overview of the results, future research directions, and some concluding remarks.

The notation and conventions in the paper are as follows. When important, we assume the $(-,+,+,+)$ signature of the spacetime metric. The Greek indices from the middle of the alphabet, $\lambda, \mu, \nu, \ldots$, represent spacetime indices and take values $0, 1, \ldots, D-1$, where D is the dimension of the spacetime manifold $\mathcal{M}_D$ under consideration. The Greek indices from the beginning of the alphabet, $\alpha, \beta, \gamma, \ldots$, represent group indices, as well as Latin indices $a, b, c, \ldots$ and uppercase Latin indices $A, B, C, \ldots$ and $I, J, K, \ldots$. All these indices will be assigned to various Lie groups under consideration. Lowercase Latin indices from the middle of the alphabet, $i, j, k, \ldots$, are generic and will be used to count all fields in a given theory or for some other purpose depending on the context. Throughout the paper, we denote the space of algebra-valued differential p-forms as

$$\mathcal{A}^p(\mathcal{M}, \mathfrak{a}) \equiv \Lambda^p(\mathcal{M}) \otimes \mathfrak{a},$$

where $\Lambda^p(\mathcal{M})$ is the ordinary space of differential p-forms over the manifold $\mathcal{M}$, while $\mathfrak{a}$ is some Lie algebra.

2. Review of HT Symmetry

We begin by studying some basic general properties of HT transformations. After the definition, we demonstrate that the group of HT transformations represents a normal subgroup of the *total* gauge group of a given theory, and we discuss the triviality of HT transformations and that they exhaust all possible trivial transformations. Finally, before moving on to concrete theories, we study the subtleties of the dependence of HT symmetry on the choice of the action.

2.1. Definition of HT Transformations

Given an action $S[\phi^i]$ as a functional of fields $\phi^i(x)$ ($i \in \{1, \ldots, N\}$ where we assume $N \geqslant 2$), the infinitesimal HT transformation is defined as

$$\phi^i(x) \to \phi'^i(x) = \phi^i(x) + \delta_0\phi^i(x)\,, \tag{3}$$

where the form variations of the fields are defined as

$$\delta_0\phi^i(x) = \epsilon^{ij}(x)\frac{\delta S}{\delta\phi^j(x)}\,. \tag{4}$$

The variation of the action under HT transformations then gives

$$\delta S = \frac{\delta S}{\delta\phi^i}\delta_0\phi^i = \frac{\delta S}{\delta\phi^i}\frac{\delta S}{\delta\phi^j}\epsilon^{ij}\,. \tag{5}$$

If the HT parameters are chosen to be antisymmetric,

$$\epsilon^{ij}(x) = -\epsilon^{ji}(x)\,, \tag{6}$$

the variation of the action (5) is identically zero, and HT transformations (4) represent a gauge symmetry of the theory.

The most-striking thing in the above definition is the fact that we did not specify the action in any way. Aside from the assumption $N \geqslant 2$, which excludes only actions describing a single real scalar field, every action is invariant with respect to the HT transformations. In other words, *HT transformations are a gauge symmetry of essentially every theory*.

The second striking property of the definition is that the form variations of fields become zero on-shell, according to (4). In this sense, the HT symmetry is sometimes called *trivial symmetry*, in contrast to ordinary gauge symmetries that a theory may have, which transform the fields in a nontrivial way on-shell. Triviality is also the reason why HT gauge symmetry does not feature in any way in the Hamiltonian analysis of a theory, so only the presence of ordinary gauge symmetries can be deduced from the Hamiltonian formalism.

2.2. HT Symmetry Group and Its Properties

There are two general properties that can be formulated for HT transformations. The first is that HT transformations form a normal subgroup within the full group of gauge symmetries, while the second is that HT transformations exhaust the set of all possible trivial transformations. The consequence of these properties is that one can always write the total symmetry group of any theory as

$$\mathcal{G}_{\text{total}} = \mathcal{G}_{\text{nontrivial}} \ltimes \mathcal{G}_{HT}\,, \tag{7}$$

where $\mathcal{G}_{\text{nontrivial}}$ is the symmetry group of ordinary gauge transformations (if there are any), $\mathcal{G}_{HT}$ is the HT symmetry group, and the symbol $\ltimes$ stands for a semidirect product. One can also reformulate (7) as

$$\mathcal{G}_{\text{nontrivial}} = \mathcal{G}_{\text{total}}/\mathcal{G}_{HT}\,, \tag{8}$$

so that the group of ordinary gauge symmetries is represented as a quotient group.

The easiest way to demonstrate (7) is to prove that the Lie algebra corresponding to $\mathcal{G}_{HT}$ represents an ideal within the Lie algebra corresponding to $\mathcal{G}_{\text{total}}$. To that end, pick an arbitrary form variation of fields that represents a symmetry of the action and write it in the form

$$\hat{\delta}_0\phi^i(x) = F^i(x)\,, \qquad \text{such that} \qquad \hat{\delta}S = \frac{\delta S}{\delta\phi^i}F^i \equiv 0\,. \tag{9}$$

Then, using (4), we can take concatenated variations of this form variation and the HT form variation as

$$\delta_0\hat{\delta}_0\phi^i = \frac{\delta F^i}{\delta\phi^j}\frac{\delta S}{\delta\phi^k}\epsilon^{jk}\,,$$

and

$$\hat{\delta}_0\delta_o\phi^i = \frac{\delta}{\delta\phi^k}\left(\epsilon^{ij}\frac{\delta S}{\delta\phi^j}\right)F^k = \frac{\delta\epsilon^{ij}}{\delta\phi^k}\frac{\delta S}{\delta\phi^j}F^k + \epsilon^{ij}\frac{\delta}{\delta\phi^j}\left(\frac{\delta S}{\delta\phi^k}F^k\right) - \epsilon^{ij}\frac{\delta S}{\delta\phi^k}\frac{\delta F^k}{\delta\phi^j}\,.$$

The term in the second parentheses is zero by (9), so the commutator of two-form variations becomes

$$[\delta_0\,,\hat{\delta}_0]\phi^i = \left(\epsilon^{jk}\frac{\delta F^i}{\delta\phi^j} - \epsilon^{ji}\frac{\delta F^k}{\delta\phi^j} - \frac{\delta\epsilon^{ik}}{\delta\phi^j}F^j\right)\frac{\delta S}{\delta\phi^k}\,, \tag{10}$$

which is again an HT transformation, since the expression in the parentheses is antisymmetric with respect to indices i, k. Therefore, the commutator is always an element of HT algebra, which means that HT algebra itself is an ideal of the total symmetry algebra. At the Lie group level, this translates into (7).

The second general property is the statement that there are no other trivial transformations beside the HT transformations. Assuming that some transformation described by the form variation $\bar{\delta}_0\phi^i$ is a gauge symmetry of the action that vanishes on-shell, i.e., that it satisfies

$$\frac{\delta S}{\delta\phi^i}\bar{\delta}_0\phi^i = 0\,, \qquad \text{and} \qquad \bar{\delta}_0\phi^i \approx 0\,,$$

then one can prove that this transformation is an HT transformation, i.e., there exists a choice of antisymmetric HT parameters ϵ^{ij} such that the form variation $\bar{\delta}_0\phi^i$ is of type (4):

$$\bar{\delta}_0\phi^i = \epsilon^{ij}\frac{\delta S}{\delta\phi^j}\,. \tag{11}$$

Provided certain suitable regularity conditions for the action S, this statement can be rigorously formulated as a theorem. However, we omitted the proof since it is technical and off topic for the purposes of this paper. The interested reader can find the details of both the theorem and the proof in [12], Appendix 10.A.2.

To sum up, the first property (10) tells us that one can always factorize the total gauge symmetry group into the form (7), while the second property (11) guarantees that the quotient group (8) contains only nontrivial gauge transformations. This factorization of the total symmetry group is a key result that lays the groundwork for any subsequent analysis of HT transformations in particular and gauge symmetry in general.

2.3. Dependence of HT Symmetry on the Action

The final property of HT transformations that needs to be discussed is their dependence on the choice of the action. Suppose we are given some action $S_{\text{old}}[\phi^i]$, where $i \in \{1, \dots, N\}$, which has the corresponding HT transformation described as in (4):

$$\delta_0^{\text{old}} \phi^i = \epsilon^{ij} \frac{\delta S_{\text{old}}}{\delta \phi^j} \,. \tag{12}$$

Now, suppose that we modify that action into another one, $S_{\text{new}}[\phi^i, \chi^k]$, where $k \in \{N + 1, \dots, N + M\}$, by adding an extra term to the old action:

$$S_{\text{new}}[\phi^i, \chi^k] = S_{\text{old}}[\phi^i] + S_{\text{extra}}[\phi^i, \chi^k] \,. \tag{13}$$

Here, χ^j are additional fields that may be introduced into the new action. The HT transformation corresponding to the new action can be written in the block-matrix form, made of blocks of sizes N and M, as follows:

$$\begin{pmatrix} \delta_0^{\text{new}} \phi^i \\ \delta_0^{\text{new}} \chi^k \end{pmatrix} = \left(\begin{array}{c|c} \epsilon^{ij} & \zeta^{il} \\ \hline \theta^{kj} & \psi^{kl} \end{array} \right) \begin{pmatrix} \dfrac{\delta S_{\text{new}}}{\delta \phi^j} \\ \dfrac{\delta S_{\text{new}}}{\delta \chi^l} \end{pmatrix} , \qquad \begin{array}{l} i, j \in \{1, \dots, N\} \,, \\ k, l \in \{N + 1, \dots, N + M\} \,. \end{array} \tag{14}$$

Here, $\epsilon = -\epsilon^T$ is an antisymmetric $N \times N$ block of parameters ϵ^{ij}, ζ is a rectangular $N \times M$ block of parameters ζ^{il}, θ is a rectangular $M \times N$ block such that $\theta = -\zeta^T$, and finally, $\psi = -\psi^T$ is an antisymmetric $M \times M$ block of parameters ψ^{kl}. Overall, the total parameter matrix is antisymmetric, as required by (6).

The question one can now study is what is the relation between the two HT gauge symmetry groups $\mathcal{G}_{HT}^{\text{old}}$ and $\mathcal{G}_{HT}^{\text{new}}$ that correspond to the two actions. In practice, this question is most often relevant in cases when one introduces the piece S_{extra} as a gauge-fixing term, whose purpose is to break the ordinary gauge symmetry down to its subgroup:

$$G_{\text{nontrivial}}^{\text{new}} \subset G_{\text{nontrivial}}^{\text{old}} \,.$$

Naively, one might expect a similar relationship between the HT symmetry groups, $\mathcal{G}_{HT}^{\text{new}} \subset \mathcal{G}_{HT}^{\text{old}}$. However, looking at (12) and (14), this is obviously wrong. Namely, if $M \geqslant 1$, the HT symmetry of the new action is *larger* than the HT symmetry of the old action. Counting the number of independent parameters of both, one easily sees that

$$\dim(\mathcal{G}_{HT}^{\text{old}}) = \frac{N(N-1)}{2} \,, \qquad \dim(\mathcal{G}_{HT}^{\text{new}}) = \frac{(N+M)(N+M-1)}{2} \,,$$

so that the only possible relationship would be the opposite, $\mathcal{G}_{HT}^{\text{old}} \subset \mathcal{G}_{HT}^{\text{new}}$. However, in fact, this can also be shown to be wrong. Namely, one can choose the extra parameters ζ, θ and ψ to be zero in (14), reducing it to the form that is formally similar to (12):

$$\delta_0^{\text{new}} \phi^i = \epsilon^{ij} \frac{\delta S_{\text{new}}}{\delta \phi^j} \,.$$

However, taking into account the relationship (13) between the two actions, the HT transformation takes the form

$$\delta_0^{\text{new}} \phi^i = \epsilon^{ij} \frac{\delta S_{\text{old}}}{\delta \phi^j} + \epsilon^{ij} \frac{\delta S_{\text{extra}}}{\delta \phi^j} \,,$$

which is explicitly different from (12), due to the presence of the term S_{extra} in the action. Therefore, the gauge group $\mathcal{G}_{HT}^{\text{old}}$ is not a subgroup of $\mathcal{G}_{HT}^{\text{new}}$ either.

The overall conclusion is that introducing additional terms to the action changes the total gauge symmetry in a nontrivial way. On the one hand, the ordinary gauge symmetry group typically becomes *smaller* due to explicit symmetry breaking by the extra term. On the other hand, the HT gauge symmetry group may become *larger* if the extra term contains additional fields, but either way becomes *different*, as a consequence of the very presence of the extra term. Given this, one can conclude that the *total* symmetry groups for the two actions will always be mutually different:

$$\mathcal{G}_{\text{total}}^{\text{new}} = \mathcal{G}_{\text{nontrivial}}^{\text{new}} \ltimes \mathcal{G}_{HT}^{\text{new}} \qquad \neq \qquad \mathcal{G}_{\text{total}}^{\text{old}} = \mathcal{G}_{\text{nontrivial}}^{\text{old}} \ltimes \mathcal{G}_{HT}^{\text{old}} \,.$$

Specifically, one cannot claim that the group $\mathcal{G}_{\text{total}}^{\text{old}}$ is being broken down into $\mathcal{G}_{\text{total}}^{\text{new}}$ as its subgroup; such a relationship may hold exclusively for the quotient groups of ordinary gauge transformations.

In the next two sections, we will turn to explicit examples of all general properties and features of the HT symmetry that have been discussed above. Moreover, we will also discuss some additional particular properties, such as the fact that some nontrivial gauge subgroups of $\mathcal{G}_{\text{total}}$ are not simultaneously subgroups of $\mathcal{G}_{\text{nontrivial}}$, which is a consequence of the semidirect product in (7). One such example will be the diffeomorphism symmetry in the Chern–Simons and $3BF$ actions.

Let us conclude this section with one conceptual comment. Throughout the literature, the typical practice is to always take the quotient between the total and HT symmetry groups as in (8), in order to isolate the nontrivial gauge transformations, and call the latter simply as the "gauge symmetry" of a theory. This approach is in fact advocated for in [12]. However, we believe that this practice can be misleading and that one should instead describe the group $\mathcal{G}_{\text{total}}$ as "the gauge symmetry" of a theory, explicitly including the HT subgroup as a legitimate gauge symmetry group. Namely, despite the fact that it is often called "trivial", the consequences of its presence in $\mathcal{G}_{\text{total}}$ are far from trivial. Granted, it may often be enough to discuss the gauge symmetry on-shell, and then, one can indeed calculate all symmetry transformations only "up to equations of motion", with no mention of the HT subgroup. However, whenever one needs to discuss the gauge transformations off-shell, the HT subgroup simply cannot be ignored anymore. Typical situations include the Batalin–Vilkovisky formalism [1], various generalizations of gauge symmetry in the context of higher gauge theories and quantum gravity [33], and even the traditional contexts such as the Coleman–Mandula theorem [34]. The situations in which HT transformations play a significant role may be rare, but nevertheless, they tend to be important. Thus, in our opinion, it would be prudent to always be aware that, for any given theory, its total gauge symmetry group is in fact bigger, and more feature-rich, than just the group of ordinary gauge transformations that are typically discussed in the literature.

3. HT Symmetry in Chern–Simons Theory

As an illustrative example of the general properties of HT symmetry from the previous section, let us discuss the HT transformations for the simple case of the Chern–Simons theory. The Chern–Simons theory represents an excellent toy example since it is well known in the literature and most readers should be familiar with it.

Given any Lie group G, its corresponding Lie algebra $\mathfrak{g}$, and a three-dimensional manifold $\mathcal{M}_3$, the Chern–Simons theory can be defined as a topological field theory over a trivial principal bundle $G \to \mathcal{M}_3$, given by the action:

$$S_{CS} = \int_{\mathcal{M}_3} \langle A \wedge \mathrm{d}A \rangle_{\mathfrak{g}} + \frac{1}{3} \langle A \wedge [A \wedge A] \rangle_{\mathfrak{g}} \,. \tag{15}$$

Here, $A \in \mathcal{A}^1(\mathcal{M}_3, \mathfrak{g})$ is a $\mathfrak{g}$-valued connection one-form over a manifold $\mathcal{M}_3$, and $\langle \_, \_ \rangle_{\mathfrak{g}}$ is a G-invariant symmetric nondegenerate bilinear form on $\mathfrak{g}$. One often rewrites the Chern–Simons action within the framework of the enveloping algebra of $\mathfrak{g}$, introducing the notion of a *trace* as

$$\mathrm{Tr}(XY) \equiv \langle X , Y \rangle_{\mathfrak{g}} \,,$$

for every $X, Y \in \mathfrak{g}$. Then, the Chern–Simons action can be rewritten as

$$S_{CS} = \int_{\mathcal{M}_3} \mathrm{Tr}\left(A \wedge \mathrm{d}A + \frac{2}{3} A \wedge A \wedge A \right) , \tag{16}$$

where, for the second term, one employs the identity $\mathrm{Tr}(X[Y, Z]) = \mathrm{Tr}(XYZ) - \mathrm{Tr}(XZY)$ for every $X, Y, Z \in \mathfrak{g}$.

The gauge symmetry of the Chern–Simons action consists of G-gauge transformations, determined with the parameters $\epsilon_{\mathfrak{g}}{}^I(x)$. Using the basis of generators T_I to expand the connection A into components as

$$A = A^I{}_\mu(x)\, \mathrm{d}x^\mu \otimes T_I \,,$$

the form variation of the connection components $A^I{}_\mu$ corresponding to gauge transformations can then be written as

$$\delta_0 A^I{}_\mu = \partial_\mu \epsilon_{\mathfrak{g}}{}^I - f_{JK}{}^I \epsilon_{\mathfrak{g}}{}^J A^K{}_\mu \,, \tag{17}$$

where $f_{JK}{}^I$ are the structure constants corresponding to the generators T_I. Therefore, the gauge symmetry of the Chern–Simons theory is usually quoted as the initially chosen Lie group G:

$$\mathcal{G}_{CS} = G \,. \tag{18}$$

However, as we have seen in the previous section, this is not the complete set of gauge transformations, and the *total* gauge group should in fact be

$$\mathcal{G}_{\text{total}} = \mathcal{G}_{CS} \ltimes \mathcal{G}_{HT} \,. \tag{19}$$

Let us define the HT transformations for the Chern–Simons action (15). If we denote the dimension of the Lie algebra $\mathfrak{g}$ as $\dim(\mathfrak{g}) = p$, the number of independent field components $A^I{}_\mu$ is $N = 3p$. The HT transformation is then defined with the HT parameters $\epsilon^{IJ}{}_{\mu\nu}(x)$ as

$$\delta_0 A^I{}_\mu = \epsilon^{IJ}{}_{\mu\nu} \frac{\delta S}{\delta A^J{}_\nu} \,. \tag{20}$$

The requirement that the variation of the action vanishes:

$$\delta S = \frac{\delta S}{\delta A^I{}_\mu} \frac{\delta S}{\delta A^J{}_\nu} \epsilon^{IJ}{}_{\mu\nu} = 0 \,,$$

enforces the antisymmetry restriction on the HT parameters:

$$\epsilon^{IJ}{}_{\mu\nu} = -\epsilon^{JI}{}_{\nu\mu} \,.$$

Note that this equation can be satisfied in two different ways—the parameters can be either antisymmetric with respect to group indices IJ and symmetric with respect to spacetime indices $\mu\nu$, or vice versa. We, therefore, have two possible choices for their symmetry properties. The first possibility is defined as

$$\epsilon^{IJ}{}_{\mu\nu} = \epsilon^{IJ}{}_{\nu\mu} = -\epsilon^{JI}{}_{\mu\nu} = -\epsilon^{JI}{}_{\nu\mu} \,, \tag{21}$$

while the second possibility is defined as

$$\epsilon^{IJ}{}_{\mu\nu} = \epsilon^{JI}{}_{\mu\nu} = -\epsilon^{IJ}{}_{\nu\mu} = -\epsilon^{JI}{}_{\nu\mu} \,. \tag{22}$$

Varying the action, one obtains an explicit form of the HT transformation:

$$\delta_0 A^I{}_\mu = \epsilon^{IJ}{}_{\mu\nu}\varepsilon^{\nu\rho\sigma}\Big(\partial_\rho A_{J\sigma} - \partial_\sigma A_{J\rho} + f_{KLJ}\, A^K{}_\rho A^L{}_\sigma\Big) \,. \tag{23}$$

In order to demonstrate that HT transformations have highly nontrivial implications, despite being trivial on-shell, it is instructive to discuss diffeomorphisms. Namely, looking at the action (15), one expects that the theory has diffeomorphism symmetry, since it is formulated in a manifestly covariant way using differential forms. However, one can check that diffeomorphisms are not a subgroup of the ordinary gauge symmetry group $\mathcal{G}_{CS}$ given by (18), but nevertheless can be obtained as a subgroup of the total gauge group (19). In other words, one can demonstrate that

$$Diff(\mathcal{M}_3) \not\subset \mathcal{G}_{CS} \,, \qquad \text{but} \qquad Diff(\mathcal{M}_3) \subset \mathcal{G}_{\text{total}} = \mathcal{G}_{CS} \ltimes \mathcal{G}_{HT} \,.$$

Let us examine this in detail. The diffeomorphism transformation

$$x^\mu \to x'^\mu = x^\mu + \xi^\mu(x) \,, \tag{24}$$

determined by the parameter $\xi^\mu(x)$ represents a subgroup $Diff(\mathcal{M})$ of the full gauge symmetry of some given action, if for every field $\phi(x)$ in the theory and every choice of diffeomorphism parameters $\xi^\mu(x)$, there exists a choice of the gauge parameters $\epsilon^{\text{gauge}}(x)$ and the HT parameters $\epsilon^{\text{HT}}(x)$, such that:

$$\delta_0{}^{\text{diff}}\,\phi = \delta_0{}^{\text{gauge}}\phi + \delta_0{}^{\text{HT}}\phi \,. \tag{25}$$

In other words, if a theory has diffeomorphism symmetry, the diffeomorphism form variations of all the fields in the theory should be expressible in terms of their ordinary gauge and HT form variations.

In the case of Chern–Simons theory, this can be demonstrated explicitly. If one chooses the gauge parameters $\epsilon_{\mathfrak{g}}{}^I$ and the HT parameters $\epsilon^{IJ}{}_{\mu\nu}$ as

$$\epsilon_{\mathfrak{g}}{}^I = -\xi^\lambda A^I{}_\lambda \,, \qquad \epsilon^{IJ}{}_{\mu\nu} = -\frac{1}{2}\xi^\lambda \varepsilon_{\lambda\mu\nu} g^{IJ} \,, \tag{26}$$

where g^{IJ} is the inverse of $g_{IJ} \equiv \langle T_I \,, T_J \rangle_{\mathfrak{g}}$, one can apply Equations (25) using (17) and (23) to reproduce precisely the well-known diffeomorphism form variation of the connection $A^I{}_\mu$:

$$\delta_0{}^{\text{diff}} A^I{}_\mu = -A^I{}_\lambda \partial_\mu \xi^\lambda - \xi^\lambda \partial_\lambda A^I{}_\mu \,. \tag{27}$$

Therefore, as expected, despite the fact that $Diff(\mathcal{M}_3) \not\subset \mathcal{G}_{CS}$, one obtains that $Diff(\mathcal{M}_3) \subset \mathcal{G}_{\text{total}} = \mathcal{G}_{CS} \ltimes G_{HT}$. Note that the choice of HT parameters in (26) is nontrivial, which emphasizes the role of HT transformations and the fact that the full group of gauge symmetries is $\mathcal{G}_{\text{total}}$ rather than $\mathcal{G}_{CS}$. As we shall see in the next section, this property is not specific only to the Chern–Simons theory.

4. HT Symmetry in 3*BF* Theory

After discussing the Chern–Simons theory as a toy example, we move to the more important case of the 3*BF* theory. This theory is relevant for building models of quantum gravity; see [8,20,21,33,35]. Therefore, it is important to study its gauge symmetry and, in particular, the role of HT transformations.

4.1. Review of the 3*BF Theory*

Analogous to the fact that Chern–Simons theory is a topological theory based on a Lie group and a 3-dimensional manifold, the $3BF$ theory is also a topological theory based on a notion of a three-group and a 4-dimensional manifold. The notion of a three-group represents a categorical generalization of the notion of a group, in the context of higher gauge theory (HGT); see [15] for a review and motivation. For the purpose of defining the $3BF$ theory, we are interested in particular in a strict Lie three-group, which is known to be isomorphic to a so-called Lie two-crossed module; see [17–19] for details.

A Lie two-crossed module, denoted as $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \triangleright\,, \{\_\,,\_\}_{\mathrm{pf}})$, is an algebraic structure specified by three Lie groups G, H, and L, together with the homomorphisms $\delta : L \to H$ and $\partial : H \to G$, an action $\triangleright$ of the group G on all three groups, and a G-equivariant map, called the Peiffer lifting:

$$\{\_\,,\_\}_{\mathrm{pf}} : H \times H \to L\,.$$

In order for this structure to form a two-crossed module, the structure constants of algebras $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$ (the Lie algebras corresponding to the Lie groups G, H, and L, respectively), as well as the maps ∂ and δ, the action $\triangleright$, and the Peiffer lifting, must satisfy certain axioms; see [20] for details.

Given a two-crossed module and a four-dimensional compact and orientable spacetime manifold $\mathcal{M}_4$, one can introduce the notion of a trivial principal three-bundle, in analogy with the notion of a trivial principal bundle constructed from an ordinary Lie group and a manifold; see [15]. Then, one can introduce the notion of a three-connection, an ordered triple (α, β, γ), where α, β, and γ are algebra-valued differential forms, $\alpha \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{g})$, $\beta \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{h})$, and $\gamma \in \mathcal{A}^3(\mathcal{M}_4, \mathfrak{l})$; see [17–19]. The corresponding fake hree-curvature $(\mathcal{F}, \mathcal{G}, \mathcal{H})$ is defined as:

$$\begin{gathered} \mathcal{F} = \mathrm{d}\alpha + \alpha \wedge \alpha - \partial\beta\,, \qquad \mathcal{G} = \mathrm{d}\beta + \alpha \wedge^{\triangleright} \beta - \delta\gamma\,, \\ \mathcal{H} = \mathrm{d}\gamma + \alpha \wedge^{\triangleright} \gamma + \{\beta \wedge \beta\}_{\mathrm{pf}}\,. \end{gathered} \tag{28}$$

Then, for a four-dimensional manifold $\mathcal{M}_4$, one can define the gauge-invariant topological $3BF$ action, based on the structure of a two-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \triangleright\,, \{\_\,,\_\}_{\mathrm{pf}})$, by the action

$$S_{3BF} = \int_{\mathcal{M}_4} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} + \langle C \wedge \mathcal{G} \rangle_{\mathfrak{h}} + \langle D \wedge \mathcal{H} \rangle_{\mathfrak{l}}\,, \tag{29}$$

where $B \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{g})$, $C \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{h})$, and $D \in \mathcal{A}^0(\mathcal{M}_4, \mathfrak{l})$ are Lagrange multipliers and $\mathcal{F} \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{g})$, $\mathcal{G} \in \mathcal{A}^3(\mathcal{M}_4, \mathfrak{h})$, and $\mathcal{H} \in \mathcal{A}^4(\mathcal{M}_4, \mathfrak{l})$ represent the fake three-curvature given by Equation (28). The forms $\langle\_\,,\_\rangle_{\mathfrak{g}}$, $\langle\_\,,\_\rangle_{\mathfrak{h}}$, and $\langle\_\,,\_\rangle_{\mathfrak{l}}$ are G-invariant symmetric nondegenerate bilinear forms on $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$, respectively. The action (29) is an example of the so-called higher gauge theory.

By choosing the three bases of generators $\tau_\alpha \in \mathfrak{g}$, $t_a \in \mathfrak{h}$, and $T_A \in \mathfrak{l}$ of the three respective Lie algebras, one can expand all fields in the theory into components as

$$\begin{aligned} B &= \frac{1}{2} B^\alpha{}_{\mu\nu}(x)\, \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \otimes \tau_\alpha\,, & \alpha &= \alpha^\alpha{}_\mu(x)\, \mathrm{d}x^\mu \otimes \tau_\alpha\,, \\ C &= C^a{}_\mu(x)\, \mathrm{d}x^\mu \otimes t_a\,, & \beta &= \frac{1}{2} \beta^a{}_{\mu\nu}(x)\, \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \otimes t_a\,, \\ D &= D^A(x) T_A\,, & \gamma &= \frac{1}{3!} \gamma^A{}_{\mu\nu\rho}(x)\, \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho \otimes T_A\,. \end{aligned}$$

One can also make use of the following notation for the components of all maps present in the theory, in the same three bases:

$$
\begin{array}{llll}
[\tau_\alpha\,,\tau_\beta] = f_{\alpha\beta}{}^{\gamma}\tau_\gamma\,, & g_{\alpha\beta} = \langle\tau_\alpha\,,\tau_\beta\rangle_{\mathfrak{g}}\,, & \tau_\alpha \triangleright \tau_\beta = \triangleright_{\alpha\beta}{}^{\gamma}\tau_\gamma\,, & \delta T_A = \delta_A{}^a t_a\,, \\
[t_a\,,t_b] = f_{ab}{}^{c}t_c\,, & g_{ab} = \langle t_a\,,t_b\rangle_{\mathfrak{h}}\,, & \tau_\alpha \triangleright t_a = \triangleright_{\alpha a}{}^{b}t_b\,, & \partial t_a = \partial_a{}^{\alpha}\tau_\alpha\,, \\
[T_A\,,T_B] = f_{AB}{}^{C}T_C\,, & g_{AB} = \langle T_A\,,T_B\rangle_{\mathfrak{l}}\,, & \tau_\alpha \triangleright T_A = \triangleright_{\alpha A}{}^{B}T_B\,, & \{t_a\,,t_b\}_{\rm pf} = X_{ab}{}^{A}T_A\,.
\end{array}
$$

The complete gauge symmetry of the $3BF$ action was studied in [8] using the techniques of Hamiltonian analysis. It consists of five types of gauge transformations, G-, H-, L-, M-, and N-gauge transformations, determined with the independent parameters $\epsilon_{\mathfrak{g}}{}^{\alpha}(x)$, $\epsilon_{\mathfrak{h}}{}^{a}{}_{\mu}(x)$, $\epsilon_{\mathfrak{l}}{}^{A}{}_{\mu\nu}(x)$, $\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu}(x)$, and $\epsilon_{\mathfrak{n}}{}^{a}(x)$, respectively. The form variations of the fields B, C, D, α, β, and γ, obtained in [8] are given as follows:

$$
\begin{array}{rcl}
\delta_0 B^{\alpha}{}_{\mu\nu} & = & f_{\beta\gamma}{}^{\alpha}\epsilon_{\mathfrak{g}}{}^{\beta}B^{\gamma}{}_{\mu\nu} + 2C_{a[\mu|}\epsilon_{\mathfrak{h}}{}^{b}{}_{|\nu]}\triangleright_{\beta b}{}^{a}g^{\alpha\beta} - D_A\triangleright_{\beta B}{}^{A}\epsilon_{\mathfrak{l}}{}^{B}{}_{\mu\nu}g^{\alpha\beta} - 2\nabla_{[\mu|}\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{|\nu]} \\
 & & +\beta_{b\mu\nu}\triangleright_{\beta a}{}^{b}\epsilon_{\mathfrak{n}}{}^{a}g^{\alpha\beta}\,, \\
\delta_0 C^{a}{}_{\mu} & = & \triangleright_{\alpha b}{}^{a}\epsilon_{\mathfrak{g}}{}^{\alpha}C^{b}{}_{\mu} + 2D_A X_{(ab)}{}^{A}\epsilon_{\mathfrak{h}}{}^{b}{}_{\mu} - \partial^{a}{}_{\alpha}\epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu} - \nabla_{\mu}\epsilon_{\mathfrak{n}}{}^{a}\,, \\
\delta_0 D^{A} & = & \triangleright_{\alpha B}{}^{A}\epsilon_{\mathfrak{g}}{}^{\alpha}D^{B} + \delta^{A}{}_{a}\epsilon_{\mathfrak{n}}{}^{a}\,, \\
\delta_0 \alpha^{\alpha}{}_{\mu} & = & -\partial_{\mu}\epsilon_{\mathfrak{g}}{}^{\alpha} - f_{\beta\gamma}{}^{\alpha}\alpha^{\beta}{}_{\mu}\epsilon_{\mathfrak{g}}{}^{\gamma} - \partial_{a}{}^{\alpha}\epsilon_{\mathfrak{h}}{}^{a}{}_{\mu}\,, \\
\delta_0 \beta^{a}{}_{\mu\nu} & = & \triangleright_{\alpha b}{}^{a}\epsilon_{\mathfrak{g}}{}^{\alpha}\beta^{b}{}_{\mu\nu} - 2\nabla_{[\mu|}\epsilon_{\mathfrak{h}}{}^{a}{}_{|\nu]} + \delta_{A}{}^{a}\epsilon_{\mathfrak{l}}{}^{A}{}_{\mu\nu}\,, \\
\delta_0 \gamma^{A}{}_{\mu\nu\rho} & = & \triangleright_{\alpha B}{}^{A}\epsilon_{\mathfrak{g}}{}^{\alpha}\gamma^{B}{}_{\mu\nu\rho} + 3!\beta^{a}{}_{[\mu\nu}\epsilon_{\mathfrak{h}}{}^{b}{}_{\rho]}X_{(ab)}{}^{A} + \nabla_{\mu}\epsilon_{\mathfrak{l}}{}^{A}{}_{\nu\rho} - \nabla_{\nu}\epsilon_{\mathfrak{l}}{}^{A}{}_{\mu\rho} + \nabla_{\rho}\epsilon_{\mathfrak{l}}{}^{A}{}_{\mu\nu}\,.
\end{array}
\quad (30)
$$

The gauge transformations (30) form a group $\mathcal{G}_{3BF}$:

$$
\mathcal{G}_{3BF} = \tilde{G} \ltimes (\tilde{H}_L \ltimes (\tilde{N} \times \tilde{M}))\,, \quad (31)
$$

where $\tilde{G}$ denotes the group of G-gauge transformations, the H-gauge transformations together with the L-gauge transformations form the group $\tilde{H}_L$, while $\tilde{M}$ and $\tilde{N}$ are the groups of M- and N-gauge transformations, respectively. All these groups are determined from the structure of the initial chosen two-crossed module that defines the theory; see [8] for details.

However, as we have seen in the general theory in Section 2 and in the example of the Chern–Simons theory in Section 3, the symmetry group $\mathcal{G}_{3BF}$ determined by the Hamiltonian analysis does not include HT transformations, and therefore, the *total* gauge group should in fact be

$$
\mathcal{G}_{\rm total} = \mathcal{G}_{3BF} \ltimes \mathcal{G}_{HT}\,. \quad (32)
$$

4.2. Explicit HT Transformations

Let us explicitly define the HT transformations for the $3BF$ action (29). If we denote the dimensions of the Lie algebras $\mathfrak{g}, \mathfrak{h}, \mathfrak{l}$ as

$$
\dim(\mathfrak{g}) = p\,, \qquad \dim(\mathfrak{h}) = q\,, \qquad \dim(\mathfrak{l}) = r\,,
$$

the number of independent field components in the theory can be counted according to the following table:

$B^{\alpha}{}_{\mu\nu}$	$C^{a}{}_{\mu}$	D^{A}	$\alpha^{\alpha}{}_{\mu}$	$\beta^{a}{}_{\mu\nu}$	$\gamma^{A}{}_{\mu\nu\rho}$
$6p$	$4q$	r	$4p$	$6q$	$4r$

The total number of independent field components is, therefore,

$$
N = 6p + 4q + r + 4p + 6q + 4r = 10p + 10q + 5r\,.
$$

Let ϕ^i denote all field components, where $i = 1, 2, \ldots, N$. We can write the fields schematically as a column-matrix with six blocks:

$$\phi^i = \begin{pmatrix} B^{\alpha}{}_{\mu\nu} \\ C^{a}{}_{\mu} \\ D^{A} \\ \alpha^{\alpha}{}_{\mu} \\ \beta^{a}{}_{\mu\nu} \\ \gamma^{A}{}_{\mu\nu\rho} \end{pmatrix} .$$

The HT transformation is then defined via the parameters $\epsilon^{ij}(x)$ as

$$\delta_0\phi^i = \epsilon^{ij}\,\frac{\delta S}{\delta\phi^j} .$$

The requirement that the variation of the action vanishes enforces the antisymmetry restriction on the parameters, $\epsilon^{ij} = -\epsilon^{ji}$, for all $i, j \in \{1, \ldots, N\}$. These transformations can be represented more explicitly as a tensorial 6×6 block-matrix equation, in the following form:

$$\begin{pmatrix} \delta_0 B^{\alpha}{}_{\mu\nu} \\ \delta_0 C^{a}{}_{\mu} \\ \delta_0 D^{A} \\ \delta_0 \alpha^{\alpha}{}_{\mu} \\ \delta_0 \beta^{a}{}_{\mu\nu} \\ \delta_0 \gamma^{A}{}_{\mu\nu\rho} \end{pmatrix} = \left(\begin{array}{c|c|c|c|c|c} \epsilon^{\alpha\beta}{}_{\mu\nu\sigma\lambda} & \epsilon^{\alpha b}{}_{\mu\nu\sigma} & \epsilon^{\alpha B}{}_{\mu\nu} & \epsilon^{\alpha\beta}{}_{\mu\nu\sigma} & \epsilon^{\alpha b}{}_{\mu\nu\sigma\lambda} & \epsilon^{\alpha B}{}_{\mu\nu\sigma\lambda\xi} \\ \hline \mu^{a\beta}{}_{\mu\sigma\lambda} & \epsilon^{ab}{}_{\mu\sigma} & \epsilon^{aB}{}_{\mu} & \epsilon^{a\beta}{}_{\mu\sigma} & \epsilon^{ab}{}_{\mu\sigma\lambda} & \epsilon^{aB}{}_{\mu\sigma\lambda\xi} \\ \hline \mu^{A\beta}{}_{\sigma\lambda} & \mu^{Ab}{}_{\sigma} & \epsilon^{AB} & \epsilon^{A\beta}{}_{\sigma} & \epsilon^{Ab}{}_{\sigma\lambda} & \epsilon^{AB}{}_{\sigma\lambda\xi} \\ \hline \mu^{\alpha\beta}{}_{\mu\sigma\lambda} & \mu^{\alpha b}{}_{\mu\sigma} & \mu^{\alpha B}{}_{\mu} & \epsilon^{\alpha\beta}{}_{\mu\sigma} & \epsilon^{\alpha b}{}_{\mu\sigma\lambda} & \epsilon^{\alpha B}{}_{\mu\sigma\lambda\xi} \\ \hline \mu^{a\beta}{}_{\mu\nu\sigma\lambda} & \mu^{ab}{}_{\mu\nu\sigma} & \mu^{aB}{}_{\mu\nu} & \mu^{a\beta}{}_{\mu\nu\sigma} & \epsilon^{ab}{}_{\mu\nu\sigma\lambda} & \epsilon^{aB}{}_{\mu\nu\sigma\lambda\xi} \\ \hline \mu^{A\beta}{}_{\mu\nu\rho\sigma\lambda} & \mu^{Ab}{}_{\mu\nu\rho\sigma} & \mu^{AB}{}_{\mu\nu\rho} & \mu^{A\beta}{}_{\mu\nu\rho\sigma} & \mu^{Ab}{}_{\mu\nu\rho\sigma\lambda} & \epsilon^{AB}{}_{\mu\nu\rho\sigma\lambda\xi} \end{array}\right) \begin{pmatrix} \frac{1}{2}\frac{\delta S}{\delta B^{\beta}{}_{\sigma\lambda}} \\ \frac{\delta S}{\delta C^{b}{}_{\sigma}} \\ \frac{\delta S}{\delta D^{B}} \\ \frac{\delta S}{\delta \alpha^{\beta}{}_{\sigma}} \\ \frac{1}{2}\frac{\delta S}{\delta \beta^{b}{}_{\sigma\lambda}} \\ \frac{1}{3!}\frac{\delta S}{\delta \gamma^{B}{}_{\sigma\lambda\xi}} \end{pmatrix} . \tag{33}$$

The coefficients multiplying the variations of the action in the column on the right-hand side are there to compensate the overcounting of the independent field components. Due to the antisymmetry of HT parameters, all μ blocks (below the diagonal) are determined in terms of the ϵ blocks (above the diagonal), as follows. For the first column of the parameter matrix in (33), we have:

$$\begin{gathered} \mu^{b\alpha}{}_{\sigma\mu\nu} = -\epsilon^{\alpha b}{}_{\mu\nu\sigma} , \qquad \mu^{B\alpha}{}_{\mu\nu} = -\epsilon^{\alpha B}{}_{\mu\nu} , \qquad \mu^{\beta\alpha}{}_{\sigma\mu\nu} = -\epsilon^{\alpha\beta}{}_{\mu\nu\sigma} , \\ \mu^{b\alpha}{}_{\sigma\lambda\mu\nu} = -\epsilon^{\alpha b}{}_{\mu\nu\sigma\lambda} , \qquad \mu^{B\alpha}{}_{\sigma\lambda\xi\mu\nu} = -\epsilon^{\alpha B}{}_{\mu\nu\sigma\lambda\xi} . \end{gathered} \tag{34}$$

For the second column, we have:

$$\begin{gathered} \mu^{Ba}{}_{\mu} = -\epsilon^{aB}{}_{\mu} , \qquad \mu^{\beta a}{}_{\sigma\mu} = -\epsilon^{a\beta}{}_{\mu\sigma} , \\ \mu^{ba}{}_{\sigma\lambda\mu} = -\epsilon^{ab}{}_{\mu\sigma\lambda} , \qquad \mu^{Ba}{}_{\sigma\lambda\xi\mu} = -\epsilon^{aB}{}_{\mu\sigma\lambda\xi} . \end{gathered} \tag{35}$$

The μ parameters in the third column are determined via:

$$\mu^{\beta A}{}_{\sigma} = -\epsilon^{A\beta}{}_{\sigma} , \qquad \mu^{bA}{}_{\sigma\lambda} = -\epsilon^{Ab}{}_{\sigma\lambda} , \qquad \mu^{BA}{}_{\sigma\lambda\xi} = -\epsilon^{AB}{}_{\sigma\lambda\xi} , \tag{36}$$

while the remaining μ parameters in the fourth and fifth columns are determined as:

$$\mu^{b\alpha}{}_{\sigma\lambda\mu} = -\epsilon^{\alpha b}{}_{\mu\sigma\lambda} , \qquad \mu^{B\alpha}{}_{\sigma\lambda\xi\mu} = -\epsilon^{\alpha B}{}_{\mu\sigma\lambda\xi} , \qquad \mu^{Ba}{}_{\sigma\lambda\xi\mu\nu} = -\epsilon^{aB}{}_{\mu\nu\sigma\lambda\xi} . \tag{37}$$

Finally, in addition to all these, the parameters in the blocks on the diagonal also have to satisfy certain antisymmetry relations, specifically:

$$\begin{gathered}\epsilon^{\alpha\beta}{}_{\mu\nu\sigma\lambda} = -\epsilon^{\beta\alpha}{}_{\sigma\lambda\mu\nu}\,, \qquad \epsilon^{ab}{}_{\mu\sigma} = -\epsilon^{ba}{}_{\sigma\mu}\,, \qquad \epsilon^{AB} = -\epsilon^{BA}\,, \\ \epsilon^{\alpha\beta}{}_{\mu\sigma} = -\epsilon^{\beta\alpha}{}_{\sigma\mu}\,, \qquad \epsilon^{ab}{}_{\mu\nu\sigma\lambda} = -\epsilon^{ba}{}_{\sigma\lambda\mu\nu}\,, \qquad \epsilon^{AB}{}_{\mu\nu\rho\sigma\lambda\xi} = -\epsilon^{BA}{}_{\sigma\lambda\xi\mu\nu\rho}\,.\end{gathered} \tag{38}$$

Like in the example of the Chern–Simons theory from the previous section, these antisymmetry relations can be satisfied in various multiple ways. All those possibilities are allowed, as long as the identities (38) are satisfied. The final ingredient in (33) is the expressions for the variation of the action with respect to the fields, and these are given as follows:

$$\begin{aligned}\frac{\delta S}{\delta B^{\beta}{}_{\nu\rho}} &= \frac{1}{2}\varepsilon^{\nu\rho\sigma\tau}\mathcal{F}_{\beta\sigma\tau}\,, \\ \frac{\delta S}{\delta C^{b}{}_{\rho}} &= \frac{1}{3!}\varepsilon^{\rho\sigma\tau\lambda}\mathcal{G}_{b\sigma\tau\lambda}\,, \\ \frac{\delta S}{\delta D^{B}} &= \frac{1}{4!}\varepsilon^{\sigma\tau\lambda\xi}\mathcal{H}_{B\sigma\tau\lambda\xi}\,, \\ \frac{\delta S}{\delta \alpha^{\beta}{}_{\rho}} &= \frac{1}{2}\varepsilon^{\rho\tau\lambda\xi}\left(\nabla_{\tau}B_{\beta\lambda\xi} - \rhd_{\beta a}{}^{b}C_{b\tau}\beta^{a}{}_{\lambda\xi} + \frac{1}{3}\rhd_{\beta B}{}^{A}D_{A}\gamma^{B}{}_{\tau\lambda\xi}\right), \\ \frac{\delta S}{\delta \beta^{b}{}_{\nu\rho}} &= \varepsilon^{\nu\rho\sigma\tau}\left(\nabla_{\sigma}C_{b\tau} - \frac{1}{2}\partial_{b}{}^{\alpha}B_{\alpha\sigma\tau} + X_{(ab)}{}^{A}D_{A}\beta^{b}{}_{\sigma\tau}\right), \\ \frac{\delta S}{\delta \gamma^{B}{}_{\mu\nu\rho}} &= \varepsilon^{\mu\nu\rho\sigma}(\nabla_{\sigma}D_{B} + \delta_{B}{}^{a}C_{a\sigma})\,.\end{aligned} \tag{39}$$

4.3. Diffeomorphisms

As in the case of the Chern–Simons theory, it is instructive to discuss diffeomorphism symmetry. The $3BF$ action (29) obviously is diffeomorphism invariant, since it is formulated in a manifestly covariant way, using differential forms. However, one can check that the diffeomorphisms are not a subgroup of the gauge symmetry group $\mathcal{G}_{3BF}$ given by Equation (31), but nevertheless can be obtained as a subgroup of the total gauge group (32):

$$Diff(\mathcal{M}_4) \not\subset \mathcal{G}_{3BF}\,, \qquad \text{but} \qquad Diff(\mathcal{M}_4) \subset \mathcal{G}_{\text{total}} = \mathcal{G}_{3BF} \ltimes \mathcal{G}_{HT}\,. \tag{40}$$

Let us demonstrate this. Like in the Chern–Simons case, we want to demonstrate that the form variation of all fields corresponding to diffeomorphisms can be obtained as a suitable combination of the form variations for the ordinary gauge transformations (30) and the HT transformations (33). In other words, for an arbitrary choice of the diffeomorphism parameters $\xi^{\mu}(x)$ from (24), Equation (25) should hold in the case of the $3BF$ theory as well:

$$\delta_0{}^{\text{diff}}\phi = \delta_0{}^{\text{gauge}}\phi + \delta_0{}^{\text{HT}}\phi\,. \tag{41}$$

Indeed, this can be shown by a suitable choice of parameters. Regarding the parameters of the gauge transformations (30), the appropriate choice is given as:

$$\begin{gathered}\epsilon_{\mathfrak{g}}{}^{\alpha} = \xi^{\lambda}\alpha^{\alpha}{}_{\lambda}\,, \qquad \epsilon_{\mathfrak{h}}{}^{a}{}_{\mu} = -\xi^{\lambda}\beta^{a}{}_{\mu\lambda}\,, \qquad \epsilon_{\mathfrak{l}}{}^{A}{}_{\mu\nu} = -\xi^{\lambda}\gamma^{A}{}_{\mu\nu\lambda}\,, \\ \epsilon_{\mathfrak{m}}{}^{\alpha}{}_{\mu} = -\xi^{\lambda}B^{\alpha}{}_{\mu\lambda}\,, \qquad \epsilon_{\mathfrak{n}}{}^{a} = \xi^{\lambda}C^{a}{}_{\lambda}\,.\end{gathered} \tag{42}$$

Regarding the parameters of the HT transformations (33), we chose the following special case, with the majority of the parameters equated to zero:

$$\begin{pmatrix} \delta_0 B^{\alpha}{}_{\mu\nu} \\ \delta_0 C^{a}{}_{\mu} \\ \delta_0 D^{A} \\ \delta_0 \alpha^{\alpha}{}_{\mu} \\ \delta_0 \beta^{a}{}_{\mu\nu} \\ \delta_0 \gamma^{A}{}_{\mu\nu\rho} \end{pmatrix} = \left(\begin{array}{c|c|c|c|c|c} 0 & 0 & 0 & \epsilon^{\alpha\beta}{}_{\mu\nu\sigma} & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \epsilon^{ab}{}_{\mu\sigma\lambda} & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & \epsilon^{AB}{}_{\sigma\lambda\xi} \\ \hline \mu^{\alpha\beta}{}_{\mu\sigma\lambda} & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & \mu^{ab}{}_{\mu\nu\sigma} & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & \mu^{AB}{}_{\mu\nu\rho} & 0 & 0 & 0 \end{array}\right) \begin{pmatrix} \frac{1}{2}\frac{\delta S}{\delta B^{\beta}{}_{\sigma\lambda}} \\ \frac{\delta S}{\delta C^{b}{}_{\sigma}} \\ \frac{\delta S}{\delta D^{B}} \\ \frac{\delta S}{\delta \alpha^{\beta}{}_{\sigma}} \\ \frac{1}{2}\frac{\delta S}{\delta \beta^{b}{}_{\sigma\lambda}} \\ \frac{1}{3!}\frac{\delta S}{\delta \gamma^{B}{}_{\sigma\lambda\xi}} \end{pmatrix}. \tag{43}$$

Of course, due to antisymmetry, the nonzero μ blocks take negative values of the corresponding ϵ blocks, in accordance with (34), (35), and (36). The three independent nonzero ϵ blocks are chosen as

$$\epsilon^{\alpha\beta}{}_{\mu\nu\sigma} = \xi^{\rho} g^{\alpha\beta} \varepsilon_{\mu\nu\sigma\rho}\,, \qquad \epsilon^{ab}{}_{\mu\sigma\lambda} = \xi^{\rho} g^{ab} \varepsilon_{\rho\mu\sigma\lambda}\,, \qquad \epsilon^{AB}{}_{\sigma\lambda\xi} = \xi^{\rho} g^{AB} \varepsilon_{\sigma\lambda\xi\rho}\,. \tag{44}$$

Finally, substituting (42) and (44) into (30) and (43), respectively, and then substituting all those results into (41), after a certain amount of work, one obtains precisely the standard form variations corresponding to diffeomorphisms:

$$\begin{aligned} \delta_0^{\rm diff} B^{\alpha}{}_{\mu\nu} &= -B^{\alpha}{}_{\lambda\nu}\partial_{\mu}\xi^{\lambda} - B^{\alpha}{}_{\mu\lambda}\partial_{\nu}\xi^{\lambda} - \xi^{\lambda}\partial_{\lambda}B^{\alpha}{}_{\mu\nu}\,, \\ \delta_0^{\rm diff} C^{a}{}_{\mu} &= -C^{a}{}_{\lambda}\partial_{\mu}\xi^{\lambda} - \xi^{\lambda}\partial_{\lambda}C^{a}{}_{\mu}\,, \\ \delta_0^{\rm diff} D^{A} &= -\xi^{\lambda}\partial_{\lambda}D^{A}\,, \\ \delta_0^{\rm diff} \alpha^{\alpha}{}_{\mu} &= -\alpha^{\alpha}{}_{\lambda}\partial_{\mu}\xi^{\lambda} - \xi^{\lambda}\partial_{\lambda}\alpha^{\alpha}{}_{\mu}\,, \\ \delta_0^{\rm diff} \beta^{a}{}_{\mu\nu} &= -\beta^{a}{}_{\lambda\nu}\partial_{\mu}\xi^{\lambda} - \beta^{a}{}_{\mu\lambda}\partial_{\nu}\xi^{\lambda} - \xi^{\lambda}\partial_{\lambda}\beta^{a}{}_{\mu\nu}\,, \\ \delta_0^{\rm diff} \gamma^{A}{}_{\mu\nu\rho} &= -\gamma^{A}{}_{\lambda\nu\rho}\partial_{\mu}\xi^{\lambda} - \gamma^{A}{}_{\mu\lambda\rho}\partial_{\nu}\xi^{\lambda} - \gamma^{A}{}_{\mu\nu\lambda}\partial_{\rho}\xi^{\lambda} - \xi^{\lambda}\partial_{\lambda}\gamma^{A}{}_{\mu\nu\rho}\,. \end{aligned} \tag{45}$$

This establishes both relations (40), as we set out to demonstrate. We note again that the HT transformations play a crucial role in obtaining the result, since we had to choose the parameters (44) in a nontrivial manner.

4.4. Symmetry Breaking in 2BF Theory

Let us now turn to the topic of symmetry breaking and the way it influences HT transformations. To that end, we studied the topological $2BF$ action, which is a special case of the $3BF$ action (29) without the last term:

$$S_{2BF} = \int_{\mathcal{M}_4} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} + \langle C \wedge \mathcal{G} \rangle_{\mathfrak{h}}\,. \tag{46}$$

In order to be even more concrete, let us fix a two-crossed module structure with the following choice of groups:

$$G = SO(3,1)\,, \qquad H = \mathbb{R}^4\,, \qquad L = \{e\}\,.$$

In other words, we interpret group G as the Lorentz group, group H as the spacetime translations group, while group L is trivial, for simplicity. This choice corresponds to the so-called Poincaré two-group; see [16] for details. Since the generators of the Lorentz group can be conveniently counted using the antisymmetric combinations of indices from the group of translations, instead of the G-group indices α, we shall systematically write $[ab] \in \{01, 02, 03, 12, 13, 23\}$, where $a, b \in \{0, 1, 2, 3\}$ are H-group indices, and the brackets denote antisymmetrization. With a further change in notation from the connection 1-form α to the spin-connection 1-form ω, the curvature 2-form $\mathcal{F}(\alpha)$ to $R(\omega)$, and interpreting the Lagrange multiplier 1-form C as the tetrad 1-form e, the $2BF$ action can be rewritten in new notation as

$$S_{2BF} = \int_{\mathcal{M}_4} B^{[ab]} \wedge R_{[ab]} + e^a \wedge \mathcal{G}_a \,. \tag{47}$$

The ordinary gauge symmetry group for this action has a form similar to (31):

$$\mathcal{G}_{2BF} = \tilde{G} \ltimes (\tilde{H} \ltimes (\tilde{N} \times \tilde{M}))\,, \tag{48}$$

while the total group of gauge symmetries is extended by the HT transformations, so that

$$\mathcal{G}_{\text{total}} = \mathcal{G}_{2BF} \ltimes \mathcal{G}_{HT} \,. \tag{49}$$

The explicit HT transformations are written as a tensorial 4×4 block-matrix equation, in the form

$$\begin{pmatrix} \delta_0 B^{[ab]}{}_{\mu\nu} \\ \delta_0 e^a{}_\mu \\ \delta_0 \omega^{[ab]}{}_\mu \\ \delta_0 \beta^a{}_{\mu\nu} \end{pmatrix} = \left(\begin{array}{c|c|c|c} \epsilon^{[ab][cd]}{}_{\mu\nu\sigma\lambda} & \epsilon^{[ab]c}{}_{\mu\nu\sigma} & \epsilon^{[ab][cd]}{}_{\mu\nu\sigma} & \epsilon^{[ab]c}{}_{\mu\nu\sigma\lambda} \\ \hline \mu^{a[cd]}{}_{\mu\sigma\lambda} & \epsilon^{ac}{}_{\mu\sigma} & \epsilon^{a[cd]}{}_{\mu\sigma} & \epsilon^{ac}{}_{\mu\sigma\lambda} \\ \hline \mu^{[ab][cd]}{}_{\mu\sigma\lambda} & \mu^{[ab]c}{}_{\mu\sigma} & \epsilon^{[ab][cd]}{}_{\mu\sigma} & \epsilon^{[ab]c}{}_{\mu\sigma\lambda} \\ \hline \mu^{a[cd]}{}_{\mu\nu\sigma\lambda} & \mu^{ac}{}_{\mu\nu\sigma} & \mu^{a[cd]}{}_{\mu\nu\sigma} & \epsilon^{ac}{}_{\mu\nu\sigma\lambda} \end{array}\right) \begin{pmatrix} \frac{1}{4}\frac{\delta S}{\delta B^{[cd]}{}_{\sigma\lambda}} \\ \frac{\delta S}{\delta e^c{}_\sigma} \\ \frac{1}{2}\frac{\delta S}{\delta \omega^{[cd]}{}_\sigma} \\ \frac{1}{2}\frac{\delta S}{\delta \beta^c{}_{\sigma\lambda}} \end{pmatrix}, \tag{50}$$

where the usual antisymmetry rules apply. Here, we have

$$\begin{aligned} \frac{\delta S}{\delta B^{[cd]}{}_{\sigma\lambda}} &= \varepsilon^{\mu\nu\sigma\lambda} R_{[cd]\mu\nu}\,, \\ \frac{\delta S}{\delta \omega^{[cd]}{}_\sigma} &= \varepsilon^{\sigma\mu\nu\rho}\left(\nabla_\mu B_{[cd]\nu\rho} - e_{[c|\mu}\beta_{|d]\nu\rho}\right), \\ \frac{\delta S}{\delta e^c{}_\sigma} &= \frac{1}{2}\varepsilon^{\sigma\mu\nu\rho}\nabla_\mu \beta_{c\nu\rho}\,, \\ \frac{\delta S}{\delta \beta^c{}_{\sigma\lambda}} &= \varepsilon^{\mu\nu\sigma\lambda}\nabla_\mu e_{c\nu}\,. \end{aligned} \tag{51}$$

The $2BF$ action (46) is topological, in the sense that it has no local propagating degrees of freedom. In this sense, it does not represent a theory of any realistic physics. In order to construct a more realistic theory, one proceeds by introducing the so-called *simplicity constraint* term into the action, which changes the equations of motion of the theory so that it does have nontrivial degrees of freedom. An example is the action

$$S_{GR} = \int_{\mathcal{M}_4} B^{[ab]} \wedge R_{[ab]} + e^a \wedge \nabla\beta_a - \lambda_{[ab]} \wedge \left(B^{[ab]} - \frac{1}{16\pi l_p^2}\varepsilon^{abcd} e_c \wedge e_d\right), \tag{52}$$

where the new constraint term features another Lagrange multiplier two-form $\lambda_{[ab]}$. By virtue of the simplicity constraint, the theory becomes equivalent to general relativity, in the sense that the corresponding equations of motion reduce to vacuum Einstein field equations (see [16] for the analysis and proof). In this sense, constraint terms of various types are important when building more realistic theories; see [20] for more examples.

However, adding the simplicity constraint term also changes the gauge symmetry of the theory. In particular, it breaks the gauge group $\mathcal{G}_{2BF}$ from (48) down to one of its subgroups, so that the symmetry group of the action S_{GR} is

$$\mathcal{G}_{GR} \subset \mathcal{G}_{2BF} \,. \tag{53}$$

This is expected and unsurprising. What is less obvious, however, is that the group of HT transformations $\tilde{\mathcal{G}}_{HT}$ of the action S_{GR} *is not a subgroup* of the HT group $\mathcal{G}_{HT}$ of the original action S_{2BF}:

$$\tilde{\mathcal{G}}_{HT} \not\subset \mathcal{G}_{HT}\,, \tag{54}$$

which implies that

$$\mathcal{G}^{GR}_{\text{total}} \not\subset \mathcal{G}^{2BF}_{\text{total}}\,, \tag{55}$$

despite (53).

Let us demonstrate this. Since the action (52) features an additional field $\lambda^{[ab]}{}_{\mu\nu}(x)$, the HT transformations (50) have to be modified to take this into account and obtain the following 5×5 block-matrix form:

$$\begin{pmatrix} \delta_0 B^{[ab]}{}_{\mu\nu} \\ \delta_0 e^a{}_\mu \\ \delta_0 \omega^{[ab]}{}_\mu \\ \delta_0 \beta^a{}_{\mu\nu} \\ \delta_0 \lambda^{[ab]}{}_{\mu\nu} \end{pmatrix} = \left(\begin{array}{c|c|c|c|c} \epsilon^{[ab][cd]}{}_{\mu\nu\sigma\lambda} & \epsilon^{[ab]c}{}_{\mu\nu\sigma} & \epsilon^{[ab][cd]}{}_{\mu\nu\sigma} & \epsilon^{[ab]c}{}_{\mu\nu\sigma\lambda} & \zeta^{[ab][cd]}{}_{\mu\nu\sigma\xi} \\ \hline \mu^{a[cd]}{}_{\mu\sigma\lambda} & \epsilon^{ac}{}_{\mu\sigma} & \epsilon^{a[cd]}{}_{\mu\sigma} & \epsilon^{ac}{}_{\mu\sigma\lambda} & \zeta^{a[cd]}{}_{\mu\sigma\xi} \\ \hline \mu^{[ab][cd]}{}_{\mu\sigma\lambda} & \mu^{[ab]c}{}_{\mu\sigma} & \epsilon^{[ab][cd]}{}_{\mu\sigma} & \epsilon^{[ab]c}{}_{\mu\sigma\lambda} & \zeta^{[ab][cd]}{}_{\mu\sigma\xi} \\ \hline \mu^{a[cd]}{}_{\mu\nu\sigma\lambda} & \mu^{ac}{}_{\mu\nu\sigma} & \mu^{a[cd]}{}_{\mu\nu\sigma} & \epsilon^{ac}{}_{\mu\nu\sigma\lambda} & \zeta^{a[cd]}{}_{\mu\nu\sigma\xi} \\ \hline \theta^{[ab][cd]}{}_{\mu\nu\sigma\lambda} & \theta^{[ab]c}{}_{\mu\nu\sigma} & \theta^{[ab][cd]}{}_{\mu\nu\sigma} & \theta^{[ab]c}{}_{\mu\nu\sigma\lambda} & \psi^{[ab][cd]}{}_{\mu\nu\sigma\xi} \end{array}\right) \begin{pmatrix} \frac{1}{4}\frac{\delta S_{GR}}{\delta B^{[cd]}{}_{\sigma\lambda}} \\ \frac{\delta S_{GR}}{\delta e^c{}_\sigma} \\ \frac{1}{2}\frac{\delta S_{GR}}{\delta \omega^{[cd]}{}_\sigma} \\ \frac{1}{2}\frac{\delta S_{GR}}{\delta \beta^c{}_{\sigma\lambda}} \\ \frac{1}{4}\frac{\delta S_{GR}}{\delta \lambda^{[cd]}{}_{\sigma\xi}} \end{pmatrix}, \tag{56}$$

where

$$\begin{aligned} \frac{\delta S_{GR}}{\delta B^{[cd]}{}_{\sigma\lambda}} &= \varepsilon^{\mu\nu\sigma\lambda}\Big(R_{[cd]\mu\nu} - \lambda_{[cd]\mu\nu}\Big)\,, \\ \frac{\delta S_{GR}}{\delta \omega^{[cd]}{}_{\sigma}} &= \varepsilon^{\sigma\mu\nu\rho}\Big(\nabla_\mu B_{[cd]\nu\rho} - e_{[c|\mu}\beta_{|d]\nu\rho}\Big)\,, \\ \frac{\delta S_{GR}}{\delta e^{c}{}_{\sigma}} &= \frac{1}{2}\varepsilon^{\sigma\mu\nu\rho}\Big(\nabla_\mu \beta_{c\nu\rho} + \frac{1}{8\pi l_p^2}\varepsilon_{abcd}\lambda^{[ab]}{}_{\mu\nu}e^d{}_\rho\Big)\,, \\ \frac{\delta S_{GR}}{\delta \beta^{c}{}_{\sigma\lambda}} &= \varepsilon^{\mu\nu\sigma\lambda}\nabla_\mu e_{c\nu}\,, \\ \frac{\delta S_{GR}}{\delta \lambda^{[cd]}{}_{\sigma\xi}} &= -\varepsilon^{\sigma\xi\mu\nu}\Big(B_{[cd]\mu\nu} - \frac{1}{8\pi l_p^2}\varepsilon_{abcd}e^a{}_\mu e^b{}_\nu\Big)\,. \end{aligned} \tag{57}$$

We can now investigate the differences in the form of HT transformations for the topological and constrained theory. First, comparing (56) to (50), we see that the HT transformations in the constrained theory feature *more gauge parameters* than are present in the topological theory. Namely, compared to S_{2BF}, the action S_{GR} features an extra Lagrange multiplier two-form $\lambda^{[ab]}$, which extends the matrix of HT parameters from 4×4 blocks to 5×5 blocks, and, therefore, introduces the new parameters ζ and ψ (and θ, which are the negative of ζ due to antisymmetry). This means that the group $\tilde{\mathcal{G}}_{HT}$ for the constrained theory is *larger* than the group $\mathcal{G}_{HT}$ for the topological theory. On the one hand, this immediately proves (54) and, consequently, (55). On the other hand, one can ask the opposite question—given that $\tilde{\mathcal{G}}_{HT}$ is larger than $\mathcal{G}_{HT}$, is the latter maybe a subgroup of the former?

The answer to this question is negative:

$$\mathcal{G}_{HT} \not\subset \tilde{\mathcal{G}}_{HT}\,, \tag{58}$$

which together with (54) implies our final conclusion:

$$\mathcal{G}_{HT} \neq \tilde{\mathcal{G}}_{HT}\,. \tag{59}$$

In order to demonstrate (58), we can try to set all extra parameters ζ, ψ, and θ to zero in (56), reducing it to the same form as (50). This would naively suggest that $\mathcal{G}_{HT}$ indeed is a subgroup of $\tilde{\mathcal{G}}_{HT}$. However, upon closer inspection, we can observe that this is not true, since the functional derivatives (57) are different from (51). Namely, even taking into account that the choice $\zeta = \psi = \theta = 0$ eliminates the fifth equation from (57), the first four equations are still different from their counterparts (51) because of the presence of the Lagrange multiplier $\lambda^{[ab]}$ in the action. The Lagrange multiplier is a field in the theory, and generically, it is not zero, since it is determined by the equation of motion:

$$\lambda^{[ab]}{}_{\mu\nu} = R^{[ab]}{}_{\mu\nu}\,.$$

Therefore, the HT transformations (56) in fact cannot be reduced to the HT transformations (50) by setting the extra parameters equal to zero, which proves (58) and (59).

The overall consequences from the above analysis are as follows. The topological action S_{2BF} has a large ordinary gauge group $\mathcal{G}_{2BF}$ and a small HT symmetry group $\mathcal{G}_{HT}$. When one changes the action to S_{GR} by adding a simplicity constraint term, two things happen—the ordinary gauge group breaks down to its subgroup $\mathcal{G}_{GR}$, so that it becomes smaller, while the HT symmetry group *grows larger* to a completely different group $\tilde{\mathcal{G}}_{HT}$. In effect, the *total* gauge groups for the two actions are intrinsically different:

$$\mathcal{G}^{2BF}_{\text{total}} = \mathcal{G}_{2BF} \ltimes \mathcal{G}_{HT} \qquad \neq \qquad \mathcal{G}^{GR}_{\text{total}} = \mathcal{G}_{GR} \ltimes \tilde{\mathcal{G}}_{HT}\,,$$

in the sense that neither is a subgroup of the other. This conclusion is often overlooked in the literature, which mostly puts emphasis on the symmetry breaking of the ordinary gauge group down to its subgroup.

Let us state here, without proof, that the action (52) represents an example of a non-topological action, for which one can also demonstrate a property analogous to (40), that diffeomorphisms are not a subgroup of its ordinary gauge group, but are a subgroup of the total gauge group. Simply put, given that the simplicity constraint term in (52) breaks the ordinary gauge symmetry group $\mathcal{G}_{2BF}$ into its subgroup $\mathcal{G}_{GR}$ (see (53)), one can expect that diffeomorphisms are not a subgroup of $\mathcal{G}_{GR}$, since they are not a subgroup of the larger group $\mathcal{G}_{2BF}$ of the topological action (46). Nevertheless, since the action (52) is written in a manifestly covariant form, diffeomorphisms are certainly a symmetry of the action and, thus, must be a subgroup of the total gauge group $\mathcal{G}^{GR}_{\text{total}} = \mathcal{G}_{GR} \ltimes \tilde{\mathcal{G}}_{HT}$, in line with the statement analogous to (40). We leave the details of the proof as an exercise for the reader. The point of this analysis was to demonstrate that the interplay (40) between diffeomorphisms and the HT symmetry is a generic property of a large class of actions, including the physically relevant ones, and not limited to examples of topological theories such as the Chern–Simons or nBF models.

As the last comment, let us remark that, in fact, almost all conclusions discussed for the cases of the Chern–Simons, $3BF$, and $2BF$ theories are not really specific to these concrete cases. One can easily generalize our analysis to any other theory, and the conclusions should remain unchanged, except maybe in some corner cases.

5. Conclusions

Let us review the results. In Section 2, we gave a short overview of HT gauge symmetry and discussed its most-important general properties. First, the HT group is a normal subgroup of the total group of gauge symmetries of any given action. Second, HT transformations exhaust all "trivial" (i.e., vanishing on-shell) symmetries, in the sense that there are no trivial symmetries that are not of the HT type. Finally, adding additional terms into the action substantially changes the HT group, often enlarging it. This may be considered a counterintuitive result, since usually adding additional terms in the action serves the purpose of fixing the gauge and, thus, is meant to reduce the gauge symmetry, rather than to enlarge it.

After these general results, in Section 3, we discussed the HT symmetry of the Chern–Simons action, which is a convenient toy example that neatly displays the general features from Section 2. Special attention was given to the issue of diffeomorphisms, and it was shown that, while they are not a subgroup of the ordinary gauge group of the Chern–Simons action, they nevertheless do represent a proper subgroup of the total gauge symmetry, and the HT subgroup plays a nontrivial role in demonstrating this.

Section 4 was devoted to the study of HT symmetry in the $2BF$ and $3BF$ theories, which are relevant for the constructions of realistic quantum gravity models within the generalized spinfoam approach and higher gauge theory. After a brief review and introduction to the notion of three-groups and the $3BF$ theory, appropriate HT transformations were explicitly constructed, complementing the ordinary group of gauge symmetries of the $3BF$ action based on a given three-group. This gave us the total gauge symmetry group for this class of theories. We again discussed the issue of diffeomorphisms and demonstrated again that they are a subgroup of the total gauge group, without being a subgroup of the ordinary gauge group, just like in the case of the Chern–Simons theory. Finally, we introduced a completely concrete example of the $2BF$ theory based on the Poincaré two-group, which becomes classically equivalent to Einstein's general relativity when one introduces the additional term into the action, called the simplicity constraint. As argued in general in Section 2, the presence of this constraint breaks the ordinary gauge group down into its subgroup, while simultaneously enlarging the HT group, since it introduces an additional Lagrange multiplier field into the action. This represents an explicit example of the general statement from Section 2 that the total gauge symmetry group changes nontrivially, as opposed to simply breaking down to its subgroup.

It should be noted that the analysis and results discussed here do not cover everything that can be said about HT symmetry. Among the topics not covered, one can mention the question of an explicit form of finite HT transformations, as opposed to infinitesimal ones. Can one write down finite HT transformations in closed form, either for some conveniently chosen action or maybe even in general? A related topic is the explicit evaluation of the commutator of two HT transformations, or equivalently, the structure constants of the HT Lie algebra, or in yet other words, the multiplication rule in the group $\mathcal{G}_{HT}$. Is the group Abelian or not and for which choices of the action? Finally, one would also like to know the topological properties of the group $\mathcal{G}_{HT}$, i.e., its global structure. All these are potentially interesting topics for future research.

As a particularly interesting topic for future research, we should mention the nontrivial change of the HT symmetry group when additional terms are being added to the action. In Section 4.4, we briefly demonstrated that HT symmetry does change in a nontrivial way, on the example action (52). Nevertheless, the precise properties and the physical interpretation of this change are yet to be studied in full and for a general choice of the action. This topic is the subject of ongoing research.

Finally, we would like to reiterate the differences in two possible approaches to the notion of "the gauge symmetry" of a theory. The overwhelmingly common approach throughout the literature is to factor out the HT group and work only with the ordinary, nontrivial gauge group as the relevant symmetry. Admittedly, this approach does feature a certain level of appeal due to its simplicity and economy, since it does not have to deal with HT symmetry at all. Nevertheless, there are important situations where this is not enough, and one really needs to take into account the *total* gauge symmetry group, which includes HT transformations. As a rule, these situations always involve the gauge symmetry off-shell, either for the purpose of quantization or otherwise. A typical example is the Batalin–Vilkovisky formalism, where one needs to explicitly keep track of HT transformations throughout the whole analysis. Another situation, which was discussed here in more detail, is the question of diffeomorphism symmetry, where HT transformations are required in order to prove that diffeomorphisms are a symmetry of the theory even off-shell. This is especially relevant for building quantum gravity models. Finally, the third scenario would be the discussion of the Coleman–Mandula theorem. One of the main assumptions of the theorem is that the Poincaré group is a subgroup of the full symmetry group of the theory. Given this assumption, and a number of other assumptions, the theorem implies that the full symmetry group must be a direct product of the Poincaré subgroup and the internal symmetry subgroup. In certain cases of theories (such as the $3BF$ action), the full symmetry group is not explicitly expressed as such a direct product, and moreover, it is not obvious that the Poincaré group is a subgroup of the full symmetry group to begin with. Therefore, in order to verify whether the above assumption of the theorem is satisfied, one needs to inspect if the Poincaré group is or is not a subgroup of the full symmetry group. At this point, one may run into a scenario similar to diffeomorphisms: the Poincaré group may fail to be a subgroup of the ordinary gauge group, but still be a subgroup of the total gauge group, once the HT symmetry is taken into account. In this sense, HT symmetry may become relevant for the proper analysis and application of the Coleman–Mandula theorem in certain contexts. This topic is the subject of ongoing research [34].

All of the above arguments suggest that it may be prudent to abandon the common approach of factoring out the HT group and instead adopt the description of the symmetry with the total gauge group, which includes HT transformations on equal footing as the ordinary gauge transformations. In the long run, this may be a conceptually cleaner approach. However, either way, we believe that HT symmetry is relevant for the overall symmetry structure of a theory and that better understanding of its properties can add value to and benefit research.

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Equivalence Principle in Classical and Quantum Gravity

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Abstract: We give a general overview of various flavours of the equivalence principle in classical and quantum physics, with special emphasis on the so-called weak equivalence principle, and contrast its validity in mechanics versus field theory. We also discuss its generalisation to a theory of quantum gravity. Our analysis suggests that only the strong equivalence principle can be considered fundamental enough to be generalised to a quantum gravity context since all other flavours of equivalence principle hold only approximately already at the classical level.

Keywords: equivalence principle; general relativity; quantum gravity

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1. Introduction

Quantum mechanics (QM) and general relativity (GR) are the two cornerstones of modern physics. Yet, merging them together in a quantum theory of gravity (QG) is still elusive despite the nearly century-long efforts of vast numbers of physicists and mathematicians. While the majority of the attempts were focused on trying to formulate the full theory of quantised gravity, such as string theory, loop quantum gravity, non-commutative geometry, and causal set theory, to name a few, a number of recent studies embraced a rather more modest approach by exploring possible consequences of basic features and principles of QM and GR, and their status, in a tentative theory of QG. Acknowledging that the superposition principle, as a defining characteristic of any quantum theory, must be featured in QG as well, led to a number of papers studying gravity-matter entanglement [1–7], genuine indefinite causal orders [8–15], quantum reference frames [16–20] and deformations of Lorentz symmetry [21–25], to name a few major research directions. Exploring spatial superpositions of masses, and in general gravitational fields, led to the analysis of the status of various versions of the equivalence principle, and their exact formulations in the context of QG. In particular, in [26], it was shown that the weak equivalence principle (WEP) should generically be violated in the presence of a specific type of superpositions of gravitational fields, describing small quantum fluctuations around a dominant classical geometry. On the other hand, a number of recent studies propose generalisations of WEP to QG framework (see for example [16,20,27–31]), arguing that it remains satisfied in such scenarios, a result *seemingly* at odds with [26] (for details, see the discussion from Section 5).

The modern formulation of WEP is given in terms of a *test particle* and it's *trajectory*: it is a *theorem* within the mathematical formulation of GR stating that the trajectory of a test particle satisfies the so-called geodesic equation [32–46], while it is *violated* within the context of QG, as shown in [26]. In this paper, we present a brief overview of WEP in GR and a critical analysis of the notions of particle and trajectory in both classical and quantum mechanics, as well as in the corresponding field theories.Our analysis demonstrates that WEP, as well as all other flavours of the equivalence principle (EP) aside from the strong one (SEP), hold only approximately. From this we conclude that neither WEP nor any other flavour of EP (aside from SEP) can be considered a viable candidate for generalisation to the quantum gravity framework.

The paper is organised as follows. In Section 2, we give a brief historical overview of various flavours of the equivalence principle, with a focus on WEP. In Section 3, we analyse the notion of a trajectory in classical and quantum mechanics, while in Section 4 we discuss the notion of a particle in field theory and QG. Finally, in the Conclusion, we briefly review and discuss our results, and present possible future lines of research.

2. Equivalence Principle in General Relativity

The equivalence principle is one of the most fundamental principles in modern physics. It is one of the two cornerstone building blocks for GR, the other being the principle of general relativity. While its importance is well understood in the context of gravity, it is often underappreciated in the context of other fundamental interactions. In addition, there have been numerous studies and everlasting debates about whether EP holds also in quantum physics, if it should be generalised to include quantum phenomena or not, etc. Finally, EP has been historically formulated in a vast number of different ways, which are often not mutually equivalent, leading to a lot of confusion about the actual statement of the principle and its physical content [47–53]. Given the importance of EP, and the amount of confusion around it, it is important to try and help clarify these issues.

The equivalence principle is best introduced by stating its purpose—in its traditional sense, the purpose of EP is to *prescribe the interaction between gravity and all other fields in nature, collectively called matter* (by "matter" we assume not just fermionic and scalar fields, but also gauge vector bosons, i.e., nongravitational interaction fields). This is important to state explicitly since EP is often mistakenly portrayed as a property of gravity alone, without any reference to matter. In a more general, less traditional, and often not appreciated sense, the purpose of EP is to prescribe the interaction between *any gauge field* and all other fields in nature (namely fermionic and scalar matter, as well as other gauge fields, including gravity), which we will reflect on briefly in the case of electrodynamics below.

Given such a purpose, let us for the moment concentrate on the gravitational version of EP, and provide its modern formulation, as it is known and understood today. The statement of the equivalence principle is the following:

> *The equations of motion for matter coupled to gravity remain locally identical to the equations of motion for matter in the absence of gravity.*

This kind of statement requires some unpacking and comments.

- When comparing the equations of motion in the presence and in the absence of gravity, the claim that they remain identical may naively suggest that gravity does not influence the motion of matter in any way whatsoever. However, on closer inspection, the statement is that the two sets of equations remain *locally* identical, emphasising that the notion of locality is a crucial feature of the EP. While equations of motion are already local in nature (since they are usually expressed as partial differential equations of finite order), the actual interaction between matter and gravity enters only when *integrating* those equations to find a solution (see Appendix A for a detailed example).
- In order to compare the equations of motion for matter in the presence of gravity to those in its absence, the equations themselves need to be put in a suitable form (typically expressed in general curvilinear coordinates, as tensor equations). The statement of EP relies on a theorem that this can always be achieved, first noted by Erich Kretschmann [54].
- Despite being dominantly a statement about the interaction between matter and gravity, EP also implicitly suggests that the best way to describe the gravitational field is as a property of the geometry of spacetime, such as its metric [55]. In that setup, EP can be reformulated as a statement of *minimal coupling* between gravity and matter, stating that equations of motion for matter may depend on the spacetime metric and its first derivatives, but not on its (antisymmetrised) second derivatives, i.e., the *spacetime curvature does not explicitly appear in the equations of motion for matter*.

- The generalisation of EP to other gauge fields is completely straightforward, by replacing the role of gravity with some other gauge field, and suitably redefining what matter is. For example, in electrodynamics, the EP can be formulated as follows:

  > *The equations of motion for matter coupled to the electromagnetic field remain locally identical to the equations of motion for matter in the absence of the electromagnetic field.*

  This statement can also be suitably reformulated as the minimal coupling between the electromagnetic (EM) field and matter, i.e., coupling matter to the electromagnetic potential A_μ but not to the corresponding field strength $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. This is in fact the standard way the EM field is coupled to matter (see Appendix A for an illustrative example). Even more generally, the gauge field sector of the whole Standard Model of elementary particles (SM) is built using the minimal coupling prescription, meaning that the suitably generalised version of the EP actually prescribes the interaction between matter and all fundamental interactions in nature, namely strong, weak, electromagnetic and gravitational. In this sense, EP is a cornerstone principle for the whole fundamental physics, as we understand it today.

Of course, much more can be said about the statement of EP, its consequences, and various other details. However, in this work, our attention will focus on the so-called *weak equivalence principle* (WEP), which is a reformulation of EP applied to matter which consists of mechanical particles. To that end, it is important to understand various flavours and reformulations of EP that have appeared through history.

As with any deep concept in physics, EP has been expressed historically through a painstaking cycle of formulating it in a precise way, understanding the formulation, understanding the drawbacks of that formulation, coming up with a better formulation, and repeating. In this sense, EP, as quoted above, is a modern product of long and meticulous refinement over several generations of scientists. Needless to say, each step in that process made its way into contemporary physics textbooks, leading to a plethora of different formulations of EP that have accumulated in the literature over the years. This can bring about a lot of confusion about what EP actually states [47–50] since various formulations from old and new literature may often be not merely phrased differently, but in fact substantively inequivalent. To that end, let us comment on several of the most common historical statements of EP (for a more detailed historical overview and classification, see [56,57]), and their relationship with the modern version:

- *Equality of gravitational and inertial mass.* This is one of the oldest variants of EP, going back to Newton's law of universal gravitation. The statement claims that the "gravitational charge" of a body is the same as the body's resistance to acceleration, in the sense that the mass appearing on the left-hand side of Newton's second law of motion exactly cancels the mass appearing in Newton's gravitational force law on the right-hand side. This allows one to relate it to the modern version of EP, in the sense that a suitably accelerated observer could rewrite Newton's law of motion as the equation for a free particle, exploiting the cancellation of the "intertial force" and the gravitational force on the right-hand side of the equation. Unfortunately, this version of EP is intrinsically nonrelativistic, and applicable only in the context of Newtonian gravity since already in GR the source of gravity becomes the full stress-energy tensor of matter fields, rather than just the total mass. Finally, this principle obviously fails when applied to photons, as demonstrated by the gravitational bending of light.
- *Universality of free fall.* Going back all the way to Galileo, this statement claims that the interaction between matter and gravity does not depend on any intrinsic property of matter itself, such as its mass, angular momentum, chemical composition, temperature, or any other property, leading to the idea that gravity couples universally (i.e., in the same way) to all matter. Formulated from experimental observations by Galileo, its validity is related to the quality of experiments used to verify it. As we shall see below,

in a precise enough setting, one can experimentally observe direct coupling between the angular momentum of a body and spacetime curvature [32–46], invalidating the statement.

- *Local equality between gravity and inertia.* Often called Einstein's equivalence principle, the statement claims that a local and suitably isolated observer cannot distinguish between accelerating and being at rest in a uniform gravitational field. While this statement is much closer in spirit to the modern formulation of EP, it obscures the crucial aspect of the principle — coupling of matter to gravity. Namely, in this formulation, it is merely implicit that the only way an observer can *attempt to distinguish* gravity from inertia is by making local experiments using some form of *matter*, i.e., studying the equations of motion of matter in the two situations and trying to distinguish them by observing whether or not matter behaves differently. Moreover, the statement is often discussed in the context of mechanics, arguing that any given particle does not distinguish between gravity and inertia. This has two main pitfalls—first, the reliance on particles is very misleading (as we will discuss below in much more detail), and second, it implicitly suggests that gravity and inertia are the same phenomenon, which is completely false. Namely, inertia can be understood as a specific form of gravity, but a general gravitational field cannot be simulated by inertia, since inertia cannot account for tidal effects of inhomogeneous configurations of gravity.
- *Weak equivalence principle.* Stating that the equations of motion of particles do not depend on spacetime curvature, or equivalently, that the motion of a free particle is always a geodesic trajectory in spacetime, WEP is in fact an application of modern EP to mechanical point-like particles (i.e., test particles). One can argue that, as far as the notion of a point-like particle is a well-defined concept in physics, WEP is a good principle. Nevertheless, as we will discuss below in detail, the notion of a point-like particle is an idealisation that does not actually have any counterpart in reality, in either classical or quantum physics. Regarding a realistic particle (with nonzero size), WEP *never holds*, due to the explicit effect of gravitational tidal forces across the particle's size. In this sense, WEP can be considered at best an *approximate* principle, which can be assumed to hold only in situations where particle size can be approximated to zero.
- *Strong equivalence principle.* This version of the principle states that the equations of motion of all fundamental fields in nature do not depend on spacetime curvature (see [55], Section 16.2, page 387). To the best of our knowledge so far, fields are indeed the most fundamental building blocks in modern physics (such as SM), while the strength of the gravitational field is indeed described by spacetime curvature (as in GR). In this sense, the statement of SEP is actually an instance of EP applied to field theory, and as such equivalent to the modern statement of EP. So far, all our knowledge of natural phenomena is consistent with the validity of SEP.

As can be seen from the above review, various formulations of EP are both mutually inequivalent and have different domains of applicability. Specifically, only SEP holds universally, while all other flavours of EP hold only approximately. In the remainder of the paper, we focus on the study of WEP since recently it gained a lot of attention in the literature [20,27–29,31], primarily in the context of its generalisation to a "quantum WEP", and in the context of a related question of particle motion in a quantum superposition of different gravitational configurations, the latter being a scenario that naturally arises in QG. Since WEP is stated in terms of a test particle and its trajectory, in order to try and generalise it to the scope of QG one should first analyse these two notions in classical and quantum mechanics and field theory in more detail.

3. The Notion of Trajectory in Classical and Quantum Mechanics

A trajectory of a physical system in three-dimensional space is a set of points that form a line, usually parameterised by time. More formally, a trajectory is a set $\{(x(t), y(t), z(t)) \in$

$\mathbb{R}^3 | t \in [t_i, t_f] \subset \mathbb{R} \wedge t_i < t_f\}$, given by three smooth functions $x, y, z : \mathbb{R} \mapsto \mathbb{R}$. Depending on the nature of the system, the choice of points that form its trajectory may vary.

In classical mechanics, one often considers an ideal "point-like particle" localised in one spatial point $(x(t), y(t), z(t))$ at each moment of time t, in which case the choice of the points forming the system's trajectory is obvious. In the case of systems continuously spread over certain volumes ("rigid bodies", or "objects") or composite systems consisting of several point-like particles or bodies, it is natural to consider their centres of mass as points that form the trajectory. While this definition is natural, widely accepted, and formally applicable to any classical mechanical system, there are cases in which the very notion of a trajectory loses its intuitive, as well as useful, meaning.

Consider for example an electrical dipole, i.e., a system of two point-like particles with equal masses and opposite electrical charges, separated by the distance $\ell(t)$. As long as this distance stays "small" and does not vary significantly with time, the notion of a trajectory of a dipole, defined as the set of centres of mass of the two particles, does meet our intuition, and can be useful. Informally, if the trajectories of each of the two particles are "close" to each other, they can be approximated, and consequently represented, by the trajectory of the system's centre of mass. However, if the separate trajectories of the two particles diverge, one going to the "left", and another to the "right", one could hardy talk of a trajectory of such a composite system, although the set of locations of its centres of mass is still well defined. In fact, the dipole itself ceases to make physical sense when the distance between its constituents is large.

Moving to the realm of quantum mechanics, due to the superposition principle, even the ideal point-like particles do not have a well-defined position, which is further quantified by the famous Heisenberg uncertainty relations. Thus, the trajectory of point-like particles (and any system that in a given regime can be approximated to be point-like) is defined as a set of expectation values of the position operator. Like in the case of composite classical systems, here as well the definition of a trajectory of a point-like particle is mathematically always well defined, yet for a very similar reason is applicable only to certain cases. Namely, in order to give a useful meaning to the above definition of trajectory, the system considered must be *well localised*. Consider for example the double-slit experiment, in which the point-like particle is highly delocalised so that we say that *its trajectory is not well defined*, even though the set of the expectation values of the position operator is.

We see that, while in mechanics both the notions of a particle and its trajectory are rather straightforward and always well defined, the latter make sense only if our system is well localised in space (see for example [58], where the authors analyse the effects of wave-packet spreading to the notion of a trajectory).

4. The Notion of a Particle in Field Theory

While in classical mechanics a point-like particle is always well localised, we have seen that in the quantum case one must introduce an additional constraint in order for it to be considered localised—the particle should be represented by a wave-packet. The source for this requirement lies in the fact that quantum particles, although mechanical, are represented by a *wavefunction*. Thus, it is only to be expected that when moving to the realm of the field ontology, the notion of a particle becomes even more involved and technical.

In field theory, the fundamental concept is the *field*, rather than a particle. The notion of a particle is considered a derived concept, and in fact in QFT one can distinguish two vastly different phenomena that are called "particles".

The first notion of a particle is an elementary excitation of a free field. For example, the state

$$|\Psi\rangle = \hat{a}^\dagger(\vec{k})|0\rangle\,,$$

is called a *single particle state* of the field, or a *plane-wave-particle*. It has the following properties:

- It is an eigenstate of the *particle number operator* for the eigenvalue 1.

- It has a sharp value of the momentum $\vec{k}$, and corresponds to a completely delocalised plane wave configuration of the field.
- It has no centre of mass, and no concept of "position" in space since the "position operator" is not a well-defined concept for the field.
- States of this kind are said to describe *elementary particles*, understood as asymptotic free states of past and future infinity, in the context of the S-matrix for scattering processes. An example of a real scalar particle of this type would be the *Higgs particle*. For fields of other types (Dirac fields, vector fields, etc.) examples would be an *electron*, a *photon*, a *neutrino*, an asymptotically free *quark*, and so on. Essentially, all particles tabulated in the Standard Model of elementary particles are of this type.

Note that all the above notions are defined within the scope of free field theory, and do not carry over to interacting field theory. In other words, free field theory is a convenient idealisation, which does not really reflect realistic physics. One should therefore understand the concept of a plane-wave-particle in this sense, merely as a convenient mathematical approximation. Moreover, the particle number operator is not an invariant quantity, as demonstrated by the Unruh effect. We should also emphasise that in an interacting QFT, the proper way to understand the notion of a particle is as a localised wave-packet, interacting with its virtual particle cloud, which does have a position in space and whose momentum is defined through its group velocity. In this sense, the particle as a wave-packet could be better interpreted as a kink, discussed below.

The second notion of the particle in field theory is a bound state of fields, also called a *kink solution*. This requires an interacting theory since interactions are necessary to form bound states. This kind of configuration of fields has the following properties:

- It is not an eigenstate of the particle number operator, and the expectation value of this operator is typically different from 1.
- It is usually well localised in space, and does not have a sharp value of momentum.
- As long as the kink maintains a stable configuration (i.e., as long as it does not decay), one can in principle assign to it the concept of *size*, and as a consequence also the concepts of *centre of mass*, *position in space*, and *trajectory*. In this sense, a kink can play the role of a test particle.
- States of this kind are said to describe *composite particles*. Given an interacting theory such as the Standard Model, under certain circumstances quarks and gluons form bound states called a *proton* and a *neutron*. Moreover, protons and neutrons further form bound states called *atomic nuclei*, which together with electrons and photons form *atoms*, *molecules*, and so on.

For a kink, the notions of centre of mass, position in space and size are described only as classical concepts, i.e., as expectation values of certain field operators, such as the stress-energy tensor. Moreover, given the nonzero size of the kink, its centre of mass and position are not uniquely defined, even classically, since in relativity different observers would assign different points as the centre of mass.

Given the two notions of particles in QFT, one can describe two different corresponding notions of WEP. In principle, one first needs to apply SEP in order to couple the matter fields to gravity, at the fundamental level. Assuming this is completed, the motions of both the plane-wave-particles and kink particles can be derived from the combined set of Einstein's equations and matter field equations, without any appeal to any notion of WEP. In this sense, once the trajectory of the particle in the background gravitational field has been determined from the field equations, one can verify *as a theorem* whether the particle satisfies WEP or not.

Specifically, in the case of a matter field coupled to general relativity such that it locally resembles a plane wave, one can apply the WKB approximation to demonstrate that the wave 4-vector $k^\mu(x)$, orthogonal to the wavefront at its every point $x \in \mathbb{R}^4$, will satisfy a geodesic equation,

$$k^\mu(x)\nabla_\mu k^\lambda(x) = 0\,. \tag{1}$$

However, given that the plane-wave-particle is completely delocalised in space, the fact that the wave 4-vector satisfies the geodesic equation could hardly be interpreted as "the particle following a geodesic trajectory", and thus obeying WEP. Indeed, identifying the vector field orthogonal to the wavefront to the notion of "particle's trajectory" is at best an abuse of terminology.

Next, in the case of the kink particle coupled to general relativity, one assumes the configuration of the background gravitational field is such that the particle maintains its structure and that its size can be completely neglected. One can then apply the procedure given in [26,32–46] to demonstrate that the 4-vector $u^\mu(\tau)$, tangent to the kink's world line (i.e., its trajectory), will satisfy a geodesic equation ($\tau \in \mathbb{R}$ represents kink's proper time),

$$u^\mu(\tau)\nabla_\mu u^\lambda(\tau) = 0\,. \tag{2}$$

Thus, one concludes that the kink obeys WEP as a *theorem* in field theory, without the necessity to actually postulate it.

Note the crucial difference between Equations (1) and (2)—while the former features 4-dimensional variable x, the latter is given in terms of only 1-dimensional proper time τ. This reflects the fact that the plane-wave-particle is a highly delocalised object, with no well-defined position and trajectory, while the kink is a highly localised object, with a well-defined position and trajectory. As a consequence, WEP can be formulated only for the kink, and not for the plane-wave particle.

In the case of the kink, it is also important to emphasise that the zero-size approximation of the kink is crucial. Namely, without this assumption, the particle will feel the tidal forces of gravity across its size, effectively coupling its angular momentum $J^{\mu\nu}(\tau)$ to the curvature of the background gravitational field [32–46] (see also [59] for a more refined analysis of tidal effects). This will give rise to an equation of motion for the kink of the form

$$u^\mu(\tau)\nabla_\mu u^\lambda(\tau) = R^\lambda{}_{\mu\rho\sigma} u^\mu(\tau) J^{\rho\sigma}(\tau)\,, \tag{3}$$

which features explicit coupling to curvature (absent from (2)) and thus fails to obey WEP. In this sense, for realistic kink solutions WEP is *always violated*, and can be considered to hold only as an approximation when the size of the particle can be completely neglected compared to the radius of curvature of the background gravitational field. If in addition the kink has negligible total energy, it can be used as a point-like test particle.

In the above discussion, while matter fields are described as quantum, using QFT, the background gravitational field is considered to be completely classical. It should therefore not be surprising that WEP may fail to hold if one allows the gravitational field to be quantum, such as matter fields, and one needs to revisit all steps of the above analysis from the perspective of QG. In fact, the case of the kink particle has been studied in precisely this scenario [26], and it has been shown that if the background gravitational field is in a specific type of quantum superposition of different configurations, the kink will fail to obey WEP even in the zero size approximation. Simply put, the equation of motion for the kink will contain extra terms due to the interference effects between superposed configurations of gravity, giving rise to an effective force that pushes the kink off the geodesic trajectory. Moreover, of course, similar to the case of classical gravity, the resulting conclusion is a *theorem*, which follows from the fundamental field equations of the theory. One of the assumptions of that theorem is that the field equations allow for kink solutions in the first place. Namely, it is entirely possible that in quantum gravity particles cannot be localised at all, as opposed to the classical case where such an approximation can be feasible. If that is the case, then one cannot even formulate (i.e., generalise from classical theory) the notion of WEP in a quantum gravity setup. However, one can instead assume that kink solutions do exist, as was performed in [26], where a particular superposition of gravitational fields was considered, describing small quantum fluctuations around a dominant classical geometry. It was then argued that such superpositions are compatible with the approximation of a well-defined localised particle (see the discussion around Equations (2.2) and (3.15), as well as Section 3.4 of that paper). As it turns out, even in such cases the trajectory of the kink fails to obey WEP. Therefore, the generalisations of WEP and other approximate versions of EP are not the best candidates for analysing the properties of quantum gravity.

Moreover, the assumption of a well-defined notion of a particle in the QG framework can also be supported from the point of view of nonrelativistic limit. Namely, in [4,5] an experiment was proposed in which the effects of QG fluctuations are expected to be observable, by measuring the motion of nonrelativistic particles. Furthermore, an extension of this experiment was also suggested [60], which aims to determine the potential difference between gravitational and inertial masses of those particles in such a setup. In fact, the relation between the two types of masses in the nonrelativistic limit has also been previously analysed in [26], predicting their difference due to quantum fluctuations of geometry. In this sense, the notion of a kink should make sense even in the QG setup, at least in the nonrelativistic limit.

For the case of the plane-wave-particle travelling through the superposed background of two gravitational field configurations, the analysis of the equation of motion for the wave-vector field $k^{\mu}(x)$, in the sense of [26,32–46], has not been performed so far (to the best of our knowledge). However, in principle, one can expect a similar interference term to appear in the WKB analysis, and give rise to a non-geodesic equation for the wave 4-vector as well. In this sense, it is to be expected that generically even the wavefronts of such plane-wave-particles would fail to obey WEP.

5. Conclusions and Discussion

In this paper, we give an overview of the equivalence principle and its various flavours formulated historically, with a special emphasis on the weak equivalence principle. We performed a critical analysis of the notions of particle and trajectory in various frameworks of physics, showing that the notion of a point-like particle and its trajectory are not always well defined. This in turn suggests that WEP might not be the best starting point for generalisation to QG, as we argue in more detail below.

As discussed in Section 4, in [26] it was shown that if superpositions of states of gravity and matter are allowed, WEP can be violated. It is important to note that the cases considered in [26] feature a specific type of superposition of three groups of states: the first consists of a single so-called dominant state—a classical state whose expectation values of the metric and the stress-energy tensors satisfy Einstein field equations; the second consists of states similar to the dominant one, with arbitrary coefficients; and the third consists of states quasi-orthogonal to the dominant one, but with negligible coefficients. Only then one may talk of a (well-localised) trajectory of the test particle in the overall superposed state and consequently about the straightforward generalisation of the classical WEP to the realm of QG. Considering that for the dominant state, being classical, the trajectory of the test particle follows the corresponding geodesic, we see that in the superposed state its trajectory would *deviate from the geodesic of the dominant state*, thus violating WEP. Note that, as discussed in Section 4, this deviation, in addition to classically weighted trajectories of the individual branches, also features purely quantum (i.e., off-diagonal) interference terms.

On the other hand, a number of recent studies propose generalisations of WEP to QG framework, arguing that it remains satisfied in such scenarios, a result *seemingly* at odds with [26]. For example, in [29–31], the authors consider superpositions of an arbitrary number of classical quasi-orthogonal states with arbitrary coefficients, arguing that since WEP is valid in each classical branch, it is valid in its superposition as well. If taken as a *definition* of what it means that a certain principle is satisfied in a superposition of different quantum states, then the above statement is manifestly true. As such, being a definition, it tells little about physics—it merely rephrases one statement ("principle A is separately satisfied in all branches of a superposition") with another, simpler ("principle A is satisfied in a superposition"). Namely, note that in [29,30], such a generalised version of EP plays no functional role in the analyses conducted in those papers. What does play a functional role is the statement of one version of classical EP (specifically, local equality between gravity and inertia) applied to each particular state in a superposition. All physically relevant (and otherwise interesting) conclusions of the two papers could be equally obtained without ever talking about the generalised EP. In addition, in [31] EP itself is not even the main focus of the paper, and its generalisation is just introduced in analogy to the analysis of the conservation laws, which is itself an interesting topic. On the other hand, in the case of weakly superposed gravitational fields, such as in proposed experiments [4,5], the violation of the equality of inertial and gravitational masses is to be expected [26,60]. Moreover, following the spirit of the above definition, one could be misled to conclude that the notions of the particle's position and trajectory are always well-defined, as long as they are defined in each (quasi-classical) branch of the superposition.

An alternative approach to the generalisation of EP to the quantum domain was proposed in [16,20,27,28]. In those works, the authors discuss the coupling of a spatially delocalised wave-particle to gravity, with the aim of generalising such a scenario to QG. To that end, they prove a theorem which essentially states that for such a delocalised wave-particle, even when it is entangled with the gravitational field, one can always find a quantum reference frame transformation, such that in the vicinity of a given spacetime point one has a locally inertial coordinate system. The theorem employs the novel techniques of quantum reference frames (QRF) to generalise to the quantum domain the well-known result from differential geometry, that in the infinitesimal neighbourhood of any spacetime point one can always choose a locally inertial coordinate system.

The authors then employ the theorem to generalise one flavour of EP to the quantum domain. Specifically, even if the wave-particle is entangled with the gravitational field, one can use the appropriate QRF transformation to switch to a locally inertial coordinate system, and then in that system "all the (nongravitational) laws of physics must take on their familiar non-relativistic form". Here, to the best of our understanding, the phrase "nongravitational laws of physics" refers to the equations of motion for a quantum-mechanical wave-particle, while "non-relativistic form" means that these equations of motion take the same form as in special-relativistic context.

Our understanding is that the above wave-particle generalisation of EP lies somewhere "in between" mechanics and field theory, i.e., it is in a sense stronger than WEP, which discusses particles, but weaker than SEP, which discusses full-blown matter fields. Since it refers to wave-particles rather than kinks, our analysis of WEP and its reliance on the particle trajectory does not apply to this version of EP.

The methodology in [16,20,27,28] is that one should try to generalise even approximate flavours of EP, as a stopgap result in a bigger research programme, in the hope that they may still shed some light on QG. This is of course a legitimate methodology, and from that point of view these kinds of generalisations of EP to the quantum domain represent interesting results. Nevertheless, we also believe it would be preferable to formulate a generalisation of SEP, and in a way which does not appeal to reference frames at all, since that would be closer to the essence of the statement of EP, as discussed in Section 2.

To conclude, our analysis suggests that, instead of trying to generalise various approximate formulations of EP, one should rather talk of operationally verifiable statements regarding the (in)equality of gravitational and inertial masses, possible deviation from the geodesic motion of test particles, the universality of free fall, etc., and study other principles and their possible generalisations to QG, such as SEP (see Section 4.2 in [26]), background independence, quantum nonlocality, and so on.

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Appendix A

Here, we provide a detailed example of the two applications of the EP. First, we discuss the gravitational EP and apply it to a real scalar field, giving all mathematical details and discussing various related aspects such as locality, symmetry localisation, and so on. Then, we turn to the application of the gauge field generalisation of EP, using electrodynamics as an example. We describe how one can couple matter to an EM field, mimicking the previous gravitational example, and emphasize the analogy between the gravitational and EM case at each step. Note also that the non-Abelian gauge fields can be studied in exactly the same way. Finally, we discuss the case of test particles, and the violation of the WEP in both gravitational and electromagnetic cases.

Throughout this section, we assume that the Minkowski metric $\eta_{\mu\nu}$ has signature $(-,+,+,+)$.

Appendix A.1. The Gravitational Case

Let us begin with an example of a real scalar field in Minkowski spacetime, and apply the equivalence principle by coupling it to gravity. The equation of motion in this case is the ordinary Klein–Gordon equation,

$$\left(\eta^{\mu\nu}\partial_\mu\partial_\nu - m^2\right)\phi(x) = 0\,. \tag{A1}$$

As it stands, it describes the free scalar field in Minkowski spacetime, in an inertial coordinate system. In order to couple it to gravity (in the framework of GR), we first rewrite this equation into an arbitrary curvilinear coordinate system, as

$$\left(\tilde{g}^{\mu\nu}\tilde{\nabla}_\mu\tilde{\nabla}_\nu - m^2\right)\phi(\tilde{x}) = 0\,. \tag{A2}$$

Here the covariant derivative $\tilde{\nabla}_\mu$ is defined in terms of the Levi-Civita connection,

$$\tilde{\Gamma}^\lambda{}_{\mu\nu} = \frac{1}{2}\tilde{g}^{\lambda\sigma}\left(\partial_\mu\tilde{g}_{\nu\sigma} + \partial_\nu\tilde{g}_{\mu\sigma} - \partial_\sigma\tilde{g}_{\mu\nu}\right), \tag{A3}$$

which is in turn defined in terms of the curvilinear Minkowski metric $\tilde{g}_{\mu\nu}$. Note that the tilde symbol denotes the fact that this metric has been obtained by a coordinate transformation $\tilde{x}^\mu = \tilde{x}^\mu(x)$ from the Minkowski metric in an inertial coordinate system, $\eta_{\mu\nu}$,

$$\tilde{g}_{\mu\nu} = \frac{\partial x^\rho}{\partial\tilde{x}^\mu}\frac{\partial x^\sigma}{\partial\tilde{x}^\nu}\eta_{\rho\sigma}\,, \tag{A4}$$

and, therefore, if one were to evaluate the Riemann curvature tensor using $\tilde{g}_{\mu\nu}$ and $\tilde{\Gamma}^{\lambda}{}_{\mu\nu}$, according to the equation

$$R^{\lambda}{}_{\rho\mu\nu} = \partial_{\mu}\tilde{\Gamma}^{\lambda}{}_{\rho\nu} - \partial_{\nu}\tilde{\Gamma}^{\lambda}{}_{\rho\mu} + \tilde{\Gamma}^{\lambda}{}_{\sigma\mu}\tilde{\Gamma}^{\sigma}{}_{\rho\nu} - \tilde{\Gamma}^{\lambda}{}_{\sigma\nu}\tilde{\Gamma}^{\sigma}{}_{\rho\mu}\,, \tag{A5}$$

one would obtain that $R^{\lambda}{}_{\mu\nu\rho} = 0$ at every point in spacetime since transforming into a different coordinate system cannot induce the curvature of spacetime.

Now one can apply EP (in this example specifically SEP) in order to couple the scalar field to gravity. The statement of SEP is that, in the presence of a gravitational field (i.e., in curved spacetime), the equation of motion for the scalar field should locally retain the same form as in the absence of the gravitational field (i.e., in flat spacetime). Since Equation (A2) depends only on the field at a given spacetime point and its first and second derivatives at the same point, the equation is in fact local—it is defined within an infinitesimal neighbourhood of a single point. Given this, EP states that the corresponding equation of motion in the presence of gravity should have precisely the same form:

$$\left(g^{\mu\nu}\nabla_{\mu}\nabla_{\nu} - m^2\right)\phi(x) = 0\,. \tag{A6}$$

The absence of the tilde now denotes the fact that the covariant derivative ∇_{μ} is defined in terms of a generic Levi-Civita connection $\Gamma^{\lambda}{}_{\mu\nu}$ which is in turn defined in terms of a generic metric $g_{\mu\nu}$, which does not necessarily satisfy (A4). In other words, EP postulates that the Equation (A6) now holds even in curved spacetime since for a generic metric and connection, the Riemann curvature tensor need not be equal to zero everywhere. The interaction between the scalar field and gravity, as postulated by EP and implemented in Equation (A6), is also known in the literature as the *minimal coupling* prescription [61].

In order to convince oneself that the preparation step of transforming (A1) to (A2) is trivial in the sense that it does not introduce any substantial modification of (A1), one can additionally demonstrate that (A6) is in fact locally equivalent to (A1) as well. Namely, according to a theorem in differential geometry (see for example the end of Chapter 85 in [62]), at any specific spacetime point x_0 one can choose the locally inertial coordinate system, in which the generic metric $g_{\mu\nu}$, the corresponding connection $\Gamma^{\lambda}{}_{\mu\nu}$ and consequently also the covariant derivative ∇_{μ} take their usual Minkowski values,

$$g_{\mu\nu}(x_0) = \eta_{\mu\nu}\,, \qquad \Gamma^{\lambda}{}_{\mu\nu}(x_0) = 0\,, \qquad \nabla_{\mu}\Big|_{x=x_0} = \partial_{\mu}\,, \tag{A7}$$

so that in the infinitesimal neighbourhood of the point x_0 Equation (A6) obtains the form precisely equal to (A1).

However, note that when *integrating* (A6), one must take into account that spacetime is curved since integration is a nonlocal operation, and the locally inertial coordinate system cannot eliminate spacetime curvature. Therefore, the *solutions* of (A6) will in general be *different* from solutions of (A1), indicating the physical interaction of the scalar field with gravity, despite the fact that the form of the equation of motion is identical in both cases.

Another thing that should be emphasised is that EP itself is not a mathematical theorem, but rather a principle with physical content, since it can be either satisfied or violated. Specifically, we could have prescribed a different coupling of the scalar field to gravity, such that in curved spacetime its equation of motion takes for example the form

$$\left(g^{\mu\nu}\nabla_{\mu}\nabla_{\nu} - m^2 + R^2 + K^2\right)\phi(x) = 0\,, \tag{A8}$$

where $R \equiv R^{\mu\nu}{}_{\mu\nu}$ and $K \equiv R^{\mu\nu\rho\sigma}R_{\mu\nu\rho\sigma}$ are the curvature scalar and Kretschmann invariant, respectively. This equation is not equivalent to (A2) and there is no coordinate system in which it can take the form (A1) since R and K are invariants. In this sense, (A8) is an example of a scalar field coupled to gravity such that EP is violated. This type of interaction between matter and gravity is also known in the literature as *non-minimal coupling* [61].

Finally, we should note that the transformation from (A1) to (A2) amounts to what is also known in the literature as *symmetry localisation* [61]. In particular, one can verify that (A1) remains invariant with respect to the group $\mathbb{R}^4$ of global translations,

$$x^\mu \to \tilde{x}^\mu = x^\mu + \zeta^\mu \,, \qquad (\zeta \in \mathbb{R}^4) \,, \tag{A9}$$

while (A2) remains invariant with respect to the group $Diff(\mathbb{R}^4)$ of spacetime diffeomorphisms, obtained by localisation of the translational symmetry group,

$$x^\mu \to \tilde{x}^\mu = x^\mu + \zeta^\mu(x) \equiv \tilde{x}^\mu(x) \,, \tag{A10}$$

which represent general curvilinear coordinate transformations, used in (A4). One can explicitly verify that all three Equations (A2), (A6) and (A8) remain invariant with respect to local translations (A10) while describing no coupling to gravity, coupling to gravity that satisfies EP, and coupling to gravity that violates EP, respectively. In this sense, contrary to a common misconception (often stated in the literature) that symmetry localisation gives rise to interactions, one can say that the process of symmetry localisation *does not* introduce nor prescribe interactions in any way whatsoever. In particular, a direct counterexample is the Equation (A4), which manifestly *does* obey local translational symmetry, while it *does not* give rise to any interaction whatsoever (see below for the analogous counterexample in electrodynamics).

Appendix A.2. The Electromagnetic Case

Let us begin with an example of a Dirac field in Minkowski spacetime, and apply the generalised equivalence principle by coupling it to the EM field. The equation of motion in this case is the ordinary Dirac equation,

$$(i\gamma^\mu \partial_\mu - m)\psi(x) = 0 \,, \tag{A11}$$

where γ^μ are standard Dirac gamma matrices, satisfying the anticommutator identity of the Clifford algebra $\{\gamma^\mu, \gamma^\nu\} = -2\eta^{\mu\nu}$. As it stands, Equation (A11) describes the free Dirac field, not coupled to an EM field in any way. Note that it is invariant with respect to global $U(1)$ transformations, defined as

$$\psi \to \psi' = e^{-i\lambda}\psi \,, \qquad e^{-i\lambda} \in U(1) \,, \qquad \lambda \in \mathbb{R} \,. \tag{A12}$$

In order to couple it to standard Maxwell electrodynamics, we first rewrite this equation into a form which is invariant with respect to local $U(1)$ transformations,

$$\psi \to \psi' = e^{-i\lambda(x)}\psi \,, \qquad \partial_\mu \to \tilde{\mathcal{D}}_\mu = \partial_\mu + i\partial_\mu \lambda(x) \,, \tag{A13}$$

so that the equation takes the form

$$(i\gamma^\mu \tilde{\mathcal{D}}_\mu - m)\psi(x) = 0 \,, \tag{A14}$$

Note that here, $\tilde{\mathcal{D}}$ denotes the covariant derivative with respect to the "pure gauge" connection

$$\tilde{A}_\mu \equiv \partial_\mu \lambda(x) \,, \tag{A15}$$

where $\lambda(x)$ denotes the arbitrary gauge function. Moreover, note that (A11) is analogous to (A1), (A14) is analogous to (A2), while the global and local $U(1)$ gauge transformations (A12) and (A13) are EM analogues of the global and local spacetime translations (A9) and (A10) from the gravitational case. Finally, note that if one were to evaluate the electromagnetic Faraday field strength tensor using $\tilde{A}_\mu$ from (A15), according to the equation

$$F_{\mu\nu} = \partial_\mu \tilde{A}_\nu - \partial_\nu \tilde{A}_\mu \,, \tag{A16}$$

one would obtain that $F_{\mu\nu} = 0$ at every point in spacetime since the potential that is a pure gauge cannot induce an EM field. Here (A16) is analogous to (A5).

Once the Dirac equation in the form (A14) is in hand, one can apply the electromagnetic generalisation of EP in order to couple the Dirac field to an EM field. The statement of EP, in this case, is that in the presence of an EM field, the equation of motion for the Dirac field should locally retain the same form as in the absence of the EM field. Since Equation (A14) depends only on the field at a given spacetime point and its first derivatives at the same point, it is therefore defined within an infinitesimal neighbourhood of a single point—in other words, it is local. Given this, electromagnetic EP states that the corresponding equation of motion in the presence of EM field should have precisely the same form (the analogue of (A6)):

$$(i\gamma^\mu \mathcal{D}_\mu - m)\psi(x) = 0\,. \tag{A17}$$

The absence of the tilde now denotes the fact that the covariant derivative $\mathcal{D}_\mu \equiv \partial_\mu + iA_\mu$ is defined in terms of a generic $U(1)$ connection A_μ which does not necessarily satisfy (A15), but does obey the usual gauge transformation rule,

$$A_\mu \to A'_\mu = A_\mu + \partial_\mu \lambda(x)\,. \tag{A18}$$

In other words, electromagnetic EP postulates that the Equation (A17) holds even in the presence of an EM field since for a generic connection A_μ the Faraday tensor may not be equal to zero everywhere. The interaction between the Dirac field and the EM field as postulated by the electromagnetic EP and implemented in Equation (A17) is again known in the literature as the *minimal coupling* prescription [61,63].

If one wishes to convince oneself that the preparation step of transforming (A11) to (A14) is trivial in the sense that it does not introduce any substantial modification of (A11), one can additionally demonstrate that (A17) is in fact locally equivalent to (A11). To do this, at any specific spacetime point x_0 one can choose the following $U(1)$ gauge,

$$\lambda(x) = -A_\mu(x_0)x^\mu\,, \tag{A19}$$

so that, according to (A18)

$$A'_\mu(x) = A_\mu(x) - \partial_\mu(A_\nu(x_0)x^\nu) \qquad \Rightarrow \qquad A'_\mu(x_0) = 0\,, \qquad \mathcal{D}_\mu\Big|_{x=x_0} = \partial_\mu\,. \tag{A20}$$

This choice of gauge is the EM analogue of the choice of a locally inertial coordinate system (A7). Substituting this into the primed version of (A17) and evaluating the whole equation at $x = x_0$, it reduces precisely to the form (A11) in the infinitesimal neighbourhood at that point, despite the presence of nonzero EM field.

Again note that when *integrating* (A17), one must take into account that the EM field is nonzero since integration is a nonlocal operation, and the choice of gauge (A19) eliminates the EM potential from (A17) only at the point x_0, while the Faraday tensor is gauge invariant. Therefore, the *solutions* of (A17) will in general be *different* from solutions of (A11), indicating the physical interaction of the Dirac field with EM field, despite the fact that the form of the equation of motion for the Dirac field is identical in both cases.

As in the case of gravity, we should emphasise that the electromagnetic EP is not a mathematical theorem, but rather a principle with physical content, since it can be either satisfied of violated. Specifically, we could have prescribed a different coupling of the Dirac field to electrodynamics, such that in the presence of an EM field its equation of motion takes for example the form (analogue of (A8))

$$(i\gamma^\mu \mathcal{D}_\mu - m + I_1 + I_2)\psi(x) = 0\,, \tag{A21}$$

where $I_1 \equiv F^{\mu\nu}F_{\mu\nu}$ and $I_2 \equiv \varepsilon^{\mu\nu\rho\sigma}F_{\mu\nu}F_{\rho\sigma}$ are the two fundamental invariants of the Faraday tensor. This equation is not equivalent to (A14), and there exists no local $U(1)$ gauge in which it could take the form (A11), since I_1 and I_2 are invariants. In this sense, (A21) is an example of a Dirac field coupled to the EM field such that the electromagnetic EP is violated. This is also known in the literature as *non-minimal coupling* [61,63].

Finally, we should also note that the transformation from (A11) to (A14) amounts to what is also known in the literature as *symmetry localisation* [61,63]. Specifically, one can explicitly verify that all three Equations (A14), (A17) and (A21) remain invariant with respect to local $U(1)$ gauge transformations, while describing no coupling to an EM field, coupling to an EM field that satisfies the electromagnetic EP, and coupling to an EM field that violates electromagnetic EP, respectively. In this sense, one can again say that the process of symmetry localisation *does not* introduce nor prescribe interactions in any way whatsoever. In the case of electrodynamics and other gauge theories, this is quite often misrepresented in literature—the step of symmetry localisation is silently joined together with the step of applying the electromagnetic version of EP; thus, in the end, giving rise to an interacting theory, and the resulting presence of the interaction is then mistakenly attributed to the localisation of symmetry, rather than to the application of EP. Similar to the gravitational case above, the equation of motion (A14) is an explicit counterexample to such an attribution, since it *does* have local $U(1)$ symmetry, but *does not* have any interaction with an EM field.

Appendix A.3. The Test Particle Case

The last topic we should address is the context in which the statement of electromagnetic EP is compatible with the existence of the Lorentz force law, acting on charged test particles. Namely, one often distinguishes the motion of a test particle in a gravitational field from a motion of a test particle in an EM field, by comparing the geodesic Equation (2)

$$u^{\mu}(\tau)\nabla_{\mu}u^{\lambda}(\tau) = 0\,, \tag{A22}$$

where u^{μ} is the 4-velocity of the test particle, with the Lorentz force equation

$$u^{\mu}(\tau)\nabla_{\mu}u^{\lambda}(\tau) = \frac{q}{m}F^{\lambda\rho}\,u_{\rho}(\tau)\,, \tag{A23}$$

where q/m is the charge-to-mass ratio of a test particle moving in an external EM field, described by the Faraday tensor $F_{\mu\nu}$. A typical conclusion one draws from this comparison is that the interaction with the EM field gives rise to a "real force", while the interaction with the gravitational field does not.

However, it is highly misleading to compare (A22) to (A23) in the first place. Namely, as we have discussed in detail in Section 4, in field theory the notion of a particle can be defined only approximately, and this applies equally for electrodynamics as well as for gravity. Specifically, given the example discussed above, of a Dirac field coupled to an EM field via Equation (A17), we have seen that in the infinitesimal neighbourhood of a given point x_0 one can completely gauge away any presence of the coupling to EM field from (A17). In this sense, the notion of a test particle that satisfies (A23) cannot be identified with an idealised point-particle, that has exactly zero size. Instead, the realistic test particle is a wave-packet configuration of a Dirac field (a kink), and as such has a small but nonzero size. As it evolves, the different parts of the wave-packet are subject to interaction with the EM potential A_{μ} at *different* points of spacetime, giving rise to an effective non-minimal coupling with the Faraday tensor $F_{\mu\nu}$. This is completely analogous to the case of a test particle with small but nonzero size interacting with spacetime curvature due to tidal forces—both effects are equally nonlocal since both kinks have nonzero size. On the other hand, a test particle that satisfies (A22) represents an idealised point-particle (a leading order approximation in the multipole expansion of the matter field), i.e., a kink which thus has precisely zero size.

In this sense, the Lorentz force Equation (A23) rather ought to be compared with the Papapetrou Equation (3),

$$u^{\mu}(\tau)\nabla_{\mu}u^{\lambda}(\tau) = R^{\lambda}{}_{\mu\rho\sigma}\,u^{\mu}(\tau)J^{\rho\sigma}(\tau)\,. \tag{A24}$$

Indeed, one can see quite a reasonable analogy between (A23) and (A24). There are of course small technical differences due to the precise nature of the coupling to various moments of the kink, but nevertheless, the two equations are strikingly similar. Given this, while one can still draw the conclusion that the interaction of a kink with the EM field gives rise to a "real force", one can draw precisely the same conclusion for the interaction of a kink with the gravitational field. There is no distinction between gravity and the other gauge interactions at this level—all four interactions in nature (strong, weak, electromagnetic and gravitational) are equally "real". In addition, all four interactions satisfy EP at the fundamental field theory level (i.e., in the sense of strong generalised EP), while at the level of mechanics, a corresponding weak generalised EP is manifestly violated in all four cases.

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Standard Model and 4-groups

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Abstract – We show that a categorical generalization of the the Poincaré symmetry which is based on the n-crossed modules becomes natural and simple when $n = 3$ and that the corresponding 3-form and 4-form gauge fields have to be a Dirac spinor and a Lorentz scalar, respectively. Hence by using a Poincaré 4-group we naturally incorporate fermionic and scalar matter into the corresponding 4-connection. The internal symmetries can be included into the 4-group structure by using a 3-crossed module based on the $SL(2,\mathbb{C})\times K$ group, so that for $K = U(1)\times SU(2)\times SU(3)$ we can include the Standard Model into this categorification scheme.

Introduction. – The central mathematical idea for the construction of the Standard Model (SM) was the concept of a Lie group and the corresponding connection on the principal bundle, *i.e.*, the gauge symmetry. The SM group uniquely fixes the SM forces (the strong, the weak and the electro-magnetic force), while the matter content is not restricted by the SM group. Namely, the SM matter fields, *i.e.*, the scalars and the fermions, can be *a priori* in any representation of the SM group. The SM representation is determined from the experiments and it is given by

$$\rho_{SM} = \left(1,2,-\frac{1}{2}\right) \oplus \sum_{i=1}^{3} \left(3,2,\frac{1}{6}\right)_i \oplus \left(\bar{3},1,\frac{1}{3}\right)_i \oplus \left(\bar{3},1,-\frac{2}{3}\right)_i \oplus \left(1,2,-\frac{1}{2}\right)_i \oplus (1,1,1)_i \oplus (1,1,0)_i, \tag{1}$$

where (m,n,q) are the irreps of the SM group $SU(3)\times SU(2)\times U(1)$, see [1] for a mathematical review, and i denotes a generation.

The spacetime symmetry properties of the SM fields are determined by the universal cover of the Lorentz group $SL(2,\mathbb{C})$, while gravity, as the fourth fundamental force in Nature, can be understood via the gauge symmetry principle for the Poincaré group, *i.e.*, as the Cartan connection

$$(\omega^{ab}, e^a) = (\omega^{ab}{}_\mu \mathrm{d}x^\mu, e^a{}_\mu \mathrm{d}x^\mu), \tag{2}$$

where ω^{ab} and e^a are the spin connection and the tetrad 1-forms, $a,b = 1,2,3,4$ and $x^\mu \in (x,y,z,t)$ are the spacetime coordinates.

One then wonders if there is a mathematical structure in a 4-dimensional spacetime which can incorporate the matter fields with the gauge fields and explain why the matter fields appear as the scalar and the spinor representations of the universal cover of the Lorentz group, as well as why the representation ρ_{SM} appears. Note that the superstring theory is an example of such a structure, but it requires a 10-dimensional spacetime [2].

As far as the internal symmetry group is concerned, the first attempt to explain ρ_{SM} was via the grand unification (GUT), for a review see [3]. Although the fermionic part of one generation of ρ_{SM} neatly fits into the spinorial irrep of $SO(10)$, the GUT approach is problematic because of the appearance of many new gauge fields, *i.e.*, new forces, so that the problem of symmetry breaking is the central problem to solve. One can even incorporate the Lorentz group (more precisely, its universal cover) into the GUT group, so that the Cartan connection becomes a part of the

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GUT group connection, see [4]. However, this leads to an even larger GUT group so that the problem of symmetry breaking becomes even more difficult.

As far as the spacetime symmetry group is concerned, although the Poincaré gauge symmetry accommodates gravity and coupling of fermions, it does not restrict the $SL(2,\mathbb{C})$ representations for the matter fields, since the Cartan connection contains only the spin connection and the tetrads. In this letter we will propose a generalization of the local Poincaré symmetry, which will be given by the concept of a 4-group, defined as a 3-crossed module [5], so that one can include spinor and scalar fields as the components of the generalized connection associated to the Poincaré 4-group. Since n-groups are special categories which generalize the notion of symmetry, see [6], we also show that the SM group can be easily included into the 4-group structure.

General Relativity and categorical groups. – In [7] it was pointed out that General Relativity (GR) can be reformulated as a constrained $2BF$ theory for the Poincaré 2-group, which is defined as the crossed module

$$\mathbb{R}^4 \xrightarrow{\partial} SL(2,\mathbb{C}), \tag{3}$$

where the map ∂ is trivial ($\partial(\vec{v}) = 1_{SL(2,\mathbb{C})}$ for all $\vec{v} \in \mathbb{R}^4$) while $SL(2,\mathbb{C})$ acts on $\mathbb{R}^4$ as the vector representation. The Poincaré group then appears as the group of 2-morphisms of the 2-category which is equivalent to the crossed module (3).

The Einstein-Cartan (EC) action can be obtained by constraining the $2BF$ action,

$$S_2 = \int_{\mathcal{M}} (B^{ab} \wedge R_{ab} + e^a \wedge G_a), \tag{4}$$

where B^{ab} is a 2-form, e^a is a tetrad,

$$R_{ab} = \mathrm{d}\omega_{ab} + \omega_a{}^c \wedge \omega_{cb}, \quad G_a = \mathrm{d}\beta_a + \omega_a{}^b \wedge \beta_b, \tag{5}$$

are the components of the 2-curvature associated to the 2-connection

$$\mathcal{A}_2 = (\omega^{ab}, \beta^a) = (\omega^{ab}{}_\mu \, \mathrm{d}x^\mu, \beta^a{}_{\mu\nu} \, \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu), \tag{6}$$

and β is the connection 2-form. The 2-connection $\mathcal{A}_2$ represents a categorical generalization (categorification) of the spin-connection.

The constraint that transforms S_2 into the EC action is given by

$$B^{ab} = \epsilon^{abcd} e_c \wedge e_d, \tag{7}$$

where ϵ^{abcd} is the totally antisymmetric tensor for the Poincaré group [7]. The constraint (7) is also known as the simplicity constraint.

The Poincaré 2-group structure does not restrict the matter representations, and in [8] it was pointed out that a Poincaré 3-group defined as a 2-crossed module based on the following group complex,

$$\mathbb{C}^4 \xrightarrow{\partial'} \mathbb{R}^4 \xrightarrow{\partial} SL(2,\mathbb{C}), \tag{8}$$

where the maps ∂ and ∂' are trivial while $SL(2,\mathbb{C})$ acts as the vector and the Dirac representation on $\mathbb{R}^4$ and $\mathbb{C}^4$, naturally gives the Dirac equation for the corresponding spinor field.

Namely, one can associate the 3-connection,

$$\mathcal{A}_3 = (\omega^{ab}, \beta^a, \Gamma^\alpha) = (\omega^{ab}{}_\mu \, \mathrm{d}x^\mu, \beta^a{}_{\mu\nu} \, \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu, \Gamma^\alpha{}_{\mu\nu\rho} \, \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\rho), \tag{9}$$

to the 2-crossed module (8), where Γ is a spinorial 3-form. The corresponding $3BF$ action is then given by

$$S_3 = \int_{\mathcal{M}} (B^{ab} \wedge R_{ab} + e^a \wedge G_a + D_\alpha \wedge H^\alpha), \tag{10}$$

where D_α are 0-forms, while

$$H^\alpha = \mathrm{d}\Gamma^\alpha + \omega^\alpha{}_\beta \wedge \Gamma^\beta, \quad \omega^\alpha{}_\beta = (\gamma_a)^\alpha{}_\delta (\gamma_b)^\delta{}_\beta \, \omega^{ab} \tag{11}$$

is the curvature 4-form for Γ, where γ_a are the gamma matrices.

The action S_3 can be converted into the EC action coupled to a Dirac fermion ψ^α by using the constraints

$$\Gamma^\alpha = \epsilon_{abcd} \, e^a \wedge e^b \wedge e^c \, (\gamma^d)^\alpha{}_\beta \psi^\beta, \quad D_\alpha = \psi_\alpha, \tag{12}$$

together with the simplicity constraint (7).

In order to obtain the complete EC Dirac action, one also has to add the spin torsion and the mass term to S_3,

$$S_{Tm} = \int_{\mathcal{M}} \epsilon_{abcd} \, e^a \wedge e^b \wedge \beta^c \, \bar{\psi}\gamma^d\psi + \int_{\mathcal{M}} |e| \, m\bar{\psi}\psi \, \mathrm{d}^4x, \tag{13}$$

where $|e| = |\det(e^a{}_\mu)|$.

However, if we want to associate some other $SL(2,\mathbb{C})$ representation to the 3-form Γ, then the task of obtaining the corresponding matter-field equation of motion becomes non-trivial, since it is not easy to find the constraints for the corresponding $3BF$ action. For example, in the case of a real scalar field ϕ, one has a 2-crossed module

$$\mathbb{R} \xrightarrow{\partial'} \mathbb{R}^4 \xrightarrow{\partial} SL(2,\mathbb{C}), \tag{14}$$

and the constraints are given by

$$\begin{aligned} &D = \phi, \qquad \Gamma = h_{abc} \, e^a \wedge e^b \wedge e^c, \\ &h_{abc}\epsilon^{cdef} e_d \wedge e_e \wedge e_f = e_a \wedge e_b \wedge \mathrm{d}\phi, \end{aligned} \tag{15}$$

plus the simplicity constraint [8]. Since the Standard Model features the Higgs boson, it is important to be able to accommodate scalar fields in the formalism.

The last two constraints in (15) are not easy to guess, so that one wonders: is it possible to resolve this difficulty by some higher categorical group? This can be done if we use a 4-group, which can be defined as a 3-crossed module [5].

Let us consider the following 3-crossed module (3CM):

$$\mathbb{R} \xrightarrow{\partial''} \mathbb{C}^4 \xrightarrow{\partial'} \mathbb{R}^4 \xrightarrow{\partial} SL(2,\mathbb{C}), \tag{16}$$

where $SL(2,\mathbb{C})$ acts on $\mathbb{R}^4$, $\mathbb{C}^4$ and $\mathbb{R}$ as the vector, the Dirac spinor and the scalar representation, while all other 3CM maps and actions are trivial.

Note that a complex of Lie groups

$$U \xrightarrow{\partial''} W \xrightarrow{\partial'} V \xrightarrow{\partial} G, \qquad (17)$$

where U, W and V are Abelian groups corresponding to vector spaces of representations of G, is a 3-crossed module if

1) $\partial''\vec{u} = \vec{0}_W$, $\partial'\vec{w} = \vec{0}_V$, $\partial\vec{v} = 1_G$;
2) $g \triangleright \vec{v} = R_g\vec{v}$, $g \triangleright \vec{w} = R'_g\vec{w}$, $g \triangleright \vec{u} = R''_g\vec{u}$ (action of G on V, W and U);
3) $\vec{v} \triangleright' \vec{w} = \vec{w}$, $\vec{v} \triangleright' \vec{u} = \vec{u}$, $\vec{w} \triangleright'' \vec{u} = \vec{u}$ (action of V on W and U and action of W on U);
4) $\{\vec{v},\vec{v}'\}_1 = \vec{0}_W$, $\{\vec{w},\vec{w}'\}_2 = \vec{0}_U$, $\{\vec{v},\vec{w}'\}_3 = \vec{0}_U$, $\{\vec{w},\vec{v}'\}_4 = \vec{0}_U$ (the Peiffer maps $V \times V \to W$, $W \times W \to U$, $V \times W \to U$ and $W \times V \to U$).

Given the Poincaré 4-group (16), we can construct the corresponding 4-connection as a collection of p-forms, $p = 1, 2, 3, 4$,

$$\mathcal{A}_4 = (\omega^{ab}, \beta^a, \Gamma^\alpha, \delta). \qquad (18)$$

One can also promote $\mathcal{A}_4$ into a Lie-algebra–valued 4-connection by defining

$$\hat{\mathcal{A}}_4 = (\omega^{ab} J_{ab}, \beta^a P_a, \Gamma^\alpha Y_\alpha, \delta X), \qquad (19)$$

where J, P, Y and X are the generators of the Lie algebras for $SL(2,\mathbb{C}), \mathbb{R}^4, \mathbb{C}^4$ and $\mathbb{R}$ Lie groups.

Note that the 4-form δ can be written as

$$\delta = f(x,y,z,t)\,\mathrm{d}x \wedge \mathrm{d}y \wedge \mathrm{d}z \wedge \mathrm{d}t. \qquad (20)$$

Since f is a scalar density, we will write $f = |e|\phi$ and define the corresponding 1-form curvature as

$$J = \mathrm{d}\phi. \qquad (21)$$

Note that ϕ transforms as a 0-form, *i.e.*, as a scalar field, and is dual to the 4-form δ. Then the 4-curvature for the 4-connection (18) will be given by

$$\mathcal{F}_4 = (R^{ab}, G^a, H^\alpha, J), \qquad (22)$$

where the R, G and H curvatures are given by (5) and (11).

The $4BF$ action is then given by

$$S_4 = \int_{\mathcal{M}} (B^{ab} \wedge R_{ab} + e^a \wedge G_a + \psi^\alpha \wedge H_\alpha + E \wedge J), \qquad (23)$$

where E is a 3-form. The EC action coupled to a Dirac and a scalar field is then obtained by imposing the constraints (7), (12) and

$$E_{\mu\nu\rho} = |e|\,\epsilon_{\mu\nu\rho\sigma} g^{\sigma\lambda} \partial_\lambda \phi, \qquad (24)$$

where $g^{\sigma\lambda}$ is the inverse metric of $g_{\mu\nu} = \eta_{ab} e^a{}_\mu e^b{}_\nu$ and $\epsilon_{\mu\nu\rho\sigma}$ is the Levi-Civita symbol. Note that now the scalar-field constraints are more natural and simpler than in the 2-crossed module case.

The complete EC action is then obtained by adding the fermion mass and the spin-torsion terms (13) to S_4, as well as the scalar-field potential energy,

$$S_V = \int_{\mathcal{M}} |e| V(\phi)\,\mathrm{d}^4x. \qquad (25)$$

Here $V(\phi)$ is the potential for the scalar field. For the purpose of spontaneous symmetry breaking and the Higgs mechanism, one can introduce a doublet of complex scalar fields, and choose the standard Mexican hat potential,

$$V(\phi, \phi^\dagger) = \lambda(\phi^\dagger\phi - v^2)^2, \qquad (26)$$

where λ is the quartic self-coupling of the scalar field, v is the vacuum expectation value, and

$$\phi = \begin{pmatrix} \phi_+ \\ \phi_0 \end{pmatrix} \in \mathbb{C}^2 \qquad (27)$$

is the doublet of complex scalar fields. In order to accommodate a doublet of complex scalar fields, the first group $\mathbb{R}$ in the 3CM chain complex (16) should be substituted by $\mathbb{C}^2$, giving

$$\mathbb{C}^2 \xrightarrow{\partial''} \mathbb{C}^4 \xrightarrow{\partial'} \mathbb{R}^4 \xrightarrow{\partial} SL(2,\mathbb{C}). \qquad (28)$$

This choice of the 3CM will give rise to the complex doublet of the connection 4-forms δ (see (20)), whose dual will then be a doublet of 0-forms (27).

Standard Model and categorical groups. – The Poincaré 4-group (16) can be easily modified in order to include the internal symmetries. Let us consider a 3-crossed module (17) given by

$$\mathbb{C}^r \xrightarrow{\partial''} \mathbb{C}^{2s'+2s''} \xrightarrow{\partial'} \mathbb{R}^4 \xrightarrow{\partial} SL(2,\mathbb{C}) \times K, \qquad (29)$$

where K is a compact Lie group and $\mathbb{C}^{s'}$ is a vector space for a representation of K for the left-handed fermions and $\mathbb{C}^{s''}$ is a vector space for a representation of K for the right-handed fermions. The left/right-handed fermions are described by the 2-component Weyl spinors corresponding to the $SL(2,\mathbb{C})$ irreps $(\frac{1}{2},0)$ and $(0,\frac{1}{2})$ so that

$$\mathbb{C}^2 \otimes \mathbb{C}^{s'} \oplus \mathbb{C}^2 \otimes \mathbb{C}^{s''} \cong \mathbb{C}^{2s'+2s''}. \qquad (30)$$

The 4-connection which corresponds to (29) is given by a collection of p-forms, where $p = 1, 2, 3, 4$, and they can take values in the corresponding Lie algebras, so that

$$\hat{\mathcal{A}}_4 = (\omega^{ab} J_{ab} + A^k T_k, \beta^a P_a, \Gamma_j^\alpha Y_\alpha^j, \delta_i X^i). \qquad (31)$$

Here T, Y and X denote the generators of the Lie algebras for K, $\mathbb{C}^{2(s'+s'')}$ and $\mathbb{C}^r$ Lie groups. The 4-curvature for (31) will be given by

$$\hat{\mathcal{F}}_4 = (R^{ab} J_{ab} + F^k T_k, G^a P_a, H_j^\alpha Y_\alpha^j, J_i X^i), \qquad (32)$$

where

$$F^k T_k = \mathrm{d}A + \frac{1}{2}[A \wedge A], \qquad A = A^k T_k,$$
$$H_j^\alpha = \mathrm{d}\Gamma_j^\alpha + \omega^\alpha{}_\beta \wedge \Gamma_j^\beta, \qquad J_i = d\phi_i. \tag{33}$$

The $4BF$ action is then given by

$$S_{4YM} = \int_{\mathcal{M}} (B^{ab} \wedge R_{ab} + B^k \wedge F_k + e^a \wedge G_a + \psi_j^\alpha \wedge H_\alpha^j + E^i \wedge J_i), \tag{34}$$

where B^k are 2-forms, ψ_j^α are 0-forms and E^i are 3-forms.

The SM action coupled to GR is then obtained by using $K = SU(3) \times SU(2) \times U(1)$ and by constraining the $4BF$ action (34) with the constraints (7) and with copies of the constraints (24) and (12) for each i and j.

One also has to add to S_{4YM} the potential terms quadratic in B^k

$$S_{YMP} = \int_{\mathcal{M}} g^{\mu\nu} g^{\rho\sigma} B^k{}_{\mu\rho} B_{k\nu\sigma}\, \mathrm{d}^4x, \tag{35}$$

in order to obtain the Yang-Mills action as well as the potential, the torsion and the Yukawa coupling terms for the matter fields ϕ_i and ψ_j^α.

The number of SM scalars ϕ_i is determined by the Higgs doublet, see (1), hence $r = 2$, similarly as in (28). Using this choice, and including into the action the scalar potential action (25) with the choice (26), the Higgs mechanism applies in the standard way —the $SU(2) \times U(1)$ subgroup of K is spontaneously broken down to $U(1)_{em}$, three real-valued components in (27) are absorbed by the three gauge fields rendering them massive, while the fourth real component in (27) is interpreted as the Higgs field.

Finally, from (1) it follows that the number of SM fermions ψ_j^α is given by

$$2s' + 2s'' = 2 \cdot 12 \cdot 3 + 2 \cdot 4 \cdot 3 = 96, \tag{36}$$

so that $s' = 36$ and $s'' = 12$. The total number of fermionic components corresponds to 6 quarks plus 2 leptons, considered as Dirac spinors, for three generations, so that $8 \cdot 4 \cdot 3 = 96$.

Conclusions. – We showed that a natural and simple categorification of GR based on n-crossed modules requires that $n = 3$ and that the corresponding 2-form, 3-form and 4-form gauge fields have to be a vector, a Dirac spinor and a scalar, respectively. Hence by using a categorical generalization of the Poincaré group, we naturally incorporate fermionic and scalar matter into the corresponding connection. The corresponding Poincaré 4-group gauge field theory structure can be preserved by introducing the internal symmetries via the 3-crossed module (29), which can be considered as a categorical generalization of the $SL(2,\mathbb{C}) \times K$ symmetry group of SM.

Note that in the 3-group approach to SM [8], one uses the 2-crossed module of the type

$$U \times W \xrightarrow{\partial'} V \xrightarrow{\partial} G, \tag{37}$$

which can be considered as a decategorification of the 3-crossed module (17). This is analogous to what happens in the case of pure gravity, where the Poincaré 2-group can be substitued by the Poincaré group, *i.e.*, the $2BF$ action (4) can be viewed as the BF action for the Poincaré group, see [9].

The 4-group (29) does not restrict the dimensions r, s' and s'' so it would be interesting to explore if there exists another 4-group which is based on the group complex (29) but with different maps and actions such that r, s' and s'' are related.

The ultimate goal would be to find a mathematical structure based on the 4-dimensional spacetime which can explain the dimensions r, s' and s''. Our results suggest that categorical generalizations of groups can be useful for this goal, although some additional algebraic tools may be neccessary. See for example [10], where the McKay correspondence was proposed, or see [11], where the exceptional Jordan algebras were used. Whether the determination of r, s' and s'' can be done classically or at the quantum level remains to be seen.

* * *

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Article

Hamiltonian Analysis for the Scalar Electrodynamics as 3*BF* Theory

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Abstract: The higher category theory can be employed to generalize the *BF* action to the so-called 3*BF* action, by passing from the notion of a gauge group to the notion of a gauge 3-group. The theory of scalar electrodynamics coupled to Einstein–Cartan gravity can be formulated as a constrained 3*BF* theory for a specific choice of the gauge 3-group. The complete Hamiltonian analysis of the 3*BF* action for the choice of a Lie 3-group corresponding to scalar electrodynamics is performed. This analysis is the first step towards a canonical quantization of a 3*BF* theory, an important stepping stone for the quantization of the complete scalar electrodynamics coupled to Einstein–Cartan gravity formulated as a 3*BF* action with suitable simplicity constraints. It is shown that the resulting dynamic constraints eliminate all propagating degrees of freedom, i.e., the 3*BF* theory for this choice of a 3-group is a topological field theory, as expected.

Keywords: Hamiltonian analysis; higher gauge theory; BF theory; topological theory; scalar electrodynamics

1. Introduction

The vast majority of physics community agrees that the quantum theory of gravity is necessary, even if they disagree on the quantization approach. The theory of loop quantum gravity is one of the well-formulated possible candidates for the desired theory of quantum gravity [1–3]. There are two approaches within the theory—the canonical and the covariant quantization method. The covariant quantization method is focused on obtaining a generating functional, by considering a triangulated spacetime manifold and defining the functional as a state sum over all configurations of a field living on simplices of the triangulation [2].

One of the key tools in the covariant quantization approach is the so-called *BF* theory. Given a Lie group G and its corresponding Lie algebra $\mathfrak{g}$, one considers a $\mathfrak{g}$-valued connection 1-form A, and its corresponding field strength 2-form $F \equiv \mathrm{d}A + A \wedge A$. Multiplying F with a $\mathfrak{g}$-valued Lagrange multiplier 2-form B and integrating over a four-dimensional spacetime manifold $\mathcal{M}$, one obtains the action of the *BF* theory,

$$S_{BF}[A,B] = \int_{\mathcal{M}} \langle B \wedge F \rangle_{\mathfrak{g}} \,,$$

where $\langle \_ , \_ \rangle_{\mathfrak{g}}$ is a G-invariant non-degenerate symmetric bilinear form. The *BF* theory derives its name from the symbols B and F for the Lagrange multiplier and the field strength present in the action. As it is defined, the *BF* theory is topological, containing no local propagating degrees of freedom. Therefore, for the purpose of building physically relevant actions, attention usually focuses not on the pure *BF* theory, but rather on the theory with constraints. The constrained *BF* models are based on deformations of the *BF* theory [4], by adding constraints to the topological *BF* action that promote some of the gauge degrees of freedom into physical ones. The well known example is the Plebanski model for general relativity [5]. Constrained BF models represent a starting point in the spinfoam approach to the construction of quantum gravity models [2].

The main shortcoming of building a quantum gravity model using a BF theory is the fact that it is very hard, if not impossible, to write the action for matter fields (specifically scalar and fermion fields) in the form of a constrained BF theory. Thus, the spinfoam quantization method is limited to pure gravity, and the problem of consistently coupling matter fields to gravity in this framework becomes highly nontrivial. One of the proposed ways to circumvent this issue is to generalize the notion of a BF theory using the mathematical apparatus of higher category theory.

The higher category theory [6] can be employed to generalize the BF action to the so-called nBF action, by passing from the notion of a gauge group to the notion of a gauge n-group (for a comprehensive review of n-groups see for example [7], and also Appendix C). Specifically, the notion of a 3-group in the framework of higher category theory is introduced as a 3-category with only one object where all the morphisms, 2-morphisms and 3-morphisms are invertible. Based on this generalization, recently a constrained $3BF$ action has been introduced, which describes the full Standard Model coupled to Einstein–Cartan gravity [8].

As a first step to the study of the Hamiltonian structure of such theories, in this work, we discuss the simplest nontrivial toy example, namely the theory of scalar electrodynamics coupled to gravity. The standard way to define scalar electrodynamics coupled to gravity is by the action:

$$S = \int \mathrm{d}^4x \sqrt{-g} \left[-\frac{1}{16\pi l_p^2} R - \frac{1}{4} g^{\mu\rho} g^{\nu\sigma} F_{\mu\nu} F_{\rho\sigma} + g^{\mu\nu} \nabla_\mu \phi^* \nabla_\nu \phi - m^2 \phi^* \phi \right] . \tag{1}$$

Here, $g_{\mu\nu}$ is the spacetime metric, $g \equiv \det(g_{\mu\nu})$ is its determinant, R is the corresponding curvature scalar, and l_p is the Planck length, its square being equal to the Newton's gravitational constant, $l_p^2 = G$, in the natural system of units $\hbar = c = 1$. The total covariant derivative ∇_μ of the complex scalar field ϕ is defined as $\nabla_\mu \phi = (\partial_\mu + iqA_\mu)\phi$, and thus coupled to the electromagnetic potential A_μ via the coupling constant q (the electric charge of the field ϕ). See Appendix A for more detailed notation. In the next section, we will reformulate this model as a classically equivalent constrained $3BF$ theory for a specific choice of the gauge 3-group. Moreover, for reasons of simplicity, in the Hamiltonian analysis, we will focus only on the topological sector, disregarding the simplicity constraints. The Hamiltonian structure of the theory is important for various reasons, primarily for the canonical quantization program.

The layout of the paper is as follows. In Section 2, we introduce the 3-group structure corresponding to the theory of scalar electrodynamics coupled to Einstein–Cartan gravity and the corresponding constrained $3BF$ action. Section 3 contains the Hamiltonian analysis for the topological, $3BF$ sector of the action, with the resulting first-class and second-class constraints present in the theory, and their mutual Poisson brackets. In Section 4, we analyze the Bianchi identities that the first-class constraints satisfy, which enforce restrictions in the sense of Hamiltonian analysis, and reduce the number of independent first-class constraints present in the theory. Section 5 focuses on the counting of the dynamical degrees of freedom present in the theory, based on the results from Sections 3 and 4. Encouraged by these results, in Section 6, we construct the generator of the gauge symmetries for the topological theory and we find the form variations of all variables and their canonical momenta. Finally, Section 7 is devoted to the discussion of the results and the possible future lines of research. The Appendices contain various technical details.

The notation and conventions are as follows. The local Lorentz indices are denoted by the Latin letters $a, b, c, \dots$, take values $0, 1, 2, 3$, and are raised and lowered using the Minkowski metric η_{ab} with signature $(-, +, +, +)$. Spacetime indices are denoted by the Greek letters $\mu, \nu, \dots$, and are raised and lowered by the spacetime metric $g_{\mu\nu} = \eta_{ab} e^a{}_\mu e^b{}_\nu$, where $e^a{}_\mu$ are the tetrad fields. The inverse tetrad is denoted as $e^\mu{}_a$, so that the standard orthogonality conditions hold: $e^a{}_\mu e^\mu{}_b = \delta^a_b$ and $e^a{}_\mu e^\nu{}_a = \delta^\nu_\mu$. When needed, spacetime indices will be split into time and space indices, denoted with a 0 and lowcase Latin indices $i, j, \dots$, respectively. All other indices that appear in the paper are dependent on the context, and their usage is explicitly defined in the text where they appear. The antisymmetrization over two indices is introduced with the factor one half that is $A_{[a_1|a_2\dots a_{n-1}|a_n]} = \frac{1}{2}\left(A_{a_1 a_2\dots a_{n-1}a_n} - A_{a_n a_2\dots a_{n-1}a_1}\right)$, and the total antisymmetrization is introduced as $A_{[a_1\dots a_n]} = \frac{1}{n!}\sum_{\sigma\in S_n}(-1)^{\text{sign}(\sigma)} A_{a_{\sigma(1)}\dots a_{\sigma(n)}}$.

2. Scalar Electrodynamics as a Constrained 3*BF* Action

Let us begin by providing a short introduction into the construction and structure of a 3*BF* theory, after which we will impose appropriate simplicity constraints, in order to obtain the equations of motion for scalar electrodynamics coupled to gravity.

As was discussed in detail in [8], one formulates a topological 3*BF* action by specifying a particular gauge Lie 3-group. It has been proved that any strict 3-group is equivalent to a 2-crossed module [9,10]. A gauge theory for the manifold $\mathcal{M}_4$ and 2-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \triangleright\,, \{\_\,,\_\})$ can be constructed for the following choice of the three Lie groups as:

$$G = SO(3,1) \times U(1)\,, \quad H = \mathbb{R}^4\,, \quad L = \mathbb{R}^2\,.$$

The maps ∂ and δ are chosen to be trivial. The action of the algebra $\mathfrak{g}$ on $\mathfrak{h}$ and $\mathfrak{l}$ is chosen as:

$$\begin{aligned} &M_{ab} \triangleright P_c = \triangleright_{ab,c}{}^{d}\, P_d = \delta_{[a|}{}^{d}\eta_{|b]c}\, P_d = \eta_{[b|c}\, P_{|a]}\,, && T \triangleright P_a = 0\,, \\ &M_{ab} \triangleright P_A = 0\,, && T \triangleright P_A = \triangleright_A{}^B\, P_B \end{aligned} \tag{2}$$

where M_{ab} denote the six generators of $\mathfrak{so}(3,1)$, T is the sole generator of $\mathfrak{u}(1)$, P_a are the four generators of $\mathbb{R}^4$ and P_A are the two generators of $\mathbb{R}^2$. In the previous expression, the action of the algebra $\mathfrak{u}(1)$ on the algebra $\mathbb{R}^2$ is defined via

$$\triangleright_A{}^B = iq \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The action of the algebra $\mathfrak{g}$ on itself is by definition given via the adjoint representation and, for the choice $\mathfrak{g} = \mathfrak{so}(3,1) \times \mathfrak{u}(1)$, one obtains

$$\begin{gathered} M_{ab} \triangleright M_{cd} = \triangleright_{ab\,,cd}{}^{ef}\, M_{ef} = f_{ab\,,cd}{}^{ef}\, M_{ef} = \eta_{ad}M_{bc} + \eta_{bc}M_{ad} - \eta_{ac}M_{bd} - \eta_{bd}M_{ac}\,, \\ M_{ab} \triangleright T = 0\,, \quad T \triangleright M_{ab} = 0\,, \quad T \triangleright T = 0\,, \end{gathered} \tag{3}$$

as the consequence of the direct product structure and the Abelian nature of the subgroup $U(1)$. The Peiffer lifting

$$\{\_\,,\_\} : H \times H \to L$$

is also trivial, i.e., all the coefficients $X_{ab}{}^A$ are equal to zero:

$$\{P_a\,, P_b\} \equiv X_{ab}{}^A T_A = 0\,. \tag{4}$$

Given Lie algebras $\mathfrak{g}$, $\mathfrak{h}$, and $\mathfrak{l}$, one can introduce a 3-connection (α, β, γ) given by the algebra-valued differential forms $\alpha \in \mathcal{A}^1(\mathcal{M}_4\,, \mathfrak{g})$, $\beta \in \mathcal{A}^2(\mathcal{M}_4\,, \mathfrak{h})$ and $\gamma \in \mathcal{A}^3(\mathcal{M}_4\,, \mathfrak{l})$. The corresponding fake 3-curvature $(\mathcal{F}\,, \mathcal{G}\,, \mathcal{H})$ is then defined as:

$$\mathcal{F} = \mathrm{d}\alpha + \alpha \wedge \alpha - \partial\beta\,, \qquad \mathcal{G} = \mathrm{d}\beta + \alpha \wedge^{\triangleright} \beta - \delta\gamma\,, \qquad \mathcal{H} = \mathrm{d}\gamma + \alpha \wedge^{\triangleright} \gamma + \{\beta \wedge \beta\}\,, \tag{5}$$

see [9,10] for details. For this specific choice of a 3-group, where $\alpha = \omega + A$, given by the algebra-valued differential forms $\omega \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{so}(3,1))$, $A \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{u}(1))$, $\beta \in \mathcal{A}^2(\mathcal{M}_4\,,\mathbb{R}^4)$ and $\gamma \in \mathcal{A}^3(\mathcal{M}_4\,,\mathbb{R}^2)$, the corresponding 3-curvature $(\mathcal{F}\,,\mathcal{G}\,,\mathcal{H})$ is defined as

$$
\begin{aligned}
\mathcal{F} &= R^{ab}M_{ab} + FT &&= \left(\mathrm{d}\omega^{ab} + \omega^{a}{}_{c} \wedge \omega^{cb}\right)M_{ab} + \mathrm{d}A\;T\,, \\
\mathcal{G} &= \mathcal{G}^{a}P_{a} &&= \left(\mathrm{d}\beta^{a} + \omega^{a}{}_{b} \wedge \beta^{b}\right)P_{a}\,, \\
\mathcal{H} &= \mathcal{H}^{A}P_{A} &&= \left(\mathrm{d}\gamma^{A} + \rhd_{B}{}^{A} A \wedge \gamma^{B}\right)P_{A}\,.
\end{aligned}
\tag{6}
$$

Note that the connection ω^{ab} is not present in the last expression, as follows from the definition of the action $\rhd$ and the Peiffer lifting $\{\_\,,\_\}$, see Equations (2) and (4):

$$
\begin{aligned}
\mathcal{H} &= \mathrm{d}\gamma + \alpha \wedge^{\rhd} \gamma + \{\beta \wedge \beta\} \\
&= \mathrm{d}\gamma^{A}P_{A} + (\omega^{ab}M_{ab} + AT) \wedge^{\rhd} (\gamma^{A}P_{A}) \\
&= \mathrm{d}\gamma^{A}P_{A} + \omega^{ab} \wedge \gamma^{A} M_{ab} \rhd P_{A} + A \wedge \gamma^{A} T \rhd P_{A} \\
&= \mathrm{d}\gamma^{A}P_{A} + A \wedge \gamma^{A} \rhd_{A}{}^{B} P_{B} \\
&= (\mathrm{d}\gamma^{A} + \rhd_{B}{}^{A} A \wedge \gamma^{B})P_{A}\,.
\end{aligned}
\tag{7}
$$

The coefficients of the differential 2-forms F and R^{ab}, 3-form $\mathcal{G}$, and 4-form $\mathcal{H}$ are:

$$
\begin{aligned}
F_{\mu\nu} &= \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}\,, \\
R^{ab}{}_{\mu\nu} &= \partial_{\mu}\omega^{ab}{}_{\nu} - \partial_{\nu}\omega^{ab}{}_{\mu} + \omega^{a}{}_{c\mu}\omega^{cb}{}_{\nu} - \omega^{a}{}_{c\nu}\omega^{cb}{}_{\mu}\,, \\
\mathcal{G}^{a}{}_{\mu\nu\rho} &= \partial_{\mu}\beta^{a}{}_{\nu\rho} + \partial_{\nu}\beta^{a}{}_{\rho\mu} + \partial_{\rho}\beta^{a}{}_{\mu\nu} + \omega^{a}{}_{b\mu}\,\beta^{b}{}_{\nu\rho} + \omega^{a}{}_{b\nu}\,\beta^{b}{}_{\rho\mu} + \omega^{a}{}_{b\rho}\,\beta^{b}{}_{\mu\nu}\,, \\
\mathcal{H}^{A}{}_{\mu\nu\rho\sigma} &= \partial_{\mu}\gamma^{A}{}_{\nu\rho\sigma} - \partial_{\nu}\gamma^{A}{}_{\rho\sigma\mu} + \partial_{\rho}\gamma^{A}{}_{\sigma\mu\nu} - \partial_{\sigma}\gamma^{A}{}_{\mu\nu\rho} \\
&\quad + \rhd_{B}{}^{A}A_{\mu}\gamma^{B}{}_{\nu\rho\sigma} - \rhd_{B}{}^{A}A_{\nu}\gamma^{B}{}_{\rho\sigma\mu} + \rhd_{B}{}^{A}A_{\rho}\gamma^{B}{}_{\sigma\mu\nu} - \rhd_{B}{}^{A}A_{\sigma}\gamma^{B}{}_{\mu\nu\rho}\,.
\end{aligned}
\tag{8}
$$

Now, one can define a gauge invariant $3BF$ action as:

$$
S_{3BF} = \int_{\mathcal{M}_4} \left(\langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} + \langle C \wedge \mathcal{G} \rangle_{\mathfrak{h}} + \langle D \wedge \mathcal{H} \rangle_{\mathfrak{l}} \right)\,,
\tag{9}
$$

where $B \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{so}(3,1))$, $C \in \mathcal{A}^1(\mathcal{M}_4\,,\mathbb{R}^4)$ and $D \in \mathcal{A}^0(\mathcal{M}_4\,,\mathbb{R}^2)$ are Lagrange multipliers. The forms $\langle\_\,,\_\rangle_{\mathfrak{g}}$, $\langle\_\,,\_\rangle_{\mathfrak{h}}$ and $\langle\_\,,\_\rangle_{\mathfrak{l}}$ are G-invariant bilinear symmetric nondegenerate forms on $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{l}$, respectively, defined as

$$
\langle M_{ab}\,, M_{cd}\rangle_{\mathfrak{g}} = g_{ab,cd}\,, \quad \langle T\,, T\rangle_{\mathfrak{g}} = 1\,, \quad \langle M_{ab}\,, T\rangle_{\mathfrak{g}} = 0\,, \quad \langle P_a\,, P_b\rangle_{\mathfrak{h}} = g_{ab}\,, \quad \langle P_A\,, P_B\rangle_{\mathfrak{l}} = g_{AB}\,,
$$

where

$$
g_{ab,cd} = \eta_{a[c|}\eta_{b|d]}\,, \qquad g_{ab} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad g_{AB} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.
$$

Identifying the Lagrange multiplier C^a as the tetrad field e^a, and the Lagrange multiplier D^A as the doublet of scalar fields ϕ^A,

$$
\phi = \phi^{A}P_{A} = \phi P_1 + \phi^{*}P_2\,,
$$

based on their transformation properties as discussed in [8,11], the Lagrangian of the action (9) obtains the form:

$$S_{3BF} = \int_{\mathcal{M}_4} \mathrm{d}^4x\, \epsilon^{\mu\nu\rho\sigma} \big(\frac{1}{4} B^{ab}{}_{\mu\nu} R^{cd}{}_{\rho\sigma} g_{ab,cd} + \frac{1}{4} B_{\mu\nu} F_{\rho\sigma} + \frac{1}{3!} e^a{}_\mu \mathcal{G}^b{}_{\nu\rho\sigma} g_{ab} + \frac{1}{4!} \phi^A \mathcal{H}^B{}_{\mu\nu\rho\sigma} g_{AB} \big) . \quad (10)$$

Varying the action with respect to all the variables, one obtains the equations of motion:

varied variable	equation of motion	varied variable	equation of motion
δB^{ab}	$R_{ab} = 0$	δB	$F = 0$
$\delta\omega^{ab}$	$\nabla B_{ab} - e_{[a\|} \wedge \beta_{\|b]} = 0$	δA	$\mathrm{d}B + \phi_A \rhd_B{}^A \gamma^B = 0$
δe^a	$\mathcal{G}_a = 0$	$\delta\beta^a$	$\nabla e_a = 0$
$\delta\phi^A$	$\nabla\gamma_A = 0$	$\delta\gamma^A$	$\nabla\phi_A = 0$

(11)

Since one is interested in the doublet of scalar fields ϕ^A of mass m and charge q minimally coupled to gravity and electromagnetic field, we impose additional simplicity constraint terms to the topological action (9), in order to obtain the appropriate equations of motion equivalent to the equations of motion for the action (1):

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + B \wedge F + e_a \wedge \nabla\beta^a + \phi_A \nabla\gamma^A \\ & - \lambda_{ab} \wedge \Big(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \Big) \\ & + \lambda^A \wedge \Big(\gamma_A - \frac{1}{2} H_{abcA} e^a \wedge e^b \wedge e^c \Big) + \Lambda^{abA} \wedge \Big(H_{abcA} \varepsilon^{cdef} e_d \wedge e_e \wedge e_f - \nabla\phi_A \wedge e_a \wedge e_b \Big) \\ & + \lambda \wedge \Big(B - \frac{12}{q} M_{ab} e^a \wedge e^b \Big) + \zeta^{ab} \Big(M_{ab} \varepsilon_{cdef} e^c \wedge e^d \wedge e^e \wedge e^f - F \wedge e_a \wedge e_b \Big) \\ & - \frac{1}{2\cdot 4!} m^2 \phi_A \phi^A \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d . \end{aligned} \quad (12)$$

For the notation used here and the equations of motion obtained by varying the action (12), see Appendix A.

The dynamical degrees of freedom are the tetrad fields e^a, the scalar doublet ϕ^A, and the electromagnetic potential A, while the remaining variables are algebraically determined in terms of them, as shown in Appendix A. The equation of motion for the field ϕ^A reduces to the covariant Klein-Gordon equation for the scalar field,

$$\Big(\nabla_\mu \nabla^\mu - m^2 \Big) \phi_A = 0 . \quad (13)$$

The differential equation of motion for the field A is:

$$\nabla_\mu F^{\mu\nu} = j^\nu , \qquad j^\mu \equiv \frac{1}{2} \Big(\nabla^\nu \phi^A \rhd^B{}_A \phi_B - \phi_A \rhd_B{}^A \nabla^\nu \phi^B \Big) = iq \Big(\nabla\phi^* \phi - \phi^* \nabla\phi \Big) . \quad (14)$$

Finally, the equation of motion for e^a becomes:

$$\begin{aligned} R^{\mu\nu} - \frac{1}{2} g^{\mu\nu} R &= 8\pi l_p^2\, T^{\mu\nu} , \\ T^{\mu\nu} \equiv \nabla^\mu \phi_A \nabla^\nu \phi^A - \frac{1}{2} g^{\mu\nu} \Big(\nabla_\rho \phi_A \nabla^\rho \phi^A + m^2 \phi_A \phi^A \Big) &- \frac{1}{4q} \left(F_{\rho\sigma} F^{\rho\sigma} g^{\mu\nu} + 4 F^{\mu\rho} F_\rho{}^\nu \right) . \end{aligned} \quad (15)$$

3. The Hamiltonian Analysis

The Hamiltonian analysis of the constrained $3BF$ action (12) for scalar electrodynamics is exceedingly complicated to study. A testament to this is the level of complexity of the constrained $2BF$ formulation of general relativity [12], which is merely one sector in the action (12). Therefore, in this paper, we will limit ourselves to the topological sector of the theory, namely the unconstrained $3BF$ theory (9), which consists of the terms in the first row of Equation (12), and is written in full detail in Equation (10). One should be aware that this restriction changes various properties of the theory. Namely, the simplicity constraints (everything but the first row in Equation (12)) substantially modify the dynamics of the theory—they increase the number of local propagating degrees of freedom of the theory, a property that was known since the original Plebanski model [5]. On the other hand, the unconstrained $3BF$ theory (9) is important even in its own right, and the Hamiltonian analysis may give important insight into the structure of both the unconstrained and the constrained theory.

In what follows, the complete Hamiltonian analysis for the action (9) is presented, see [13] for an overview and a comprehensive introduction of the Hamiltonian analysis. The Hamiltonian analysis for a $2BF$ action is performed in [12,14–16].

Under the standard assumption that the spacetime manifold is globally hyperbolic, $\mathcal{M}_4 = \mathbb{R} \times \Sigma_3$, the Lagrangian of the action (9) has the form:

$$L_{3BF} = \int_{\Sigma_3} \mathrm{d}^3\vec{x}\, \epsilon^{\mu\nu\rho\sigma} \Big(\frac{1}{4} B^{ab}{}_{\mu\nu}\, R^{cd}{}_{\rho\sigma}\, g_{ab,cd} + \frac{1}{4} B_{\mu\nu} F_{\rho\sigma} + \frac{1}{3!}\, e^a{}_\mu\, \mathcal{G}^b{}_{\nu\rho\sigma}\, g_{ab} + \frac{1}{4!}\, \phi^A \mathcal{H}^B{}_{\mu\nu\rho\sigma}\, g_{AB} \Big) . \tag{16}$$

The canonical momentum $\pi(q)$ corresponding for the canonical coordinate q from the set of all variables in the theory, $q \in \{B^{ab}{}_{\mu\nu}, \omega^{ab}{}_\mu, B_{\mu\nu}, A_\mu, e^a{}_\mu, \beta^a{}_{\mu\nu}, \phi^A, \gamma^A{}_{\mu\nu\rho}\}$, is obtained as a derivative of the Lagrangian with respect to the appropriate velocity,

$$\pi(q) \equiv \frac{\delta L}{\delta \partial_0 q} ,$$

giving:

$$\begin{array}{rclrcl}
\pi(B)_{ab}{}^{\mu\nu} & = & 0 , & \pi(\omega)_{ab}{}^{\mu} & = & \epsilon^{0\mu\nu\rho} B_{ab\nu\rho} , \\
\pi(B)^{\mu\nu} & = & 0 , & \pi(A)^{\mu} & = & \frac{1}{2}\epsilon^{0\mu\nu\rho} B_{\nu\rho} , \\
\pi(e)_{a}{}^{\mu} & = & 0 , & \pi(\beta)_{a}{}^{\mu\nu} & = & -\epsilon^{0\mu\nu\rho} e_{a\rho} , \\
\pi(\phi)_{A} & = & 0 , & \pi(\gamma)_{A}{}^{\mu\nu\rho} & = & \epsilon^{0\mu\nu\rho} \phi_A .
\end{array} \tag{17}$$

Since these momenta cannot be inverted for the time derivatives of the variables, they all give rise to primary constraints:

$$\begin{array}{rclrcl}
P(B)_{ab}{}^{\mu\nu} & \equiv & \pi(B)_{ab}{}^{\mu\nu} \approx 0 , & P(\omega)_{ab}{}^{\mu} & \equiv & \pi(\omega)_{ab}{}^{\mu} - \epsilon^{0\mu\nu\rho} B_{ab\nu\rho} \approx 0 , \\
P(B)^{\mu\nu} & \equiv & \pi(B)^{\mu\nu} \approx 0 , & P(A)^{\mu} & \equiv & \pi(A)^{\mu} - \frac{1}{2}\epsilon^{0\mu\nu\rho} B_{\nu\rho} \approx 0 , \\
P(e)_{a}{}^{\mu} & \equiv & \pi(e)_{a}{}^{\mu} \approx 0 , & P(\beta)_{a}{}^{\mu\nu} & \equiv & \pi(\beta)_{a}{}^{\mu\nu} + \epsilon^{0\mu\nu\rho} e_{a\rho} \approx 0 , \\
P(\phi)_{A} & \equiv & \pi(\phi)_{A} \approx 0 , & P(\gamma)_{A}{}^{\mu\nu\rho} & \equiv & \pi(\gamma)_{A}{}^{\mu\nu\rho} - \epsilon^{0\mu\nu\rho} \phi_A \approx 0 .
\end{array} \tag{18}$$

Here, the symbol "$\approx$" denotes the so-called "weak" equality, i.e., the equality that holds on a subspace of the phase space determined by the constraints, while the equality that holds for any point of the phase space is referred to as the "strong" equality and it is denoted by the symbol "$=$". The expressions "on-shell" and "off-shell" are used for weak and strong equalities, respectively, and henceforth will be used in this paper.

The fundamental Poisson brackets are defined as:

$$
\begin{aligned}
\{\, B^{ab}{}_{\mu\nu}(x)\,,\, \pi(B)_{cd}{}^{\rho\sigma}(y)\,\} &= 4\delta^{a}{}_{[c}\delta^{b}{}_{d]}\delta^{\rho}{}_{[\mu}\delta^{\sigma}{}_{\nu]}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, \omega^{ab}{}_{\mu}(x)\,,\, \pi(\omega)_{cd}{}^{\nu}(y)\,\} &= 2\delta^{a}{}_{[c}\delta^{b}{}_{d]}\delta^{\nu}{}_{\mu}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, B_{\mu\nu}(x)\,,\, \pi(B)^{\rho\sigma}(y)\,\} &= 2\delta^{\rho}{}_{[\mu}\delta^{\sigma}{}_{\nu]}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, A_{\mu}(x)\,,\, \pi(A)^{\nu}(y)\,\} &= \delta^{\nu}{}_{\mu}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, e^{a}{}_{\mu}(x)\,,\, \pi(e)_{b}{}^{\nu}(y)\,\} &= \delta^{a}{}_{b}\delta^{\nu}{}_{\mu}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, \beta^{a}{}_{\mu\nu}(x)\,,\, \pi(\beta)_{b}{}^{\rho\sigma}(y)\,\} &= 2\delta^{a}{}_{b}\,\delta^{\rho}{}_{[\mu}\delta^{\sigma}{}_{\nu]}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, \phi^{A}(x)\,,\, \pi(\phi)_{B}(y)\,\} &= \delta^{A}{}_{B}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, \gamma^{A}{}_{\mu\nu\rho}(x)\,,\, \pi(\gamma)_{B}{}^{\alpha\beta\gamma}(y)\,\} &= 3!\delta^{A}{}_{B}\,\delta^{\alpha}{}_{[\mu}\delta^{\beta}{}_{\nu}\delta^{\gamma}{}_{\rho]}\,\delta^{(3)}(\vec{x}-\vec{y})\,.
\end{aligned}
\tag{19}
$$

Using these relations, one can calculate the algebra between the primary constraints,

$$
\begin{aligned}
\{\, P(B)^{abjk}(x)\,,\, P(\omega)_{cd}{}^{i}(y)\,\} &= 4\epsilon^{0ijk}\,\delta^{a}{}_{[c}\delta^{b}{}_{d]}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, P(B)^{jk}(x)\,,\, P(A)^{i}(y)\,\} &= \epsilon^{0ijk}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, P(e)^{ak}\,,\, P(\beta)_{b}{}^{ij}(y)\,\} &= -\epsilon^{0ijk}\,\delta^{a}{}_{b}(x)\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\, P(\phi)^{A}(x)\,,\, P(\gamma)_{B}{}^{ijk}(y)\,\} &= \epsilon^{0ijk}\,\delta^{A}{}_{B}\,\delta^{(3)}(\vec{x}-\vec{y})\,,
\end{aligned}
\tag{20}
$$

while all other Poisson brackets vanish. The canonical on-shell Hamiltonian is defined by

$$
\begin{aligned}
H_c = \int_{\Sigma_3} \mathrm{d}^3\vec{x}\,\Big[&\frac{1}{4}\pi(B)_{ab}{}^{\mu\nu}\,\partial_0 B^{ab}{}_{\mu\nu} + \frac{1}{2}\pi(\omega)_{ab}{}^{\mu}\,\partial_0\omega^{ab}{}_{\mu} + \frac{1}{2}\pi(B)^{\mu\nu}\,\partial_0 B_{\mu\nu} + \pi(A)^{\mu}\,\partial_0 A_{\mu}\\
&+ \pi(e)_{a}{}^{\mu}\,\partial_0 e^{a}{}_{\mu} + \frac{1}{2}\pi(\beta)_{a}{}^{\mu\nu}\,\partial_0\beta^{a}{}_{\mu\nu} + \pi(\phi)_{A}\,\partial_0 D^{A} + \frac{1}{3!}\pi(\gamma)_{A}{}^{\mu\nu\rho}\,\partial_0\gamma^{A}{}_{\mu\nu\rho}\Big] - L\,.
\end{aligned}
\tag{21}
$$

Rewriting the Hamiltonian (21) such that all the velocities are multiplied by the first class constraints and therefore in an on-shell quantity they drop out, one obtains:

$$
\begin{aligned}
H_c = -\int_{\Sigma_3} \mathrm{d}^3\vec{x}\,\epsilon^{0ijk}\Big[&\frac{1}{2}B_{ab0i}\,R^{ab}{}_{jk} + \frac{1}{2}B_{0i}F_{jk} + \frac{1}{6}e_{a0}\,\mathcal{G}^{a}{}_{ijk} + \beta^{a}{}_{0i}\nabla_j e_{ak}\\
&+ \frac{1}{2}\omega^{ab}{}_{0}\Big(\nabla_i B_{ab\,jk} - e_{[a|i}\,\beta_{|b]jk}\Big) + \frac{1}{2}A_0\Big(\partial_i B_{jk} + \frac{1}{3}\,\phi_A \,\triangleright_B{}^{A}\,\gamma^{B}{}_{ijk}\Big) + \frac{1}{2}\gamma^{A}{}_{0ij}\nabla_k\phi_A\Big]\,.
\end{aligned}
\tag{22}
$$

This expression does not depend on any of the canonical momenta and it contains only the fields and their spatial derivatives. By adding a Lagrange multiplier λ for each of the primary constraints we can build the off-shell Hamiltonian, which is given by:

$$
\begin{aligned}
H_T = H_c + \int_{\Sigma_3} \mathrm{d}^3\vec{x}\,\Big[&\frac{1}{4}\lambda(B)^{ab}{}_{\mu\nu}P(B)_{ab}{}^{\mu\nu} + \frac{1}{2}\lambda(\omega)^{ab}{}_{\mu}P(\omega)_{ab}{}^{\mu} + \frac{1}{2}\lambda(B)_{\mu\nu}P(B)^{\mu\nu} + \lambda(A)_{\mu}P(A)^{\mu}\\
&+\lambda(e)^{a}{}_{\mu}P(e)_{a}{}^{\mu} + \frac{1}{2}\lambda(\beta)^{a}{}_{\mu\nu}P(\beta)_{a}{}^{\mu\nu} + \lambda(\phi)^{A}P(\phi)_{A} + \frac{1}{3!}\lambda(\gamma)^{A}{}_{\mu\nu\rho}P(\gamma)_{A}{}^{\mu\nu\rho}\Big]\,.
\end{aligned}
\tag{23}
$$

Since the primary constraints must be preserved in time, one must impose the following requirement:

$$
\dot{P} \equiv \{\, P\,,\, H_T\,\} \approx 0\,,
\tag{24}
$$

for each primary constraint P. By using the consistency condition (24) for the primary constraints $P(B)_{ab}{}^{0i}$, $P(\omega)_{ab}{}^{0}$, $P(B)^{0i}$, $P(A)^{0}$, $P(e)_{a}{}^{0}$, $P(\beta)_{a}{}^{0i}$, and $P(\gamma)_{A}{}^{0ij}$,

$$\begin{array}{llll} \dot{P}(B)_{ab}{}^{0i} \approx 0\,, & \dot{P}(\omega)_{ab}{}^{0} \approx 0\,, & \dot{P}(B)^{0i} \approx 0\,, & \dot{P}(A)^{0} \approx 0\,, \\ \dot{P}(e)_{a}{}^{0} \approx 0\,, & \dot{P}(\beta)_{a}{}^{0i} \approx 0\,, & \dot{P}(\gamma)_{A}{}^{0ij} \approx 0\,, & \end{array} \tag{25}$$

one obtains the secondary constraints $\mathcal{S}$,

$$\begin{array}{lcllcl} \mathcal{S}(R)_{ab}{}^{i} & \equiv & \epsilon^{0ijk} R_{ab\,jk} \approx 0\,, & \mathcal{S}(\nabla B)_{ab} & \equiv & \epsilon^{0ijk}\big(\nabla_i B_{ab\,jk} - e_{[a|i}\,\beta_{|b]\,jk}\big) \approx 0\,, \\ \mathcal{S}(F)^{i} & \equiv & \frac{1}{2}\epsilon^{0ijk} F_{jk} \approx 0\,, & \mathcal{S}(\nabla B) & \equiv & \frac{1}{2}\epsilon^{0ijk}\big(\partial_i B_{jk} + \frac{1}{3}\,\phi_A \rhd_B{}^{A}\,\gamma^{B}{}_{ijk}\big) \approx 0\,, \\ \mathcal{S}(\mathcal{G})_{a} & \equiv & \frac{1}{6}\epsilon^{0ijk}\mathcal{G}_{a\,ijk} \approx 0\,, & \mathcal{S}(\nabla e)_{a}{}^{i} & \equiv & \epsilon^{0ijk}\nabla_j e_{ak} \approx 0\,, \\ \mathcal{S}(\nabla\phi)_{A}{}^{ij} & \equiv & \epsilon^{0ijk}\nabla_k \phi_A \approx 0\,, & & & \end{array} \tag{26}$$

while in the case of $P(B)_{ab}{}^{jk}$, $P(\omega)_{ab}{}^{k}$, $P(B)^{jk}$, $P(A)^{k}$, $P(e)_{a}{}^{k}$, $P(\beta)_{a}{}^{jk}$, $P(\phi)_{A}$ and $P(\gamma)_{A}{}^{ijk}$ the consistency conditions

$$\begin{array}{llll} \dot{P}(B)_{ab}{}^{jk} \approx 0\,, & \dot{P}(\omega)_{ab}{}^{k} \approx 0\,, & \dot{P}(B)^{jk} \approx 0\,, & \dot{P}(A)^{k} \approx 0\,, \\ \dot{P}(e)_{a}{}^{k} \approx 0\,, & \dot{P}(\beta)_{a}{}^{jk} \approx 0\,, & \dot{P}(\phi)_{A} \approx 0\,, & \dot{P}(\gamma)_{A}{}^{ijk} \approx 0\,, \end{array} \tag{27}$$

determine the following Lagrange multipliers:

$$\begin{array}{lcllcl} \lambda(\omega)_{ab}{}^{i} & \approx & \nabla^i\,\omega_{ab\,0}\,, & \lambda(B)^{ij} & \approx & 2\partial^{[i|}\,B^{0|j]} + \gamma_A{}^{0ij} \rhd_B{}^{A}\,\phi^{B}\,, \\ \lambda(A)^{i} & \approx & \partial^i\,A_0\,, & \lambda(\beta)_{a}{}^{ij} & \approx & 2\nabla^{[i|}\,\beta_a{}^{0|j]} - \omega_{ab}{}^{0}\,\beta^{b\,ij}\,, \\ \lambda(\phi)^{A} & \approx & A^0 \rhd{}^{A}{}_{B}\,\phi^{B}\,, & \lambda(e)_{a}{}^{i} & \approx & \nabla^i\,e_a{}^{0} - \omega_a{}^{b\,0}\,e_b{}^{i}\,, \\ \lambda(B)_{ab}{}^{ij} & \approx & \multicolumn{4}{l}{2\nabla^{[i|}B_{ab}{}^{0|j]} + e_{[a|\,0}\beta_{|b]}{}^{ij} - 2e_{[a|}{}^{[i|}\beta_{|b]}{}^{0|j]} + 2\omega_{[a|}{}^{c}B_{|b]}{}^{c\,ij}\,,} \\ \lambda(\gamma)_{A}{}^{ijk} & \approx & \multicolumn{4}{l}{-A^0 \rhd_A{}^{B}\,\gamma_B{}^{ijk} + \nabla^i\gamma_A{}^{0jk} - \nabla^j\gamma_A{}^{0ik} + \nabla^k\gamma_A{}^{0ij}\,.} \end{array} \tag{28}$$

Note that the consistency conditions leave the Lagrange multipliers

$$\lambda(B)^{ab}{}_{0i}\,, \quad \lambda(\omega)^{ab}{}_{0}\,, \quad \lambda(B)_{0i}\,, \quad \lambda(A)_{0}\,, \quad \lambda(e)^{a}{}_{0}\,, \quad \lambda(\beta)^{a}{}_{0i}\,, \quad \lambda(\gamma)^{A}{}_{0ij} \tag{29}$$

undetermined. The consistency conditions of the secondary constraints do not produce new constraints, since one can show that

$$\begin{array}{lclcl} \dot{\mathcal{S}}(R)^{abi} & = & \{\mathcal{S}(R)^{abi}\,,\,H_T\} & = & \omega^{[a|}{}_{c0}\,\mathcal{S}(R)^{c|b]i}\,, \\ \dot{\mathcal{S}}(\nabla B) & = & \{\mathcal{S}(\nabla B),\,H_T\} & = & -\rhd_B{}^{A}\,\gamma^{B}{}_{0ij}\,\mathcal{S}(\nabla\phi)_{A}{}^{ij}\,, \\ \dot{\mathcal{S}}(\mathcal{G})^{a} & = & \{\mathcal{S}(\mathcal{G})^{a}\,,\,H_T\} & = & \beta_{b0k}\,\mathcal{S}(R)^{abk} - \omega^{ab}{}_{0}\,\mathcal{S}(\mathcal{G})_{b}\,, \\ \dot{\mathcal{S}}(\nabla e)_{a}{}^{i} & = & \{\mathcal{S}(\nabla e)_{a}{}^{i}\,,\,H_T\} & = & e^{b}{}_{0}\,\mathcal{S}(R)_{ab}{}^{i} - \omega_a{}^{b}{}_{0}\,\mathcal{S}(\nabla e)_{b}{}^{i}\,, \\ \dot{\mathcal{S}}(\nabla\phi)_{A}{}^{ij} & = & \{\mathcal{S}(\nabla\phi)_{A}{}^{ij}\,,\,H_T\} & = & A_0 \rhd_A{}^{B}\mathcal{S}(\nabla\phi)_{B}{}^{ij}\,, \\ \dot{\mathcal{S}}(F)^{i} & = & \{\mathcal{S}(F)^{i}\,,\,H_T\} & = & 0\,, \\ \dot{\mathcal{S}}(\nabla B)_{ab} & = & \{\mathcal{S}(\nabla B)_{ab}\,,\,H_T\} & = & \mathcal{S}(R)_{[a|c}{}^{k}\,B^{c}{}_{|b]0k} + \omega_{[a|}{}^{c}{}_{0}\mathcal{S}(\nabla B)_{|b]c} \\ & & & & -\beta_{[a|0k}\,\mathcal{S}(\nabla e)_{|b]}{}^{k} + e_{[a|0}\,\mathcal{S}(\mathcal{G})_{|b]}\,. \end{array} \tag{30}$$

Then, the total Hamiltonian can be written as

$$
\begin{aligned}
H_T \quad = \quad \int_{\Sigma_3} \mathrm{d}^3\vec{x} \quad & \Big[\frac{1}{2}\lambda(B)_{ab}{}^{0i}\, \Phi(B)^{ab}{}_i + \frac{1}{2}\lambda(\omega)_{ab}{}^0\, \Phi(\omega)^{ab} + \lambda(B)^{0i}\, \Phi(B)_i + \lambda(A)^0\, \Phi(A) \\
& + \lambda(e)_a{}^0\, \Phi(e)^a + \lambda(\beta)_a{}^{0i}\, \Phi(\beta)^a{}_i + \frac{1}{2}\lambda(\gamma)_A{}^{0ij}\Phi(\gamma)^A{}_{ij} \\
& - \frac{1}{2}B_{ab0i}\, \Phi(R)^{abi} - \frac{1}{2}\omega_{ab0}\, \Phi(\nabla B)^{ab} - B_{0i}\, \Phi(F)^i - A_0\, \Phi(\nabla B) \\
& - e_{a0}\, \Phi(\mathcal{G})^a - \beta_{a0i}\, \Phi(\nabla e)^{ai} - \frac{1}{2}\gamma_{A0ij}\, \Phi(\nabla\phi)^{Aij} \Big] \,,
\end{aligned} \tag{31}
$$

where

$$
\begin{array}{llllll}
\Phi(B)^{ab}{}_i & = & P(B)^{ab}{}_{0i}\,, & \Phi(\gamma)^A{}_{ij} & = & P(\gamma)^A{}_{0ij}\,, \\
\Phi(\omega)^{ab} & = & P(\omega)^{ab}{}_0\,, & \Phi(F)^i & = & \mathcal{S}(F)^i - \partial_j P(B)^{ij}\,, \\
\Phi(B)_i & = & P(B)_{0i}\,, & \Phi(R)^{abi} & = & \mathcal{S}(R)^{abi} - \nabla_j P(B)^{ab\,ij}\,, \\
\Phi(A) & = & P(A)_0\,, & \Phi(\mathcal{G})^a & = & \mathcal{S}(\mathcal{G})^a + \nabla_i P(e)^{a\,i} - \frac{1}{4}\,\beta_{b\,ij}\, P(B)^{ab\,ij}\,, \\
\Phi(e)^a & = & P(e)^a{}_0\,, & \Phi(\nabla e)^{a\,i} & = & \mathcal{S}(\nabla e)^{a\,i} - \nabla_j P(\beta)^{a\,ij} + \frac{1}{2}\, e_{b\,j}\, P(B)^{ab\,ij}\,, \\
\Phi(\beta)^a{}_i & = & P(\beta)^a{}_{0i}\,, & \Phi(\nabla\phi)^{A\,ij} & = & \mathcal{S}(\nabla\phi)^{A\,ij} + \nabla_k P(\gamma)^{A\,ijk} - \rhd_B{}^A\, \phi^B\, P(B)^{ij}\,, \\
\Phi(\nabla B) & = & \multicolumn{4}{l}{\mathcal{S}(\nabla B) + \partial_i P(A)^i + \dfrac{1}{3!}\,\gamma^A{}_{ijk}\, \rhd_A{}^B\, P(\gamma)_B{}^{ijk} - \phi_A\, \rhd_B{}^A\, P(\phi)^B\,,} \\
\Phi(\nabla B)^{ab} & = & \multicolumn{4}{l}{\mathcal{S}(\nabla B)^{ab} + \nabla_i P(\omega)^{abi} + B^{[a|}{}_{c\,ij}\, P(B)^{c|b]\,ij} - 2e^{[a|}{}_i\, P(e)^{|b]\,i} - \beta^{[a|}{}_{ij}\, P(\beta)^{|b]\,ij}\,,}
\end{array} \tag{32}
$$

are the first-class constraints, while

$$
\begin{array}{llll}
\chi(B)_{ab}{}^{jk} = P(B)_{ab}{}^{jk}\,, & \chi(B)^{jk} = P(B)^{jk}\,, & \chi(e)_a{}^i = P(e)_a{}^i\,, & \chi(\phi)_A = P(\phi)_A\,, \\
\chi(\omega)_{ab}{}^i = P(\omega)_{ab}{}^i\,, & \chi(A)^i = P(A)^i\,, & \chi(\beta)_a{}^{ij} = P(\beta)_a{}^{ij}\,, & \chi(\gamma)_A{}^{ijk} = P(\gamma)_A{}^{ijk}\,,
\end{array} \tag{33}
$$

are the second-class constraints.

The PB algebra of the first-class constraints is given by:

$$
\begin{array}{lll}
\{\, \Phi(\mathcal{G})^a(x)\,,\, \Phi(\nabla e)_b{}^i(y)\,\} & = & -\,\Phi(R)^a{}_b{}^i(x)\, \delta^{(3)}(\vec{x}-\vec{y})\,, \\
\{\, \Phi(\mathcal{G})^a(x)\,,\, \Phi(\nabla B)_{bc}(y)\,\} & = & 2\delta^a{}_{[b|}\, \Phi(\mathcal{G})_{|c]}(x)\, \delta^{(3)}(\vec{x}-\vec{y})\,, \\
\{\, \Phi(\nabla e)^a{}_i(x)\,,\, \Phi(\nabla B)_{bc}(y)\,\} & = & 2\delta^a{}_{[b|}\Phi(\nabla e)_{|c]i}(x)\, \delta^{(3)}(\vec{x}-\vec{y})\,, \\
\{\, \Phi(R)^{abi}(x)\,,\, \Phi(\nabla B)_{cd}(y)\,\} & = & -4\delta^{[a|}{}_{[c}\, \Phi(R)^{|b]}{}_{d]}{}^i(x)\, \delta^{(3)}(\vec{x}-\vec{y})\,, \\
\{\, \Phi(\nabla B)^{ab}(x)\,,\, \Phi(\nabla B)_{cd}(y)\,\} & = & -4\delta^{[a|}{}_{[c|}\, \Phi(\nabla B)^{|b]}{}_{|d]}(x)\, \delta^{(3)}(\vec{x}-\vec{y})\,, \\
\{\, \Phi(\nabla B)(x)\,,\, \Phi(\nabla\phi)_A{}^{ij}(y)\,\} & = & -2\rhd^B{}_A\; \Phi(\nabla\phi)_B{}^{ij}(x)\delta^{(3)}(\vec{x}-\vec{y})\,.
\end{array} \tag{34}
$$

The PB algebra between the first and the second-class constraints is given by:

$$
\begin{aligned}
\{\,\Phi(R)^{abi}(x)\,,\,\chi(\omega)_{cd}{}^{j}(y)\,\} &= 4\,\delta^{[a|}{}_{[c|}\,\chi(B)^{|b]}{}_{|d]}{}^{ij}(x)\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\mathcal{G})^{a}(x)\,,\,\chi(\omega)_{cd}{}^{i}(y)\,\} &= 2\,\delta^{a}{}_{[c|}\,\chi(e)_{|d]}{}^{i}(x)\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\mathcal{G})^{a}(x)\,,\,\chi(\beta)_{c}{}^{jk}(y)\,\} &= -\frac{1}{2}\,\chi(B)^{a}{}_{c}{}^{jk}(x)\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla e)^{ai}(x)\,,\,\chi(\omega)_{cd}{}^{j}(y)\,\} &= -2\,\delta^{a}{}_{[c|}\,\chi(\beta)_{|d]}{}^{ij}(x)\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla e)^{ai}(x)\,,\,\chi(e)_{b}{}^{j}(y)\,\} &= \frac{1}{2}\,\chi(B)^{a}{}_{b}{}^{ij}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla B)^{ab}(x)\,,\,\chi(\omega)_{cd}{}^{i}(y)\,\} &= 4\,\delta^{[a|}{}_{[c|}\,\chi(\omega)_{|d]}{}^{|b]i}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla B)(x)\,,\,\chi(A)^{i}(y)\,\} &= 2\,\chi(A)^{i}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla B)^{ab}(x)\,,\,\chi(\beta)_{c}{}^{jk}(y)\,\} &= -2\delta^{[a|}{}_{c}\,\chi(\beta)^{|b]jk}\,\delta^{(3)}(x-y)\,,\\
\{\,\Phi(\nabla B)(x)\,,\,\chi(\gamma)_{A}{}^{ijk}(y)\,\} &= \rhd_{A}{}^{B}\;\chi(\gamma)_{B}{}^{ijk}(x)\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla B)^{ab}(x)\,,\,\chi(B)_{cd}{}^{jk}(y)\,\} &= 4\,\delta^{[a|}{}_{[c}\,\chi(B)_{d]}{}^{|b]jk}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla B)^{ab}(x)\,,\,\chi(e)_{a}{}^{i}(y)\,\} &= -2\delta^{[a|}{}_{c}\,\chi(e)^{|b]i}\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla B)(x)\,,\,\chi(\phi)_{A}(y)\,\} &= -\rhd^{B}{}_{A}\,\chi(\phi)_{B}(x)\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla\phi)^{Aij}(x)\,,\,\chi(A)^{k}(y)\,\} &= -\rhd_{B}{}^{A}\,\chi(\gamma)^{Bijk}(x)\,\delta^{(3)}(\vec{x}-\vec{y})\,,\\
\{\,\Phi(\nabla\phi)^{Aij}(x)\,,\,\chi(\phi)_{B}(y)\,\} &= -\rhd_{B}{}^{A}\,\chi(B)^{ij}(x)\,\delta^{(3)}(\vec{x}-\vec{y})\,.
\end{aligned}
\tag{35}
$$

The PB algebra between the second-class constraints has already been calculated, and is given in Equations (20).

4. The Bianchi Identities

In order to calculate the number of degrees of freedom in the theory, one needs to make use of the *Bianchi identities* (BI), as well as additional, *generalized Bianchi identities* (GBI) that are an analogue of the ordinary BI for the additional fields present in the theory.

One uses BI associated with the 1-form fields ω^{ab} and e^a, as well as the GBI for the 1-form A. Namely, the corresponding 2-form curvatures

$$R^{ab} = \mathrm{d}\omega^{ab} + \omega^{a}{}_{c}\wedge\omega^{cb}\,, \qquad T^{a} = \mathrm{d}e^{a} + \omega^{a}{}_{b}\wedge e^{b}\,, \qquad F = \mathrm{d}A\,, \tag{36}$$

satisfy the following identities:

$$\epsilon^{\lambda\mu\nu\rho}\,\nabla_{\mu}R^{ab}{}_{\nu\rho} = 0\,, \tag{37}$$

$$\epsilon^{\lambda\mu\nu\rho}\left(\nabla_{\mu}T^{a}{}_{\nu\rho} - R^{ab}{}_{\mu\nu}\,e_{b\rho}\right) = 0\,, \tag{38}$$

$$\epsilon^{\lambda\mu\nu\rho}\,\nabla_{\mu}F_{\nu\rho} = 0\,. \tag{39}$$

Choosing the free index to be time coordinate $\lambda = 0$, these indentities, as the time-independent parts of the Bianchi identities, become the off-shell restrictions in the sense of the Hamiltonian analysis. On the other hand, choosing the free index to be a spatial coordinate, one obtains time-dependent pieces of the Bianchi identities, which do not enforce any restrictions, but can instead be derived as a consequence of the Hamiltonian equations of motion.

There are also GBI associated with the 2-form fields B^{ab}, B and β^a. The corresponding 3-form curvatures are given by

$$S^{ab} = \mathrm{d}B^{ab} + 2\omega^{[a|}{}_c \wedge B^{c\,|b]}\,, \qquad P = \mathrm{d}B\,, \qquad G^a = \mathrm{d}\beta^a + \omega^a{}_b \wedge \beta^b\,. \tag{40}$$

Differentiating these expressions, one obtains the following GBI:

$$\epsilon^{\lambda\mu\nu\rho}\left(\frac{1}{3}\nabla_\lambda S^{ab}{}_{\mu\nu\rho} - R^{[a|\,c}{}_{\lambda\mu}\, B_c{}^{|b]}{}_{\nu\rho}\right) = 0\,, \tag{41}$$

$$\epsilon^{\lambda\mu\nu\rho}\partial_\lambda\, P_{\mu\nu\rho} = 0\,, \tag{42}$$

$$\epsilon^{\lambda\mu\nu\rho}\left(\frac{2}{3}\nabla_\lambda\, G^a{}_{\mu\nu\rho} - R^{ab}{}_{\lambda\mu}\,\beta_{b\,\nu\rho}\right) = 0\,. \tag{43}$$

However, in four-dimensional spacetime, these identities will be single-component equations, with no free spacetime indices, and therefore necessarily feature time derivatives of the fields. Thus, they do not impose any off-shell restictions on the canonical variables.

Finally, there is also GBI associated with the 0-form ϕ. The corresponding 1-form curvature is:

$$Q^A = \mathrm{d}\phi^A + \rhd_B{}^A\, A \wedge \phi^B\,, \tag{44}$$

so that the GBI associated with this curvature is:

$$\epsilon^{\lambda\mu\nu\rho}\left(\nabla_\nu Q^A{}_\rho - \frac{1}{2}\rhd_B{}^A\, F_{\nu\rho}\phi^B\right) = 0. \tag{45}$$

This GBI consists of 12 component equations, corresponding to six possible choices of the free antisymmetrized spacetime indices $\lambda\mu$, and the 2 possible choices of the free group index A. However, not all of these 12 identities are independent. This can be seen by taking the derivative of the Equation (45) and obtaining eight identities of the form

$$\rhd_B{}^A\,\epsilon^{\lambda\mu\nu\rho}\,\partial_\mu\, F_{\nu\rho}\,\phi^B = 0\,, \tag{46}$$

which are automatically satisfied because of the GBI (39). One concludes there are only four independent identities (45). Now, fixing the value $\lambda = 0$, one obtains the time-independent components of both Equations (45) and (46),

$$\epsilon^{0ijk}\left(\nabla_j Q^A{}_k - \frac{1}{2}\rhd_B{}^A\, F_{jk}\phi^B\right) = 0\,, \tag{47}$$

and

$$\rhd_B{}^A\,\epsilon^{0ijk}\,\partial_i\, F_{jk}\,\phi^B = 0\,. \tag{48}$$

Of these, there are six components in Equation (47), but, because of the two components of Equation (48), there are overall only four independent GBI relevant for the Hamiltonian analysis.

5. Number of Degrees of Freedom

Let us now show that the structure of the constraints implies that there are no local degrees of freedom (DoF) in a $3BF$ theory. In the general case, if there are N initial fields in the theory and there are F independent first-class constraints per space point and S independent second-class constraints per space point, then the number of local DoF, i.e., the number of independent field components, is given by

$$n = N - F - \frac{S}{2}\,. \tag{49}$$

Equation (49) is a consequence of the fact that S second-class constraints are equivalent to vanishing of $S/2$ canonical coordinates and $S/2$ of their momenta. The F first-class constraints are equivalent to vanishing of F canonical coordinates, and since the first-class constraints generate the gauge symmetries, we can impose F gauge-fixing conditions for the corresponding F canonical momenta. Consequently, there are $2N - 2F - S$ independent canonical coordinates and momenta and therefore $2n = 2N - 2F - S$, giving rise to Equation (49).

In our case, N can be determined from the Table 1, giving rise to a total of $N = 120$ canonical coordinates. Similarly, the number of independent components for the second class constraints is determined by the Table 2, so that $S = 70$.

Table 1. The number of components for all fields present in the theory.

$\omega^{ab}{}_{\mu}$	A_{μ}	$\beta^{a}{}_{\mu\nu}$	$\gamma^{A}{}_{\mu\nu\rho}$	$B^{ab}{}_{\mu\nu}$	$B_{\mu\nu}$	$e^{a}{}_{\mu}$	ϕ^{A}
24	4	24	8	36	6	16	2

Table 2. The number of components for the second class constraints present in the theory.

$\chi(B)_{ab}{}^{jk}$	$\chi(B)^{jk}$	$\chi(e)_{a}{}^{i}$	$\chi(\phi)_{A}$	$\chi(\omega)_{ab}{}^{i}$	$\chi(A)^{i}$	$\chi(\beta)_{a}{}^{ij}$	$\chi(\gamma)_{A}{}^{ijk}$
18	3	12	2	18	3	12	2

The first-class constraints are not all independent because of BI and GBI. To see that, take the derivative of $\Phi(R)^{abi}$ to obtain

$$\nabla_i \Phi(R)^{abi} = \varepsilon^{0ijk} \nabla_i R^{ab}{}_{jk} + \frac{1}{2} R^{c[a|}{}_{ij} P(B)_c{}^{|b]ij} . \tag{50}$$

The first term on the right-hand side is zero off-shell because $\epsilon^{ijk} \nabla_i R^{ab}{}_{jk} = 0$, which is a $\lambda = 0$ component of the BI (37). The second term on the right-hand side is also zero off-shell, since it is a product of two constraints,

$$R^{c[a|}{}_{ij}\, P(B)_c{}^{|b]ij} \equiv \frac{1}{2} \epsilon_{0ijk} \mathcal{S}(R)^{c[a|k}\, P(B)_c{}^{|b]ij} = 0 . \tag{51}$$

Therefore, we have the off-shell identity

$$\nabla_i \Phi(R)^{abi} = 0 , \tag{52}$$

which means that six components of $\Phi(R)^{abi}$ are not independent of the others. In an analogous fashion, taking the derivative of $\Phi(F)^i$, one obtains

$$\partial_i \Phi(F)^i = \varepsilon^{0ijk}\, \partial_i F_{jk} + \frac{1}{2}\, F_{ij}\, P(B)^{ij} . \tag{53}$$

The first term on the right-hand side is zero off-shell because $\epsilon^{ijk}\, \partial_i F_{jk} = 0$, which is a $\lambda = 0$ component of the GBI (37). The second term on the right-hand side is also zero off-shell, since it is a product of two constraints,

$$F_{ij}\, P(B)^{ij} \equiv \frac{1}{2} \epsilon_{0ijk}\, \mathcal{S}(F)^k\, P(B)^{ij} = 0 . \tag{54}$$

Therefore, we have the off-shell identity

$$\partial_i \Phi(F)^i = 0 , \tag{55}$$

which means that one component of $\Phi(F)^i$ is not independent of the others. Similarly, one can demonstrate that

$$\nabla_i \Phi(\nabla e)_a{}^i - \frac{1}{2}\,\Phi(R)_{ab}{}^i\, e^b{}_i + \frac{1}{4}\epsilon^{0ijk}\mathcal{S}(R)_{abk}\, P(\beta)^b{}_{ij} = \frac{1}{2}\epsilon^{0ijk}\left(\nabla_i T_{ajk} - R_{ab\,ij}\, e^b{}_k\right) . \tag{56}$$

The right-hand side of the Equation (56) is the $\lambda = 0$ component of the BI (38), so that Equation (56) gives the relation:

$$\nabla_i \Phi(\nabla e)_a{}^i - \frac{1}{2}\,\Phi(R)_{ab}{}^i\, e^b{}_i = 0\,, \tag{57}$$

where we have omitted the term that is the product of two constraints. This relation means that four components of the constraints $\Phi(\nabla e)_a{}^i$ and $\Phi(R)_{ab}{}^i$ can be expressed in terms of the rest. Finally, one can also demonstrate that

$$\begin{aligned} &\nabla_i \Phi(\nabla\phi)_A{}^{ij} - \frac{1}{2}\epsilon_{0ikl} \rhd_A \mathcal{S}(F)^l\, \chi(\gamma)_B{}^{ijk} + \rhd^B{}_A\, \phi_B\, \Phi(F)^j \\ &\quad + \frac{1}{2}\epsilon_{0ilm} \rhd^B{}_A\, P(B)^{ij}\, \mathcal{S}(\nabla\phi)_B{}^{lm} = \epsilon^{0ijk}\left(\nabla_i Q_{Ak} + \frac{1}{2}\rhd^B{}_A\, F_{ik}\, \phi_B\right) , \end{aligned} \tag{58}$$

which gives

$$\nabla_i \Phi(\nabla\phi)_A{}^{ij} + \frac{1}{2}\rhd^B{}_A\, \phi_B\, \Phi(F)^j = 0\,, \tag{59}$$

for $\lambda = 0$ component of the GBI (45), where we have again used that the product of two contraints is zero off-shell. This relation suggests that six components of two first-class constraints, $\Phi(\nabla\phi)_A{}^{ij}$ and $\Phi(F)^j$, are not independent of the others. However, in the previous section, we have discussed that only four of these six identities are mutually independent, which means that we have only four independent identities (59). A rigorous proof of this statement entails the evaluation of the corresponding Wronskian, and is left for future work.

Taking into account all of the above indentites (52), (55), (57), and (59), we can finally evaluate the total number of independent first-class constraints. From the Table 3, one can see that the total number of components of the first-class constraints is given by $F^* = 100$. However, the number of independent components of the first-class constraints is $F = 85$, obtained by subtracting the six relations (52), one relation (55), four relations (57) and four relations (59).

Table 3. The number of components for the first class constraints present in the theory. The identities (52), (55), (57), and (59) reduce the number of components which are independent. This reduction is explicitly denoted in the table.

$\Phi(B)_{ab}{}^i$	$\Phi(B)^i$	$\Phi(e)_a$	$\Phi(\omega)_{ab}$	$\Phi(A)$	$\Phi(\beta)_a{}^i$	$\Phi(\gamma)_A{}^{ij}$	$\Phi(R)_{ab}{}^i$	$\Phi(F)^i$	$\Phi(\mathcal{G})_a$	$\Phi(\nabla e)_a{}^i$	$\Phi(\nabla B)_{ab}$	$\Phi(\nabla B)$	$\Phi(\nabla\phi)_A{}^{ij}$
18	3	4	6	1	12	6	$18-6$	$3-1$	4	$12-4$	6	1	$6-4$

Therefore, substituting all the obtained results into Equation (49), one gets

$$n = 120 - 85 - \frac{70}{2} = 0, \tag{60}$$

which means that there are no propagating DoF in a $3BF$ theory described by the action (10).

6. Generator of the Gauge Symmetry

Based on the results of the Hamiltonian analysis of the action (10), it can also be interesting to calculate the generator of the complete gauge symmetry of the action. The gauge generator of the theory is obtained by using the Castellani's procedure (see Chapter V in [13] for details of the procedure), and one gets the following result (see Appendix B for details of the calculation):

$$
\begin{aligned}
G \;=\; & \int_{\Sigma_3} \mathrm{d}^3\vec{x}\Bigg(\frac{1}{2}(\nabla_0\epsilon^{ab}{}_i)\Phi(B)_{ab}{}^i - \frac{1}{2}\epsilon^{ab}{}_i\Phi(R)_{ab}{}^i + \frac{1}{2}(\nabla_0\epsilon^{ab})\Phi(\omega)_{ab} - \frac{1}{2}\epsilon^{ab}\Phi(\nabla B)_{ab} \\
& + (\partial_0\epsilon_i)\Phi(B)^i - \epsilon_i\Phi(F)^i + (\partial_0\epsilon)\Phi(A) - \epsilon\Phi(\nabla B) \\
& + (\nabla_0\epsilon^a)\Phi(e)_a - \epsilon^a\Phi(\mathcal{G})_a + (\nabla_0\epsilon^a{}_i)\Phi(\beta)_a{}^i - \epsilon^a{}_i\Phi(\nabla e)_a{}^i \\
& + \frac{1}{2}(\nabla_0\epsilon^A{}_{ij})\Phi(\gamma)_A{}^{ij} - \frac{1}{2}\epsilon^A{}_{ij}\Phi(\nabla\phi)_A{}^{ij} \\
& + \epsilon^{ab}\left(\beta_{[a|0i}P(\beta)_{|b]}{}^i + e_{[a|0}P(e)_{|b]} + B_{[a|c0i}P(B)^c{}_{|b]}{}^i\right) - \epsilon\,\gamma_{A0ij}\rhd_B{}^A P(\gamma)^{Bij} \\
& + \epsilon^a\beta_{b0i}P(B)^{abi} + \epsilon^a{}_i\, e_{b0}P(B)_a{}^{bi}\Bigg)\,.
\end{aligned}
\tag{61}
$$

Here, $\epsilon^{ab}{}_i$, ϵ^{ab}, ϵ_i, ϵ, ϵ^a, $\epsilon^a{}_i$ and $\epsilon^A{}_{ij}$ are the independent parameters of the gauge transformations.

Furthermore, one can employ the gauge generator to calculate the form-variations for all canonical coordinates and their corresponding momenta, by computing the Poisson bracket of the chosen variable $A(t,\vec{x})$ and the generator (61):

$$
\delta_0 A(t,\vec{x}) = \{A(t,\vec{x})\,,G\}\,. \tag{62}
$$

The results are given as follows:

$$
\begin{aligned}
\delta_0\omega^{ab}{}_0 &= \nabla_0\epsilon^{ab}\,, & \delta_0\pi(\omega)_{ab}{}^0 &= -2\epsilon_{[a|}{}^c{}_i\pi(B)_{c|b]}{}^{0i} - 2\epsilon_{[a|}{}^c\pi(\omega)_{c|b]}{}^0\,, \\
& & & \quad +2\epsilon_{[a|}\pi(e)_{|b]}{}^0 + 2\epsilon_{[a|i}\pi(\beta)_{|b]}{}^{0i}\,, \\
\delta_0\omega^{ab}{}_i &= \nabla_i\epsilon^{ab}\,, & \delta_0\pi(\omega)_{ab}{}^i &= -2\epsilon_{[a|}{}^c{}_j\,\pi(B)_{c|b]}{}^{ij} - 2\epsilon_{[a|}{}^c{}_i\,\pi(\omega)_{|b]c}{}^i \\
& & & \quad +2\epsilon_{[a|}\,\pi(e)_{|b]i} + 2\epsilon_{[a|j}\pi(\beta)_{|b]}{}^{ij} \\
& & & \quad +2\epsilon^{0ijk}\,\nabla_{[j|}\epsilon_{ab|k]} + \epsilon^{0ijk}\epsilon_{[a|}\beta_{|b]jk}\,, \\
\delta_0 B^{ab}{}_{0i} &= \nabla_0\epsilon^{ab}{}_i + \epsilon^{[a|}{}_i e^{|b]}{}_0 & \delta_0\pi(B)_{ab}{}^{0i} &= 2\epsilon_{[a|c}\,\pi(B)_{|b]}{}^{ci}\,, \\
& \quad +2\epsilon^{[a|c}B^{|b]}{}_{c0i} + \epsilon^{[a|}\beta^{|b]}{}_{0i}\,, & & \\
\delta_0 B^{ab}{}_{ij} &= 2\nabla_{[i|}\epsilon^{ab}{}_{|j]} + 2\epsilon^{[a|c}B^{|b]}{}_{cij} & \delta_0\pi(B)_{ab}{}^{ij} &= 2\epsilon_{[a|c}\,\pi(B)_{|b]}{}^{cij}\,, \\
& \quad +2\epsilon^{[a|}{}_{[i}e^{|b]}{}_{j]} + \epsilon^{[a|}\beta^{|b]}{}_{ij}\,, & & \\
\delta_0 A_0 &= \partial_0\epsilon\,, & \delta_0\pi(A)^0 &= -\tfrac{1}{2}\epsilon^A{}_{ij}\rhd^B{}_A\,\pi(\gamma)_B{}^{0ij}\,, \\
\delta_0 A_i &= \partial_i\epsilon\,, & \delta_0\pi(A)^i &= \epsilon^{0ijk}\partial_j\epsilon_k - \tfrac{1}{2}\epsilon^A{}_{jk}\rhd^B{}_A\,\pi(\gamma)_B{}^{ijk}\,, \\
\delta_0 B_{0i} &= \partial_0\epsilon_i\,, & \delta_0\pi(B)^{0i} &= 0\,, \\
\delta_0 B_{ij} &= 2\,\partial_{[i|}\epsilon_{|j]} + \epsilon^A{}_{ij}\rhd^B{}_A\,\phi_B\,, & \delta_0\pi(B)^{ij} &= -\epsilon^{0ijk}\partial_k\epsilon\,, \\
\delta_0\beta^a{}_{0i} &= \nabla_0\epsilon^a{}_i - \epsilon^{ab}\beta_{b0i}\,, & \delta_0\pi(\beta)_a{}^{0i} &= -\epsilon_{ab}\pi(\beta)^{b0i} + \tfrac{1}{2}\epsilon^b\pi(B)_{ab}{}^{0i}\,, \\
\delta_0\beta^a{}_{ij} &= 2\nabla_{[i|}\epsilon^a{}_{|j]} - \epsilon^{ab}\,\beta_{bij}\,, & \delta_0\pi(\beta)_a{}^{ij} &= -\epsilon_{ab}\,\pi(\beta)^{bij} + \tfrac{1}{2}\epsilon^b\,\pi(B)_{ab}{}^{ij} \\
& & & \quad -\epsilon^{0ijk}\,\nabla_k\epsilon^a\,, \\
\delta_0 e^a{}_0 &= \nabla_0\epsilon^a - \epsilon^{ab}\,e_{b0}\,, & \delta_0\pi(e)_a{}^0 &= -\epsilon_{ab}\,\pi(e)^{b0} + \tfrac{1}{2}\epsilon^b{}_i\,\pi(B)_{ab}{}^{0i}\,, \\
\delta_0 e^a{}_i &= \nabla_i\epsilon^a - \epsilon^{ab}\,e_{bi}\,, & \delta_0\pi(e)_a{}^i &= -\epsilon_{ab}\,\pi(e)^{bi} + \epsilon^{0ijk}\Big(\nabla_{[j|}\epsilon_{a|k]} + \epsilon_{ab}\beta^{bjk}\Big) \\
& & & \quad +\tfrac{1}{2}\epsilon^b{}_j\,\pi(B)_{ab}{}^{ij}\,,
\end{aligned}
$$

$$
\begin{array}{rclrcl}
\delta_0 \gamma^A{}_{0ij} & = & \nabla_0 \epsilon^A{}_{ij} - \epsilon\, \gamma^B{}_{0ij} \rhd^A{}_B\,, & \delta_0 \pi(\gamma)_A{}^{0ij} & = & \epsilon \rhd^B{}_A\, \pi(\gamma)_B{}^{0ij}\,, \\
\delta_0 \gamma^A{}_{ijk} & = & -\,\epsilon\, \gamma^B{}_{ijk} \rhd_B{}^A + \nabla_i \epsilon^A{}_{jk} & \delta_0 \pi(\gamma)_A{}^{ijk} & = & \epsilon \rhd_A{}^B \left(\pi(\gamma)_B{}^{ijk} + \epsilon^{0ijk}\, \phi_B \right)\,, \\
 & & -\nabla_j \epsilon^A{}_{ik} + \nabla_k \epsilon^A{}_{ij}\,, & & & \\
\delta_0 \phi^A & = & \epsilon\, \phi^B \rhd^A{}_B\,, & \delta_0 \pi(\phi)_A & = & -\epsilon \rhd^B{}_A\, \pi(\phi)_B + \frac{1}{3!}\, \epsilon\, \epsilon^{0ijk} \rhd^B{}_A\, \gamma_{Bijk} \\
 & & & & & -\frac{1}{2} \rhd_{A\,B}\, \epsilon^B{}_{ij}\, \pi(B)^{ij} - \frac{1}{2} \epsilon^{0ijk}\, \nabla_i \epsilon^A{}_{jk}\,,
\end{array}
\tag{63}
$$

These transformations are an extension of the form-variations in the case of the Poincaré 2-group obtained in [17].

7. Conclusions

Let us summarize the results of the paper. In Section 2, we have demonstated in detail how to use the idea of a categorical ladder to introduce the 3-group structure corresponding to the theory of scalar electrodynamics coupled to Einstein–Cartan gravity. We have introduced the topological $3BF$ action corresponding to this choice of a 3-group, as well as the constrained $3BF$ action which gives rise to the standard equations of motion for the scalar electrodynamics. In order to perform the canonical quantization of this theory, the complete Hamiltonian analysis of the full theory with constraints has to be performed, but the important step towards this goal is the Hamiltonian analysis of the topological $3BF$ action. This has been done in Section 3. Here, the first-class and second-class constraints of the theory, as well as their Poisson brackets, have been obtained. In Section 4, we have discussed the Bianchi identities and also the generalized Bianchi identities, since they enforce restrictions in the sense of Hamiltonian analysis, and reduce the number of independent first-class constraints present in the theory. With this background material in hand, in Section 5, the counting of the dynamical degrees of freedom present in the theory has been performed and it was established that the considered $3BF$ action is a topological theory, i.e., the diffeomorphism invariant theory without any propagating degrees of freedom. In Section 6, we have constructed the generator of the gauge symmetries for the theory, and we found the form-variations for all the variables and their canonical momenta.

The results obtained in this paper represent the straightforward generalization of Hamiltonian analysis done in [15] for the Poincaré 2-group, and a first example of the Hamiltonian analysis of a $3BF$ action. The fact that the theory was found to be topological is nontrivial, since it relies on the existence of the generalized Bianchi identities, which have been identified for the first time. In addition to that, it was demonstrated that the algebra of constraint closes, which is an important consistency check for the theory. There is another very interesting aspect of the constraint algebra. Namely, one can recognize, looking at the structure of Equations (34) that the subalgebra generated by the first-class constraint $\Phi(\nabla\phi)_A{}^{ij}$ is in fact an *ideal* of the constraint algebra because the Poisson bracket between this constraint and all other constraints is again proportional to that constraint. It is curious that precisely the constraint $\Phi(\nabla\phi)_A{}^{ij}$ is the only one related to the Lie group L from the 3-group, according to its index structure, and also that the structure constant of the ideal is determined by the action $\rhd$ of the group G on L. Let us also note that the action $\rhd$ appears as well in the structure constants of the algebra between the first-class and second-class constraints.

The results of this work open several avenues for future research. From the point of view of mathematics, the relationship between the algebraic structures mentioned above should be understood in more detail. More generally, one should understand the correspondence between the gauge group generated by the generator (61) and the 3-group structure used to define the theory. This is not viable in the special case of the 3-group discussed in this work, but instead needs to be done in the case of a generic 3-group, where homomorphisms δ and ∂ and the Peiffer lifting $\{\_,\_\}$ are nontrivial. From the point of view of physics, the obtained results represent the fundamental building blocks for the construction of the quantum theory of scalar electrodynamics coupled to gravity, as well as a convenient model to discuss before proceeding to the Hamiltonian analysis and canonical quantization of the full Standard Model coupled to gravity, formulated as a $3BF$ action with suitable constraints [8]. Both the Hamiltonian analysis of constrained $3BF$ models and the corresponding canonical quantization programme need to be further developed in order to achieve these goals. Our work is a first step in this direction.

Finally, let us note in the end that the above list of topics for future research is by no means complete, and there are potentially many other interesting topics that can be studied in this context.

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Abbreviations

The following abbreviations are used in this manuscript:

LQG	Loop Quantum Gravity
BI	Bianchi Identities
GBI	Generalized Bianchi Identities
DoF	Degrees of Freedom
PB	Poisson Bracket

Appendix A. The Equations of Motion for the Scalar Electrodynamics

The action of scalar electrodynamics coupled to Einstein–Cartan gravity is given in the form (12):

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + B \wedge F + e_a \wedge \nabla \beta^a + \phi_A \, \nabla \gamma^A \\ & - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right) \\ & + \lambda^A \wedge \left(\gamma_A - \frac{1}{2} H_{abcA} e^a \wedge e^b \wedge e^c \right) + \Lambda^{abA} \wedge \left(H_{abcA} \varepsilon^{cdef} e_d \wedge e_e \wedge e_f - \nabla \phi_A \wedge e_a \wedge e_b \right) \\ & + \lambda \wedge \left(B - \frac{12}{q} M_{ab} e^a \wedge e^b \right) + \zeta^{ab} \left(M_{ab} \varepsilon_{cdef} e^c \wedge e^d \wedge e^e \wedge e^f - F \wedge e_a \wedge e_b \right) \\ & - \frac{1}{2 \cdot 4!} m^2 \phi_A \, \phi^A \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \,. \end{aligned} \tag{A1}$$

Varying the total action (12) with respect to the variables B_{ab}, B, ω_{ab}, β_a, λ_{ab}, Λ^{abA}, γ^A, λ^A, H_{abcA}, ζ^{ab}, M_{ab}, λ, A, ϕ^A and e^a, one obtains the equations of motion:

$$R^{ab} - \lambda^{ab} = 0 \,, \tag{A2}$$

$$F + \lambda = 0 \,, \tag{A3}$$

$$\nabla B^{ab} - e^{[a|} \wedge \beta^{|b]} = 0 \,, \tag{A4}$$

$$\nabla e^a = 0 \,, \tag{A5}$$

$$B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d = 0 \,, \tag{A6}$$

$$H_{abcA}\varepsilon^{cdef}e_d\wedge e_e\wedge e_f-\nabla\phi_A\wedge e_a\wedge e_b=0\,, \tag{A7}$$

$$\nabla\phi_A-\lambda_A=0\,, \tag{A8}$$

$$\gamma_A-\frac{1}{2}H_{abcA}e^a\wedge e^b\wedge e^c=0\,, \tag{A9}$$

$$-\frac{1}{2}\lambda^A\wedge e^a\wedge e^b\wedge e^c+\varepsilon^{cdef}\Lambda^{abA}\wedge e_d\wedge e_e\wedge e_f=0\,, \tag{A10}$$

$$M_{ab}\varepsilon_{cdef}e^c\wedge e^d\wedge e^e\wedge e^f-F\wedge e_a\wedge e_b=0\,, \tag{A11}$$

$$-\frac{12}{q}\lambda\wedge e^a\wedge e^b+\zeta^{ab}\varepsilon_{cdef}e^c\wedge e^d\wedge e^e\wedge e^f=0\,, \tag{A12}$$

$$B-\frac{12}{g}M_{ab}e^a\wedge e^b=0\,, \tag{A13}$$

$$-\,\mathrm{d}B+\mathrm{d}(\zeta^{ab}e_a\wedge e_b)-\phi_A\rhd_B{}^A\gamma^B-\Lambda^{abA}\rhd^B{}_A\phi_B\wedge e_a\wedge e_b=0\,, \tag{A14}$$

$$\nabla\gamma_A-\nabla(\Lambda^{ab}{}_A\wedge e_a\wedge e_b)-\frac{1}{4!}m^2\phi_A\varepsilon_{abcd}e^a\wedge e^b\wedge e^c\wedge e^d=0\,, \tag{A15}$$

$$\begin{aligned}&\nabla\beta_a+\frac{1}{8\pi l_p^2}\varepsilon_{abcd}\lambda^{bc}\wedge e^d+\frac{3}{2}H_{abcA}\lambda^A\wedge e^b\wedge e^c+3H^{defA}\varepsilon_{abcd}\Lambda_{efA}\wedge e^b\wedge e^c\\&-2\Lambda_{abA}\wedge\nabla\phi^A\wedge e^b-2\frac{1}{4!}m^2\phi_A\,\phi^A\varepsilon_{abcd}e^b\wedge e^c\wedge e^d\\&-\frac{24}{q}M_{ab}\lambda\wedge e^b+4\zeta^{ef}M_{ef}\varepsilon_{abcd}e^b\wedge e^c\wedge e^d-2\zeta_{ab}F\wedge e^b=0\,.\end{aligned} \tag{A16}$$

The dynamical degrees of freedom are the tetrad fields e^a, the scalar field ϕ^A, and the electromagnetic potential A, while the remaining variables are algebraically determined in terms of them. Specifically, Equations (A2)–(A13) give

$$\begin{gathered}\lambda_{ab\mu\nu}=R_{ab\mu\nu}\,,\qquad\omega^{ab}{}_\mu=\triangle^{ab}{}_\mu\,,\qquad\gamma^A{}_{\mu\nu\rho}=-\frac{1}{2e}\varepsilon_{\mu\nu\rho\sigma}\nabla^\sigma\phi^A\,,\\ \Lambda^{abA}{}_\mu=\frac{1}{12e}g_{\mu\lambda}\varepsilon^{\lambda\nu\rho\sigma}\nabla_\nu\phi^A\,e^a{}_\rho e^b{}_\sigma\,,\qquad\beta^a{}_{\mu\nu}=0\,,\qquad B_{ab\mu\nu}=\frac{1}{8\pi l_p^2}\varepsilon_{abcd}e^c{}_\mu e^d{}_\nu\,,\\ H^{abcA}=\frac{1}{6e}\varepsilon^{\mu\nu\rho\sigma}\nabla_\mu\phi^A\,e^a{}_\nu e^b{}_\rho e^c{}_\sigma\,,\qquad\lambda^A{}_\mu=\nabla_\mu\phi^A\,,\\ \lambda_{\mu\nu}=F_{\mu\nu}\,,\quad B_{\mu\nu}=-\frac{1}{2eq}\varepsilon_{\mu\nu\rho\sigma}F^{\rho\sigma}\,,\\ M^{ab}=-\frac{1}{4e}\varepsilon^{\mu\nu\rho\sigma}F_{\mu\nu}\,e^a{}_\rho e^b{}_\sigma\,,\quad\zeta^{ab}=\frac{1}{4eq}\varepsilon^{\mu\nu\rho\sigma}F_{\mu\nu}\,e^a{}_\rho e^b{}_\sigma\,.\end{gathered} \tag{A17}$$

Note that from the Equations (A4)–(A6) it follows that $\beta^a=0$, as in the pure gravity case. The equation of motion (A15) reduces to the covariant Klein–Gordon equation for the scalar field coupled to the electromagnetic potential A,

$$\left(\nabla_\mu\nabla^\mu-m^2\right)\phi_A=0\,. \tag{A18}$$

From Equation (A14), we obtain the differential equation of motion for the field A:

$$\nabla_\mu F^{\mu\nu}=j^\nu\,,\qquad j^\mu\equiv\frac{1}{2}\left(\nabla^\nu\phi^A\rhd^B{}_A\phi_B-\phi_A\rhd_B{}^A\nabla^\nu\phi^B\right)=iq\left(\nabla\phi^*\phi-\phi^*\nabla\phi\right). \tag{A19}$$

Finally, the equation of motion (A16) for e^a becomes:

$$\begin{aligned} R^{\mu\nu} - \frac{1}{2} g^{\mu\nu} R &= 8\pi l_p^2\, T^{\mu\nu}\,, \\ T^{\mu\nu} \equiv \nabla^\mu \phi_A\, \nabla^\nu \phi^A - \frac{1}{2} g^{\mu\nu} \left(\nabla_\rho \phi_A\, \nabla^\rho \phi^A + m^2 \phi_A\, \phi^A \right) &- \frac{1}{4q} \left(F_{\rho\sigma} F^{\rho\sigma} g^{\mu\nu} + 4 F^{\mu\rho} F_\rho{}^\nu \right) . \end{aligned} \tag{A20}$$

The system of Equations (A2)–(A16) is equivalent to the system of Equations (A17)–(A20).

Appendix B. The Calculation of the Gauge Generator

The gauge generator of the theory is obtained by the standard Castellani procedure (see [13] for an introduction). One starts from the generic form for the generator,

$$\begin{aligned} G \;=\; \int_{\Sigma_3} \partial^3 \vec{x} \Big(& \frac{1}{2} (\partial_0 \epsilon^{ab}{}_i) G_{1ab}{}^i + \frac{1}{2} \epsilon^{ab}{}_i G_{0ab}{}^i + \frac{1}{2} (\partial_0 \epsilon^{ab}) G_{1ab} + \frac{1}{2} \epsilon^{ab} G_{0ab} \\ & + (\partial_0 \epsilon_i) G_1{}^i + \epsilon_i G_0{}^i + (\partial_0 \epsilon) G_1 + \epsilon G_0 \\ & + (\partial_0 \epsilon^a) G_{1a} + \epsilon^a G_{0a} + (\partial_0 \epsilon^a{}_i) G_{1a}{}^i + \epsilon^a{}_i G_{0a}{}^i \\ & + \frac{1}{2} (\partial_0 \epsilon^A{}_{ij}) G_{1A}{}^{ij} + \frac{1}{2} \epsilon^A{}_{ij} G_{0A}{}^{ij} \Big)\,, \end{aligned} \tag{A21}$$

where the generators G_0 and G_1 are obtained by the standard prescription [13]:

$$\begin{aligned} G_1 &= C_{PFC}\,, \\ G_0 + \{\, G_1\,,\, H_T \,\} &= C_{PFC}\,, \\ \{\, G_0\,,\, H_T \,\} &= C_{PFC}\,, \end{aligned} \tag{A22}$$

where C_{PFC} is a primary first-class constraint. For example, one choses $G_{1ab}{}^i = \Phi(B)_{ab}{}^i$. From the conditions

$$\begin{aligned} G_{0ab}{}^i + \{\, \Phi(B)_{ab}{}^i\,,\, H_T \,\} = G_{0ab}{}^i + \Phi(R)_{ab}{}^i &= C_{PFC}\,, \\ \{\, G_{0ab}{}^i\,,\, H_T \,\} = C_{PFC}{}^* &= \{\, C_{PFC} - \Phi(R)_{ab}{}^i\,,\, H_T \,\}\,, \end{aligned} \tag{A23}$$

we solve for $G_{0ab}{}^i$ by determining C_{PFC} from the second equation. Evaluating one PB, one can reexpress the second equation in the form:

$$\{\, C_{PFC}\,,\, H_T \,\} = C_{PFC}{}^* + 2\omega_{[a|}{}^d{}_0 \Phi(R)_{|b]d}{}^i = \{\, 2\omega_{[a|}{}^d{}_0 P(B)_{|b]d}{}^i\,,\, H_T \,\}\,. \tag{A24}$$

From the second equality, we recognize that

$$C_{PFC} = 2\omega_{[a|}{}^d{}_0 P(B)_{|b]d}{}^i\,, \tag{A25}$$

which can then be substituted into the first condition above, giving

$$G_{0ab}{}^i = 2\omega_{[a|}{}^d{}_0 \Phi(B)_{|b]d}{}^i - \Phi(R)_{ab}{}^i\,. \tag{A26}$$

One thus obtains

$$\frac{1}{2} (\partial_0 \epsilon^{ab}{}_i)(G_1)_{ab}{}^i + \frac{1}{2} \epsilon^{ab}{}_i G_{0ab}{}^i = \frac{1}{2} \nabla_0 \epsilon^{ab}{}_i \Phi(B)_{ab}{}^i - \frac{1}{2} \epsilon^{ab}{}_i \Phi(R)_{ab}{}^i\,.$$

The other G_0 and G_1 terms are obtained in a similar way, and the generator (61) is derived.

Appendix C. Introduction to 3-Groups

The notion of a 3-*group* is usually introduced in the framework of higher category theory [6]. In category theory, every *group* can be understood as a *category* which has only one element, and morphisms which are all invertible. The group elements are then individual morphisms that map the category element to itself, while the group operation is the categorical composition of the morphisms. In such a case, the axioms of the category guarantee the validity of all axioms of a group. This kind of construction can be generalized to 2-*groups,* 3-*groups* and, in general, *n-groups*. Namely, a 2-group is by definition a 2-category which has only one element, and whose morphisms and 2-morhisms (i.e., morphisms between morphisms) are invertible. Similarly, a 3-group is by definition a 3-category which has only one element, while its morphisms, 2-morphisms, and 3-morphisms are invertible.

The above definition of a 3-group is very abstract, and while theoretically very important, in itself not very useful for practical calculations and applications in physics. Fortunately, there is a theorem of equivalence between 3-groups and the so-called 2-*crossed modules*, which are algebraic structures with more familiar properties [9,10]. For the applications in physics, attention focuses on the so-called *strict Lie* 3-*groups*, and their corresponding differential (Lie algebra) structure, which corresponds to the *differential Lie* 2-*crossed module*. Let us therefore give a brief overview of the latter.

A *differential Lie* 2-*crossed module* $(\mathfrak{l} \xrightarrow{\delta} \mathfrak{h} \xrightarrow{\partial} \mathfrak{g}, \triangleright, \{\_\,,\_\})$ is given by three Lie algebras $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{l}$, maps $\delta : \mathfrak{l} \to \mathfrak{h}$ and ∂: $\mathfrak{h} \to \mathfrak{g}$, together with a map called the Peiffer lifting,

$$\{\_\,,\_\} : \mathfrak{h} \times \mathfrak{h} \to \mathfrak{l}\,, \tag{A27}$$

and an action $\triangleright$ of the algebra $\mathfrak{g}$ on all three algebras.

Let us introduce the bases in the three algebras, $\tau_\alpha \in \mathfrak{g}$, $t_a \in \mathfrak{h}$ and $T_A \in \mathfrak{l}$, and structure constants in those bases, as follows:

$$[\tau_\alpha\,,\tau_\beta] = f_{\alpha\beta}{}^{\gamma}\tau_\gamma\,, \quad [t_a\,,t_b] = f_{ab}{}^{c}t_c\,, \quad [T_A\, T_B] = f_{AB}{}^{C}T_C\,. \tag{A28}$$

Now, the maps ∂ and δ can be written as

$$\partial(t_a) = \partial_a{}^{\alpha}\,\tau_\alpha\,, \qquad \delta(T_A) = \delta_A{}^{a}\,t_a\,, \tag{A29}$$

and the action of the algebra $\mathfrak{g}$ on $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{l}$ as:

$$\tau_\alpha \triangleright \tau_\beta = \triangleright_{\alpha\beta}{}^{\gamma}\,\tau_\gamma\,, \quad \tau_\alpha \triangleright t_a = \triangleright_{\alpha a}{}^{b}\,t_b\,, \quad \tau_\alpha \triangleright T_A = \triangleright_{\alpha A}{}^{B}\,T_B\,. \tag{A30}$$

Finally, the Peiffer lifting can be encoded into coefficients $X_{ab}{}^{A}$ as:

$$\{t_a,\, t_b\} = X_{ab}{}^{A}\,T_A\,. \tag{A31}$$

A differential Lie 2-crossed module has the following properties (we write all equations in the abstract and their corresponding component forms, side by side):

1. The action of the algebra $\mathfrak{g}$ on itself is via the adjoint representation, i.e., $\forall g, g_1 \in \mathfrak{g}$:

$$g \triangleright g_1 = [g, g_1]\,, \qquad \triangleright_{\alpha\beta}{}^{\gamma} = f_{\alpha\beta}{}^{\gamma}\,. \tag{A32}$$

2. The action of the algebra $\mathfrak{g}$ on algebras $\mathfrak{h}$ and $\mathfrak{l}$ is $\mathfrak{g}$-equivariant, i.e., $\forall g \in \mathfrak{g}$, $h \in \mathfrak{h}$, $l \in \mathfrak{l}$:

$$\partial(g \triangleright h) = g \triangleright \partial(h)\,, \qquad \partial_a{}^{\beta}\, f_{\alpha\beta}{}^{\gamma} = \triangleright_{\alpha a}{}^{b}\,\partial_b{}^{\gamma}\,, \tag{A33}$$

$$\delta(g \triangleright l) = g \triangleright \delta(l)\,, \qquad \delta_A{}^{a}\,\triangleright_{\alpha a}{}^{b} = \triangleright_{\alpha A}{}^{B}\,\delta_B{}^{b}\,. \tag{A34}$$

3. The Peiffer lifting is a $\mathfrak{g}$-equivariant map, i.e., for every $g \in \mathfrak{g}$ and $h_1, h_2 \in \mathfrak{h}$:

$$g \rhd \{h_1, h_2\} = \{g \rhd h_1, h_2\} + \{h_1, g \rhd h_2\}\,, \qquad X_{ab}{}^B \rhd_{\alpha B}{}^A = \rhd_{\alpha a}{}^c X_{cb}{}^A + \rhd_{\alpha b}{}^c X_{ac}{}^A\,. \tag{A35}$$

4. For every h_1, $h_2 \in \mathfrak{h}$, the following identity holds:

$$\delta(\{h_1, h_2\}) = [h_1, h_2] - \partial(h_1) \rhd h_2\,, \qquad X_{ab}{}^A \delta_A{}^c = f_{ab}{}^c - \partial_a{}^\alpha \rhd_{\alpha b}{}^c\,. \tag{A36}$$

5. For all l_1, $l_2 \in \mathfrak{l}$, the following identity holds:

$$[l_1, l_2] = \{\delta(l_1), \delta(l_2)\}\,, \qquad f_{AB}{}^C = \delta_A{}^a \delta_B{}^b X_{ab}{}^C\,. \tag{A37}$$

6. For all $h_1, h_2, h_3 \in \mathfrak{h}$:

$$\begin{aligned} \{[h_1, h_2], h_3\} = \; & \partial(h_1) \rhd \{h_2, h_3\} + \{h_1, [h_2, h_3]\} - \partial(h_2) \rhd \{h_1, h_3\} - \{h_2, [h_1, h_3]\}\,, \\ f_{ab}{}^d X_{dc}{}^B = \; & \partial_a{}^\alpha X_{bc}{}^A \rhd_{\alpha A}{}^B + X_{ad}{}^B f_{bc}{}^d - \partial_b{}^\alpha \rhd_{\alpha A}{}^B X_{ac}{}^A - X_{bd}{}^B f_{ac}{}^d\,. \end{aligned} \tag{A38}$$

7. For all $h_1, h_2, h_3 \in \mathfrak{h}$:

$$\begin{aligned} \{h_1, [h_2, h_3]\} = \; & \{\delta\{h_1, h_2\}, h_3\} - \{\delta\{h_1, h_3\}, h_2\}\,, \\ X_{ad}{}^A f_{bc}{}^d = \; & X_{ab}{}^B \delta_B{}^d X_{dc}{}^A - X_{ac}{}^B \delta_B{}^d X_{db}{}^A\,. \end{aligned} \tag{A39}$$

8. For all $l \in \mathfrak{l}$ and $\forall h \in \mathfrak{h}$:

$$\{\delta(l), h\} + \{h, \delta(l)\} = -\partial(h) \rhd l\,, \qquad 2\,\delta_A{}^a X_{\{ab\}}{}^B = -\partial_b{}^\alpha \rhd_{\alpha A}{}^B\,. \tag{A40}$$

Finally, when dealing with various algebra valued differential forms, one multiplies them as differential forms using the ordinary wedge product $\wedge$, and simultaneously as algebra elements using one of maps defined above. For example, the product with an action $\wedge^{\rhd}$ of the $\mathfrak{g}$-valued n-form ρ on the $\mathfrak{h}$-valued m-form η is defined as:

$$\begin{aligned} \rho \wedge^{\rhd} \eta = \; & \frac{1}{n!m!} \rho^\alpha{}_{\mu_1 \dots \mu_m} \eta^a{}_{\nu_1 \dots \nu_n} \tau_\alpha \rhd t_a \, dx^{\mu_1} \wedge \dots dx^{\mu_m} \wedge dx^{\nu_1} \wedge \dots \wedge dx^{\nu_n} \\ = \; & \frac{1}{n!m!} \rho^\alpha{}_{\mu_1 \dots \mu_m} \eta^a{}_{\nu_1 \dots \nu_n} \rhd_{\alpha a}{}^b t_b \, dx^{\mu_1} \wedge \dots dx^{\mu_m} \wedge dx^{\nu_1} \wedge \dots \wedge dx^{\nu_n}\,. \end{aligned} \tag{A41}$$

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Quantum gravity and elementary particles from higher gauge theory

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Abstract

We give a brief overview how to couple general relativity to the Standard Model of elementary particles, within the higher gauge theory framework, suitable for the spinfoam quantization procedure. We begin by providing a short review of all relevant mathematical concepts, most notably the idea of a categorical ladder, 3-groups and generalized parallel transport. Then, we give an explicit construction of the algebraic structure which describes the full Standard Model coupled to Einstein-Cartan gravity, along with the classical action, written in the form suitable for the spinfoam quantization procedure. We emphasize the usefulness of the 3-group concept as a superior tool to describe gauge symmetry, compared to an ordinary Lie group, as well as the possibility to employ this new structure to classify matter fields and study their spectrum, including the origin of fermion families.

1 Introduction

The quantization of the gravitational field is one of the most fundamental open problems of modern theoretical physics. Since the inceptions of general relativity (GR) and quantum field theory (QFT), many attempts have been made over the years to unify the two into a self-consistent description of gravitational and matter fields as basic building blocks of nature. Some of the attempts have developed into vast research areas, such as String Theory, Loop Quantum Gravity, Causal Set Theory, and so on. One of the prominent approaches is Loop Quantum Gravity (LQG) [1, 2], which has branched into the canonical and covariant frameworks, the latter known as the *spinfoam* approach [3].

The spinfoam approach to the quantization of the gravitational field revolves around the idea of providing a precise mathematical definition to the Feynman path integral for the gravitational field,

$$Z = \int \mathcal{D}g \; e^{iS_{GR}[g]} ,$$

where g denotes the gravitational degrees of freedom, and $S_{GR}[g]$ is the GR action expressed in terms of variables g. The strategy of defining the path integral can be roughly expressed in three main steps, called the *spinfoam quantization procedure*:

1. Choose convenient variables g and rewrite the classical action in the form

$$S_{GR}[g] = S_{\text{topological}}[g] + S_{\text{simp}}[g] , \tag{1}$$

where the first term represents a topological theory (with no propagating degrees of freedom), while the second term corresponds to the so-called *simplicity constraint* terms, whose purpose is to transform the full action into a realistic non-topological action with propagating degrees of freedom.

2. Employ the methods of topological quantum field theory (TQFT) to define the path integral for the topological part of the action. This is typically implemented by passing from a smooth spacetime manifold to a simplicial complex (triangulation), and writing the path integral in the form of a discrete state sum,

$$Z = \sum_g \prod_v \mathcal{A}_v(g) \prod_\epsilon \mathcal{A}_\epsilon(g) \prod_\Delta \mathcal{A}_\Delta(g) \prod_\tau \mathcal{A}_\tau(g) \prod_\sigma \mathcal{A}_\sigma(g) \,.$$

   Here g represents the gravitational field variables living on the vertices v, edges ϵ, triangles Δ, terahedra τ, and 4-simplices σ of the simplicial complex, describing its geometry, while the corresponding amplitudes $\mathcal{A}_v(g), \dots, \mathcal{A}_\sigma(g)$ are chosen to render the whole state sum Z independent of the particular choice of the triangulation of the spacetime manifold.

3. Enforce the simplicity constraints of the theory by a suitable deformation of the amplitudes $\mathcal{A}$ and the set of independent variables g, thereby obtaining a modified state sum Z which corresponds to one possible rigorous definition of the realistic gravitational path integral.

Since its inception, the spinfoam quantization procedure has been formulated and implemented for various choices of the classical action, leading to a plethora of *spinfoam models* of quantum gravity, starting from the Ponzano-Regge model for $3D$ gravity [4], and leading up to the currently most sophisticated EPRL/FK model for the realistic $4D$ case [5, 6]. However, one property common to all spinfoam models is the fact that they all describe pure gravity, without matter fields. This is due to the common choice of the classical action — it is the well known BF theory [7], which is usually defined for the Lorentz group $SO(3,1)$, with some form of the simplicity constraint terms. The prototype description of GR in this form is the Plebanski action [8]. The reason why matter fields are absent from all such models lies in the fact that the BF action does not feature tetrad fields at the fundamental level. Instead, the tetrads appear as a consequence of classical equations of motion, and are thus inherently classical, on-shell quantities. This renders the approach based on the BF theory incapable of adding matter fields at the quantum level, since matter is coupled to gravity using precisely the tetrad fields.

The issue of the absence of the tetrad fields at the fundamental level has been successfully resolved in [9], where a categorical generalization has been made, and the $2BF$ action (introduced in [10, 11]) has been employed to build an action for GR, featuring tetrads explicitly in the topological sector of the action. The categorical generalization is based on a concept of a *categorical ladder*, an abstraction scheme introducing a chain of new objects: from categories to 2-categories to 3-categories and so forth. This powerful mathematical language gave rise to the idea that the notion of gauge symmetry in physics may be described by objects other than Lie groups. The new approach is called *higher gauge theory* (HGT), see [12] for an introduction. In the context of the spinfoam quantization procedure, HGT has been successfully applied to build a quantum gravity model, based on the Poincaré 2-group [13] as a gauge symmetry structure, and the corresponding $2BF$ action, leading to the so-called *spincube model* of quantum gravity [9]. Having the tetrads as fundamental fields in the $2BF$ action, the new model could be extended to include matter fields in a straightforward way. Nevertheless, the matter field action does not have the form analogous to (1), which renders the steps 2 and 3 of the spinfoam quantization procedure moot, since they can be applied only to the gravitational sector of the theory.

Thus, a natural need appeared to generalize the theory once more, in order to include the matter fields into the topological sector of the theory, in a similar way that was done to include the tetrad fields. The basic idea was to pass from the notion of a 2-group to a notion of a 3-group as a mathematical descriptor of gauge symmetry [12, 14, 15], giving rise to a topological $3BF$ action. With suitable simplicity constraint terms added, a $3BF$ action perfectly fits together all fields necessary for a unified description of quantum gravity coupled to matter fields — it features tetrads, spin connection, gauge fields, scalar fields and fermions. The explicit construction was done in [16], where the full Standard Model (SM) coupled to GR in the Einstein-Cartan formulation was rewritten in the form (1), suitable for the implementation of the spinfoam quantization procedure and building a full quantum theory. This demostrates the power and expressiveness of the HGT approach, and it provides us with novel mathematical tools to study the algebraic properties of the matter sector of the SM, in analogy to the gauge field sector which is being described in terms of ordinary Lie groups. In this paper we will review the essential properties of the new approach.

The layout of the paper is the following. In section 2 we give a brief introduction to the category theory, categorical ladder, and the notion of n-groups. Our attention focuses on 3-groups, in particular their representation in terms of 2-crossed modules. Section 3 reviews the construction and general properties of the $3BF$ action, and its relationship with the 3-group structure. Then, in section 4 we apply this developed formalism to construct the *Standard Model* 3*-group*, and explicitly build the action for the Standard Model coupled to Einstein-Cartan gravity in the form of the $3BF$ action with suitable simplicity constraints. Section 5 contains our concluding remarks.

2 Category theory and 3-groups

Let us begin by giving a short introduction to the category theory, and in particular the notion of *category theory ladder*, a concept used in higher gauge theory to generalize the notion of gauge symmetry. A nice introduction to this topic can be found in [12] and further technical details in [14, 15].

A category $\mathcal{C} = (Obj, Mor)$ is a structure which has objects and morphisms between them,

$$X, Y, Z, \dots \in Obj\,, \qquad f, g, h, \dots \in Mor\,,$$

where

$$f : X \to Y, \quad g : Z \to X, \quad h : X \to Y, \dots$$

such that certain rules are respected, like the associativity of composition of morphisms, and similar. Similarly, a 2-category $\mathcal{C}_2 = (Obj, Mor_1, Mor_2)$ is a structure which has objects, morphisms between them, and morphisms between morphisms, called 2-morphisms,

$$X, Y, Z, \dots \in Obj\,, \qquad f, g, h, \dots \in Mor_1\,, \qquad \alpha, \beta, \dots \in Mor_2\,,$$

where

$$f : X \to Y, \quad g : Z \to X, \quad h : X \to Y, \dots \qquad \alpha : f \to h\,, \dots$$

such that similar rules about compositions are respected. Then, a 3-category $\mathcal{C}_3 = (Obj, Mor_1, Mor_2, Mor_3)$ additionally has morphisms between 2-morphisms, called 3-morphisms,

$$\Theta, \Phi, \dots \in Mor_3\,, \qquad \Theta : \alpha \to \beta\,, \dots$$

again with a certain set of axioms about compositions of various n-morphisms. One can further generalize these structures to introduce 4-categories, n-categories, ∞-categories, etc. The process of raising the "dimensionality" of a categorical structure is called a *categorical ladder*.

It is useful to understand other algebraic structures as special cases of categories. As a particularly important example, the algebraic structure of a *group* is a special case of a category — it is a category with only one object, while all morphisms (i.e., group elements) are invertible. It is straightforward to verify that axioms of a group follow from this definition and the axioms of a category. Any group can be represented in this way, for example finite groups, Lie groups, and so on.

The notion of a categorical ladder then provides us with a natural way to introduce novel, more general algebraic structures, by extending the above definition to 2-categories, 3-categories, etc. In particular,

- a 2-group is a 2-category with only one object, while all 1-morphisms and 2-morphisms are invertible;
- a 3-group is a 3-category with only one object, while all 1-morphisms, 2-morphisms and 3-morphisms are invertible.

It is important to emphasize that an n-group is not a particular type of group. Instead, it is a different algebraic structure, which shares some of the features of groups, but is governed by a qualitatively different set of axioms.

The framework of higher gauge theory is centered around the idea that gauge symmetries in physics can be better described using these alternative algebraic structures than using the ordinary Lie groups. To that end, our attention will mostly focus on the so-called Lie 3-groups and their corresponding Lie 3-algebras. While the abstract definition in terms of n-category theory is particularly appealing from the conceptual point of view, for applications in physics there exists a more practical way to talk about 3-group. Namely, every strict Lie 3-group is known to be equivalent to a so-called 2-*crossed module*, defined as an exact sequence of three Lie groups G, H and L,

$$L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \tag{2}$$

and equipped with two "boundary homomorphisms" δ and ∂, an action $\triangleright$ of G onto G, H and L,

$$\triangleright : G \times G \to G\,, \qquad \triangleright : G \times H \to H\,, \qquad \triangleright : G \times L \to L\,,$$

and a bracket operation called *Peiffer lifting* over H to L,

$$\{\_\,,\_\} : H \times H \to L\,.$$

Certain set of axioms is assumed to hold true among all these maps. In particular, for all $g \in G$, $h \in H$ and $l \in L$, we have:

- the axiom stating that (2) is an exact sequence,

$$\partial\delta = 1_G\,, \tag{3}$$

- the axiom specifying that the action of G onto itself is conjugation,

$$g \triangleright g_0 = g\, g_0\, g^{-1} \,, \tag{4}$$

- the axioms stating that the action of G on H and L is equivariant with respect to homomorphisms ∂ and δ and the Peiffer lifting,

$$\begin{array}{lcl} g \triangleright \partial h & = & \partial(g \triangleright h) \,, \\ g \triangleright \delta l & = & \delta(g \triangleright l) \,, \\ g \triangleright \{h_1, h_2\} & = & \{g \triangleright h_1, g \triangleright h_2\} \,, \end{array} \tag{5}$$

- and finally the axioms determining the properties of the Peiffer lifting,

$$\begin{array}{lcl} \delta\,\{h_1, h_2\} & = & h_1 h_2 h_1^{-1} (\partial h_1) \triangleright h_2^{-1} \,, \\ \{\delta l_1, \delta l_2\} & = & l_1 l_2 l_1^{-1} l_2^{-1} \,, \\ \{h_1 h_2, h_3\} & = & \{h_1, h_2 h_3 h_2^{-1}\}\, \partial h_1 \triangleright \{h_2, h_3\} \,, \\ \{\delta l, h\}\,\{h, \delta l\} & = & l(\partial h \triangleright l^{-1}) \,. \end{array} \tag{6}$$

Since it is constructed from three Lie groups, a Lie 3-group has a corresponding Lie 3-algebra, also called a *differential* 2-*crossed module*,

$$\mathfrak{l} \xrightarrow{\delta} \mathfrak{h} \xrightarrow{\partial} \mathfrak{g} \,,$$

where $\mathfrak{l}$, $\mathfrak{h}$, $\mathfrak{g}$ are Lie algebras of L, H, G, the maps δ, ∂, $\triangleright$ and $\{\_\,,\_\}$ are inherited from the 3-group via natural linearization, and finally, the set of corresponding axioms applies. In addition to all this, Lie algebras have their own usual Lie structure — the generators,

$$T_A \in \mathfrak{l} \,, \qquad t_a \in \mathfrak{h} \,, \qquad \tau_\alpha \in \mathfrak{g}$$

the corresponding structure constants,

$$[T_A, T_B] = f_{AB}{}^C T_C \,, \qquad [t_a, t_b] = f_{ab}{}^c t_c \,, \qquad [\tau_\alpha, \tau_\beta] = f_{\alpha\beta}{}^\gamma \tau_\gamma \,,$$

and G-invariant nondegenerate symmetric bilinear forms (for example Killing forms),

$$\langle T_A, T_B \rangle_{\mathfrak{l}} = g_{AB} \,, \qquad \langle t_a, t_b \rangle_{\mathfrak{h}} = g_{ab} \,, \qquad \langle \tau_\alpha, \tau_\beta \rangle_{\mathfrak{g}} = g_{\alpha\beta} \,.$$

The main purpose of the 3-group structure is to *generalize the notion of parallel transport* from curves to surfaces to volumes. Namely, given a 4-dimensional manifold $\mathcal{M}$, one defines a 3-connection (α, β, γ) as a triple of 3-algebra-valued differential forms,

$$\begin{array}{lcll} \alpha & = & \alpha^\alpha{}_\mu(x)\, \tau_\alpha\, \mathbf{d}x^\mu & \in \Lambda^1(\mathcal{M}, \mathfrak{g}) \,, \\ \beta & = & \dfrac{1}{2} \beta^a{}_{\mu\nu}(x)\, t_a\, \mathbf{d}x^\mu \wedge \mathbf{d}x^\nu & \in \Lambda^2(\mathcal{M}, \mathfrak{h}) \,, \\ \gamma & = & \dfrac{1}{3!} \gamma^A{}_{\mu\nu\rho}(x)\, T_A\, \mathbf{d}x^\mu \wedge \mathbf{d}x^\nu \wedge \mathbf{d}x^\rho & \in \Lambda^3(\mathcal{M}, \mathfrak{l}) \,. \end{array}$$

Then one can introduce the line, surface and volume holonomies,

$$g = \mathcal{P}\mathrm{exp} \int_{\mathcal{P}_1} \alpha\,, \qquad h = \mathcal{S}\mathrm{exp} \int_{\mathcal{S}_2} \beta\,, \qquad l = \mathcal{V}\mathrm{exp} \int_{\mathcal{V}_3} \gamma\,,$$

and corresponding curvature forms,

$$\begin{array}{rcl} \mathcal{F} & = & \mathbf{d}\alpha + \alpha \wedge \alpha - \partial\beta\,, \\ \mathcal{G} & = & \mathbf{d}\beta + \alpha \wedge^{\triangleright} \beta - \delta\gamma\,, \\ \mathcal{H} & = & \mathbf{d}\gamma + \alpha \wedge^{\triangleright} \gamma - \{\beta \wedge \beta\}\,. \end{array}$$

The 3-group structure ensures that all these quantities are well defined, in particular the surface- and volume-ordered exponentials and the respective holonomies.

3 Higher gauge theories

The basic idea behind the higher gauge theory approach is to employ the structure of n-groups as a mathematical representation of gauge symmetries in physics, generalizing the ordinary notion of gauge symmetry described via a Lie group. Namely, in ordinary gauge theory, the prototype action functional was the so-called BF action [7], based on a chosen gauge group G. In the HGT approach, one generalizes the BF action in accord with the chosen n-group structure, leading to the nBF action. For the case of 3-groups, one defines a $3BF$ action as:

$$S_{3BF} = \int_{\mathcal{M}} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} + \langle C \wedge \mathcal{G} \rangle_{\mathfrak{h}} + \langle D \wedge \mathcal{H} \rangle_{\mathfrak{l}}\,.$$

Here B, C, and D are Lagrange multipliers, in particular a $\mathfrak{g}$-valued 2-form, an $\mathfrak{h}$-valued 1-form, and an $\mathfrak{l}$-valued 0-form, respectively.

As in the case of a BF theory, one can demonstrate that $3BF$ theory is a topological gauge theory, having no local propagating degrees of freedom. Nevertheless, it can be transformed into a physically relevant action by adding the so-called *simplicity constraint terms* to the action, changing the dynamical structure of the theory. The prototype of this procedure is represented by transforming the topological BF theory based on the Lorentz group $SO(3,1)$ into a Plebanski action [8], which describes general relativity.

One can even do more, and provide a physical interpretation of the Lagrange multipliers C and D in the $3BF$ action, as follows:

- the $\mathfrak{h}$-valued 1-form C can be interpreted as the tetrad field, if $H = \mathbb{R}^4$ is the spacetime translation group,

$$C \to e = e^a{}_\mu(x)\, t_a\, \mathbf{d}x^\mu\,,$$

- the $\mathfrak{l}$-valued 0-form D can be interpreted as the set of real-valued matter fields, given some Lie group L,

$$D \to \phi = \phi^A(x)\, T_A\,.$$

An interested reader can see [16] for further details.

4 The Standard Model

One natural question that can be asked is what choice of a 3-group can be relevant for physics. There are various answers to this question, but perhaps the most illustrative example is a choice of the 3-group which reproduces the Standard Model of elementary particles, coupled to general relativity in the Einstein-Cartan version. This is called the *Standard Model 3-group*, and in the remainder of this section we will demonstrate how it can be constructed, step by step.

The first step is to specify the groups G and H as the usual Lorentz, internal, and translational symmetries:

$$G = SO(3,1) \times SU(3) \times SU(2) \times U(1) \,, \qquad H = \mathbb{R}^4 \,.$$

Note that the Poincaré group has been broken into the separate Lorentz and translational parts, and these have been associated with two different groups within the 3-group structure.

The next step is to define the homomorphisms δ and ∂, as well as the Peiffer lifting, to be trivial,

$$\delta l = 1_H = 0 \,, \qquad \partial \vec{v} = 1_G \,,$$

and

$$\{\vec{u}, \vec{v}\} = 1_L \,,$$

for all $l \in L$ and $\vec{u}, \vec{v} \in H$. Additionally, we define the action of the group G on H via vector representation for the $SO(3,1)$ sector and via trivial representation for the $SU(3) \times SU(2) \times U(1)$ sector. Finally, the choice of the group L and the action of G on L will be discussed below. But already now one can verify that all axioms (3)–(6) are satisfied, thus making sure that these choices represent one genuine 3-group.

The next step is to choose the group L. One general property of L that can be determined immediately comes from the second axiom in (6). Namely, due to the trivial choices for the Peiffer lifting and the homomorphism δ, the axiom implies that L must be Abelian. Aside from this, the choice of the group L is guided by physical requirements, as follows.

Begin by rewriting the $3BF$ action in the form

$$S_{3BF} = \int_{\mathcal{M}} B^{\alpha} \wedge \mathcal{F}^{\beta} g_{\alpha\beta} + e^a \wedge \mathcal{G}^b g_{ab} + \phi^A \mathcal{H}^B g_{AB} \,.$$

Since the group G is a direct product of the Lorentz and internal groups, the corresponding indices α of G split according to this structure, as $\alpha = (ab\,,\, i)$, leading to the corresponding splitting of the connection α and its curvature $\mathcal{F}$,

$$\alpha = \omega^{ab} J_{ab} + A^i \tau_i \,, \qquad \mathcal{F} = R^{ab} J_{ab} + F^i \tau_i \,.$$

Here ω^{ab} is the ordinary spin connection 1-form, J_{ab} are Lorentz generators, while A^i are internal gauge potential 1-forms and τ_i the generators of $SU(3) \times SU(2) \times U(1)$. Also, R^{ab} and F^i are the Riemann curvature and gauge field strength 2-forms, respectively. Also, given that the action of $SO(3,1)$ onto $H = \mathbb{R}^4$ is via vector representation, and given that the bilinear symmetric nondegenerate form for H must be G-invariant, the only available choice is

$$g_{ab} = \eta_{ab} \equiv \text{diag}(-1, +1, +1, +1) \,.$$

Finally, given that the matter fields are elements in the Lie algebra $\mathfrak{l}$ of the group L, namely $\phi = \phi^A T_A$, we observe that there should be precisely one real-valued field $\phi^A(x)$ for each generator $T_A \in \mathfrak{l}$. This information allows us to determine the dimension of the algebra $\mathfrak{l}$, by counting the total number of real-valued components of all matter fields in the Standard Model. The matter fields have two sectors — fermions and the Higgs.

The number of the real-valued components of all fermion fields can be counted according to the following scheme:

$$\left.\begin{matrix} \begin{pmatrix} \nu_e \\ e^- \end{pmatrix}_L & \begin{pmatrix} u_r \\ d_r \end{pmatrix}_L & \begin{pmatrix} u_g \\ d_g \end{pmatrix}_L & \begin{pmatrix} u_b \\ d_b \end{pmatrix}_L \\ & & & \\ (\nu_e)_R & (u_r)_R & (u_g)_R & (u_b)_R \\ & & & \\ (e^-)_R & (d_r)_R & (d_g)_R & (d_b)_R \end{matrix}\right\} = 16 \; \frac{\text{Weyl spinors}}{\text{family}} \times$$

$$\times 3 \text{ families } \times 4 \; \frac{\text{real-valued fields}}{\text{Weyl spinor}} \; = 192 \text{ real-valued fields } \phi^A \, .$$

Similarly, the Higgs sector gives us:

$$\left.\begin{pmatrix} \phi^+ \\ \phi_0 \end{pmatrix}\right\} = 2 \text{ complex scalar fields } = 4 \text{ real-valued fields } \phi^A \, .$$

This suggests the structure for L in the form:

$$L = L_{\text{fermion}} \times L_{\text{Higgs}} \, , \qquad \dim L_{\text{fermion}} = 192 \, , \qquad \dim L_{\text{Higgs}} = 4 \, .$$

The structure of L can be further understood by looking at the action of the gauge group G on various components of fields ϕ^A. This is fixed by the choice of the action of G on L, chosen as follows. Given that G is constructed from Lorentz and internal gauge symmetry groups, the action $\triangleright : G \times L \to L$ specifies the transformation properties of each real-valued field ϕ^A with respect to those symmetries. For example, if we look at a Weyl spinor u_b that sits in the doublet

$$\begin{pmatrix} u_b \\ d_b \end{pmatrix}_L \, ,$$

the action $g \triangleright u_b$ (where $g \in SO(3,1) \times SU(3) \times SU(2) \times U(1)$) encodes that u_b consists of 4 real-valued fields which transform as:

- a left-handed spinor with respect to $SO(3,1)$,
- as a "blue" component of the fundamental representation of $SU(3)$,
- and as "isospin $+\frac{1}{2}$" of the left doublet with respect to $SU(2) \times U(1)$.

The action $\triangleright : G \times L \to L$ similarly defines the transformation properties for all other fermions in the theory, as well as for the Higgs field.

From such a definition of the action $\triangleright$, one can observe that G acts on L in precisely the same way across the three fermion families. This implies that L_{fermion} can be written as

$$L_{\text{fermion}} = L_{\text{1st family}} \times L_{\text{2nd family}} \times L_{\text{3rd family}} \, , \qquad \dim L_{k\text{-th family}} = 64 \, .$$

Ultimately, given that the components of Weys spinors mutually anticommute, given that the group L is Abelian, and given that it has the structure and dimension as given above, we can fix the choice of the group L which corresponds to the Standard Model as

$$L = \mathbb{R}^4(\mathbb{C}) \times \mathbb{R}^{64}(\mathbb{G}) \times \mathbb{R}^{64}(\mathbb{G}) \times \mathbb{R}^{64}(\mathbb{G}) \,,$$

where $\mathbb{G}$ is the algebra of Grassmann numbers. This completes the construction of the Standard Model 3-group.

The final step in specifying the theory is to spell out its classical action. As was previously discussed, the action has the form of a $3BF$ action, with the addition of appropriate simplicity constraints which will transform it into a non-topological theory, i.e., a theory with local propagating degrees of freedom. The choice of the Standard Model 3-group completely fixes the structure of the $3BF$ action, and the only thing left to do is to add the appropriate simplicity constraints. The details of the construction of these terms is given in detail in [16], and will not be repeated here. We will only quote the result,

$$S_{SM+EC} = S_{3BF} + S_{\text{simp}} \,,$$

where

$$S_{3BF} = \int B_{\hat{\alpha}} \wedge \mathcal{F}^{\hat{\alpha}} + e_{\hat{a}} \wedge \mathcal{G}^{\hat{a}} + \phi_{\hat{A}} \wedge \mathcal{H}^{\hat{A}} \,,$$

and

$$\begin{aligned} S_{\text{simp}} = & \left(B_{\hat{\alpha}} - C_{\hat{\alpha}}{}^{\hat{\beta}} M_{cd\hat{\beta}} e^c \wedge e^d\right) \wedge \lambda^{\hat{\alpha}} - \left(\gamma_{\hat{A}} - e^a \wedge e^b \wedge e^c C_{\hat{A}}{}^{\hat{B}} M_{abc\hat{B}}\right) \wedge \lambda^{\hat{A}} \\ & -4\pi i \, l_p^2 \, \varepsilon_{abcd} e^a \wedge e^b \wedge \beta^c \phi_{\hat{A}} T^{d\hat{A}}{}_{\hat{B}} \phi^{\hat{B}} \\ & +\zeta^{ab}{}_{\hat{\alpha}} \wedge \left(M_{ab}{}^{\hat{\alpha}} \varepsilon^{cdef} e_c \wedge e_d \wedge e_e \wedge e_f - F^{\hat{\alpha}} \wedge e_c \wedge e_d\right) \\ & +\zeta^{ab}{}_{\hat{A}} \wedge \left(M_{abc}{}^{\hat{A}} \varepsilon^{cdef} e_d \wedge e_e \wedge e_f - F^{\hat{A}} \wedge e_a \wedge e_b\right) \\ & -\varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \left(\Lambda + M_{\hat{A}\hat{B}} \phi^{\hat{A}} \phi^{\hat{B}} + Y_{\hat{A}\hat{B}\hat{C}} \phi^{\hat{A}} \phi^{\hat{B}} \phi^{\hat{C}} + L_{\hat{A}\hat{B}\hat{C}\hat{D}} \phi^{\hat{A}} \phi^{\hat{B}} \phi^{\hat{C}} \phi^{\hat{D}}\right) . \end{aligned}$$

See [16] for details and notation.

By varying the action with respect to all variables, and with a little technical effort, one can demonstrate that the corresponding equations of motion are precisely the classical equations of the Standard Model, coupled to general relativity in the Einstein-Cartan formulation.

5 Conclusions

Let us summarize the results of the paper. In section 2 we have given a short introduction into the category theory, introduced the notions of categorical ladder and n-categories, and in the resulting framework, provided a definition for the notion of an n-group. Our attention focused on the case of 3-groups, which are relevant for applications in physics, and the equivalent notion of a 2-crossed module, which is more convenient for practical applications. Section 3 was devoted to introducing the higher gauge theory formalism and the $3BF$ action corresponding to a choice of a 3-group, as a generalization of the well known BF action in terms of the categorical ladder. Also, we have interpreted the additional Lagrange multipliers appearing in the $3BF$ action as the tetrad and matter fields, providing the setup for the application in physics. This application was then demonstrated in detail in section 4, where the Standard Model 3-group has been defined, and utilized to construct a physically relevant constrained $3BF$ action, which is classically equivalent to the Standard Model of elementary particles coupled to general relativity in the Einstein-Cartan formulation. This is the main result, which successfully establishes the first step of the spinfoam quantization procedure, and opens up a possibility of straightforward implementation of the second and third steps, hopefully leading to a full model of quantum gravity with matter.

It should be noted that the most important feature of the higher gauge theory framework is its ability to treat gravity, gauge fields, fermions and scalar fields on completely equal footing, describing all of them via the underlying algebraic structure of a 3-group. The 3-group also provides us with a natural geometric description of a generalized notion of parallel transport, namely along a surface and along a volume, in addition to the standard notion of parallel transport along a curve. This relationship opens up a possibility for a fully geometric interpretation of all fields present in physics.

Moreover, just as the gauge group dictates the number and properties of gauge fields in Yang-Mills theories, the sector of the 3-group described by the Lie group L determines the number and properties of the fermion and scalar fields. This fact enables us to classify the spectrum of matter fields in terms of group theory, generalizing the constructions present in the Standard Model, where only gauge fields are classified in such terms. The choice of the group L thus opens up novel avenues for research on the unification of all fields, and specifically the origin of particle families, Higgs and fermion sectors, and so on.

Finally, the higher gauge theory framework may have applications in other areas of physics and mathematics as well, and various possible research directions are yet to be explored.

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Possibilities for Parallelizing Simplicial Complexes Simulation

Dušan Cvijetić, Nenad Korolija, and Marko Vojinović

***Abstract*—This manuscript presents potentials for parallelizing simulation of simplicial comple es. The implementation of most important fields and methods of classes for storing simplicial comple es and -simplices is followed by wrapper classes for simplicial comple es and -simplices respectively. Infrastructure for communication between essage Passing Interface (PI) processes along with helper functions is e plained further in the manuscript. nce multiple data are prepared to be sent from each PI process to other PI processes, sending and receiving is performed in the bac ground. ecause of the stall introduced by using PI directives, the amount of data to be transmitted is ma imized by processing multiple operations over simplicial comple es in parallel. This requires the method for loc ing simplicial comple es and -simplices by the owner PI process until all the requests are processed. oc ing mechanism and supporting simplicial comple class actions regarding loc ing is not in the scope of this manuscript.**

***Index Terms*— implicial comple ; -simple ; triangulation; manifold; PI; parallelization.**

I. Introduction

In modern theoretical physics, a lot of problems are too complicated for study using analytical methods, and one needs to resort to numerical techniques. Among those problems, an especially important class deals with evaluation of functions over simplicial complexes. A simplicial complex [1] is a piecewise-linear approximation of a smooth spacetime manifold [2] and is typically 4-dimensional or higher. Functions over a simplicial complex represent physical fields on spacetime, and one commonly employs path integral evaluations of such structures to extract expectation values of observables. For example, in Lattice Quantum Chromo-dynamics, one employs such numerical techniques to predict the theoretical values for the masses of elementary particles called hadrons [3]. Also, in Causal Dynamical Triangulations approach to quantum gravity [4,5], one uses these techniques to evaluate spectral dimension of spacetime, and study various properties of phase space of triangulated manifolds. Finally, in the Regge Quantum Gravity approach [6,7,8] one can study the entanglement properties of matter fields and gravity described by the Hartle-Hawking wavefunction [9,10], again using the techniques of numerical evaluation of path integrals over simplicial complexes.

It goes without saying that all such calculations are exceptionally expensive in computation time. Typically, one develops custom-made code, heavily optimized to solve precisely one specific problem, and executes it over months-long periods on hardware dedicated for high performance computing (HPC), usually clusters with thousands of work nodes. Such enormous calculational efforts are usually unavoidable due to the nature of the problems that need to be solved.

Nevertheless, at least for one class of such problems, it may be possible to construct a more general algorithm and structures which would provide a common basis for solving an all-encompassing class of problems using the same underlying software, while intrinsically exploiting the parallelization possibilities of the code itself and the distributed nature of the underlying hardware. Our aim is to develop such a generic software library, which could be used to solve a whole host of physics problems in the same way and optimize it for parallelized HPC environments. In this work we present the first steps towards the construction of such a library. This approach of developing common code for a whole class of problems has not been attempted so far because research teams are usually concentrated on solving only one specific problem and opt to construct custom code for that problem. However, in our opinion, a generic software library, which would provide support for a whole class of problems simultaneously, would open new avenues for numerical research, since one could use the same code to study new, yet unexplored problems as well as old well-known ones.

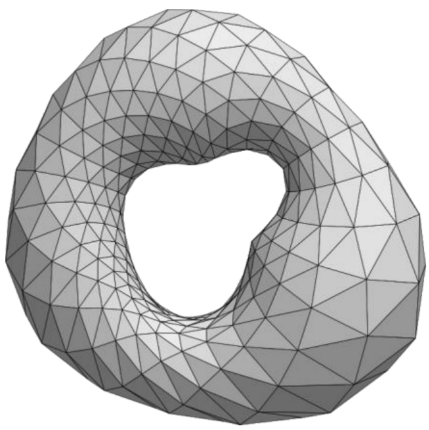

Fig. 1. Simplicial complex of a torus (source: Wikipedia).

The fundamental structure which lies at the core of the whole numerical method is the notion of a *simplicial comple* . A simplicial complex is a combinatorial structure which is easiest to understand as a generic lattice-like mesh,

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whose cells are called *simplices*, and are connected to each other along their boundaries to form the simplicial complex of a given dimension. The purpose of the whole structure is to approximate the smooth spacetime manifold with a discrete structure which is more convenient for numerical methods.

The most elementary simplex is a simplex of level zero, often called *0-simple* or *erte* – it is just a dimensionless point with no structure. Next is the *1-simple* , also called an *edge* – it is a one-dimensional line with two vertices at its boundaries. At level two we have the *2-simple* or *triangle*, whose boundary are three edges and their vertices. The *3-simple* , also known as the *tetrahedron*, has the boundary made of four triangles and their edges and vertices. The procedure of constructing simplices can be done for arbitrary dimension, giving rise to the notion of a *k-simple* , whose level (i.e. natural dimension of space in which it is defined) is equal to any positive integer k. The most commonly used example is the *4-simple* , also called *pentachoron* – a 4-dimensional figure whose boundary consists of 5 tetrahedra, 10 triangles, 10 edges and 5 vertices. In most applications in physics, the spacetime manifold is considered to be 4-dimensional, and it is cut into a lattice-like structure made of 4-simplices, which are glued together along their boundary tetrahedra. The resulting structure is a simplicial complex of dimension 4. Fig. 1 depicts an intuitive example of a 2-dimensional simplicial complex of a torus.

Given a simplicial complex, one typically wants to introduce functions that are evaluated on it. These are commonly called *colors* and are assigned via their values to each k-simplex within in the complex. In other words, some colors live on vertices, some on edges, some on triangles, and so on. The colors are a natural discretization of the notion of a *field* over a manifold. For example, just like electric and magnetic fields have a value at each point of a smooth spacetime, analogously the colors have values at each k-simplex in the simplicial complex.

Depending on the type of the problem at hand, algorithms that are used to evaluate required quantities on a simplicial complex can vary in complexity, from conceptually simple Monte Carlo integration techniques, to vastly complicated traversal and ray-tracing algorithms, to various methods for solving functional partial differential equations. Due to the variability of the complexity of all these algorithms, dictated by the nature of the problem at hand, it is helpful to develop the underlying software simulator to exploit the parallelization avenues that are intrinsic to the simplicial complexes and k-simplices themselves, so that the simulator can exploit parallel hardware environments even for algorithms that are themselves hard to parallelize. This helps the code developer with overall optimization and application to HPC hardware architectures. In what follows, we shall demonstrate a set of possible approaches to these intrinsic parallelization techniques.

II. N-Dimensional Simplicial Complexes

This section describes data structures used in the simulator of simplicial complexes from the point of view of their suitability for parallelizing the simulator execution. Data demanding structures are of main interest for optimizing the communication between processing units. Along with those, data that describes the structure and needs to be updated on multiple processing units will be described in detail. Further, the amount of data that needs to be exchanged and the frequency of expected changes will be compared to the pyramid, where top elements demand less memory, but require more often communication.

The parallelization is simulated using the MPI framework. The simulator is implemented in C++, and, as a result, the parallelization framework is built on top of the simulator. As improving the simulator of simplicial complexes is an ongoing process, the possibility for accelerating the computation is simulated based on the requirements.

Simplicial complexes are formed out of k-simplices at various levels. Simplicial complexes at level zero represent vertices. The structure of each vertex is stored in *Simple* class. Simplicial complexes at level one represent edges. Each edge consists of two vertices. As it is the case with vertices, information about edges are also kept in a *Simple* class. However, while vertices can be independent of other vertices, representing separate simplicial complexes, each edge must have at least two vertices defined as neighbors. Neighbor of an k-simplex is defined also as a k-simplex that the first k-simplex relies on. Neighboring relation is symmetrical. Therefore, if two vertices are neighbors of an edge, edge is also the neighbor of both vertices. Further, edges can form a triangle. By analogy, neighbors of triangle are three edges, but also the triangle is neighbor of these edges. The neighboring relation spans more than one level up or down. The triangle has also three vertices as neighbors and the opposite.

Simplicial complex representing a triangle consists of a k-simplex representing a triangle along with all neighbors of the triangle. Simplicial complex class is used for storing information about simplicial complexes. As it has elements field that is a pointer to pointer of k-simplices, it is also used for keeping neighbors of each k-simplex.

III. Parallelizing Simplicial Complexes Simulation

Parallelizing operations over simplicial complexes is implemented by splitting the structure over multiple MPI processes. First, we can consider a single simplicial complex system, as the most general approach. If no screen coordinates for k-simplices are assigned, we can artificially assign this type of color, so that we can present k-simplices in 2D space. Further, we can imagine multiple planes, where each plane is responsible for keeping k-simplices of one dimension. This way, we can consider n-dimensional simplicial complex as a pyramid that we observe from the bird's eye view. Now we could have a bottom-up approach, where k-simplices of dimension zero are divided onto MPI processes based on their screen coordinates. Going up, each MPI process would store higher dimensional k-simplices that have those that are one level below as their neighbors. When a k-simplex has neighbors on one level below that belong to multiple MPI processes, this k-simplex gets copied to all MPI processes involved. Finally, all MPI processes would keep the highest-level k-simplex. In the case of multiple simplicial complexes, they could be split over MPI processes based on the same bottom-up approach.

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The notion of determining the MPI process where a k-simplex is located is hidden by using wrapper functions, so that the calculation operations are performed as if all k-simplices would have been on the same MPI process, i.e. as if the simulation was executed serially. Each wrapper function can keep either a pointer to the structure, if it exists on the same MPI process, and the ID used for finding the structure on the owner MPI process.

Algorithm 1 describes the most important aspects of simplicial complex classes. First, a basic *SimpComp* class is given, followed by the wrapper class *irtualSimpComp* used for parallelization.

Algorithm 1: Declaration of simplicial complex classes.

```
class SimpComp{
public:
    SimpComp(int dim);
    SimpComp(string s, int dim);
    ~SimpComp();
    // Creating new KSimplex
    // at level k:
    VirtualKSimplex* create_ksimplex(
        int k);
    void update_owner(int owner);

    string name;
    int D;
    vector< vector<
        VirtualKSimplex *> > elements;
};
class VirtualSimpComp{
public:
    SimpComp *find_simpcomp;

    int id;
    int ownerRank;
    SimpComp *simpComp;
};
```

Algorithm 2 describes the most important aspects of k-simplices classes. A basic *Simple* class is followed by the wrapper class *irtual Simple* used for parallelization.

Algorithm 2: Declaration of k-simplex classes.

```
class KSimplex{
public:
    KSimplex();
    KSimplex(int k, int D);
    ~KSimplex();
    bool find_neighbor(
            VirtualKSimplex *k1);
    void add_neighbor(
            VirtualKSimplex *k1);

    int k; // level
    int D; // dimension
    VirtualSimpComp *neighbors;
    vector<Color *> colors;
};
class VirtualKSimplex{
public:
    KSimplex *find_ksimplex();

    int id;
    int ownerRank;
    KSimplex *ksimplex;
};
```

In both algorithms, wrapper functions store a pointer to the base class object, if such exists on a local MPI process. Otherwise, the value is *nullptr*, and the data is searched for on the so called *owner ank* based on unique identifier called *id*. Owner of this k-simplex can issue multiple requests while it holds a lock.

IV. Infrastructure for Communication Between MPI Processes

The communication between MPI processes is organized as follows. Each MPI process is preparing the data to be sent to other MPI processes. Order of operations prepared for other MPI processes is not important. All requests to other MPI processes for processing are packed in to_rank vector of vectors of unsigned char.

Each type of primitive data is serialized into the array of unsigned characters as it will be explained in the following section. Each prepared byte is pushed to the back of the vector of unsigned characters. Once all the data is prepared, the data is sent to other MPI processes in the background using *MPI Isend* directive. If a reference to the vector of array of unsigned characters is called *ec*, the pointer to the array is obtained by calling member function *data* of vector class from standard template library. After issuing all *MPI Isend* directives, waiting for each of sending to finish is achieved using *MPI Wait*.

Similarly receiving the data from other MPI processes is implemented in the background using *MPI Irec* , followed by *MPI Wait*, once the data is needed for the processing. The data is received into array of unsigned characters, that is further packed into vector of vectors of unsigned characters called from_rank for simple processing.

V. MPI Supporting Functions

As already mentioned, variables are serialized into the array of unsigned characters using the following syntax:

```
*( (__typeof__ (variable) *) (array + nArray) ) = variable;
nArray += sizeof(variable);
```

Here, *array* is array of unsinged characters where the data stored in the variable is serialized, and *nArray* is the number serialized bytes in the array.

Similarly, a variable is read and prepared into the to_rank using the following syntax:

```
__typeof__ (variable) temp_var = variable; \
int nBytes = sizeof(temp_var); \
for(int iByte = 0; iByte < nBytes; iByte++) \
   to_rank[rankNumber].push_back(
         ((unsigned char *) &temp_var) [iByte] );
```

This can be further optimized, but the optimization is out of the scope of this research.

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The communication between MPI processes is continued for as long as any MPI process requires further communication with other MPI processes. This is achieved using the following source code, where the MPI process that requires further communication sets variable *to send* to one:

```
int to_receive = 0; // A rank required communication
MPI_Allreduce(&to_send, &to_receive, 1, MPI_INT,
      MPI_SUM, MPI_COMM_WORLD);
```

After *MPI Allreduce* is executed, all MPI processes will have the information whether they have to communicate further in *to recei e* variable.

VI. Parallelization Possibilities Using Dataflow Paradigm

This simulator issues the same set of computer architecture instructions repeatedly. As in majority simulator of physical phenomena, the number of instructions is dependent on the precision of the model and is limited by the computing resources and the total simulation time requirement. These conditions are exactly what is required for a program to be suitable for acceleration using the dataflow paradigm [11]. Programming dataflow architectures requires programming skills that are higher than those needed for programming conventional von Neumann architectures. One of the possibilities is to write a program in a VHDL. More suitable solution to most of the programmers would be to exploit the framework that enables writing source code in a Java-like language, which gets automatically translated into the FPGA image [12,13]. Even in this case, the effort needed for programming such architectures is higher [14]. Besides programming dataflow architecture for the simplicial complex simulator, appropriate scheduling scheme is also needed for efficient running of multiple jobs simultaneously [15].

As the number of operations that can be applied to simplicial complexes can lead to several days' simulation time or even more, having in mind the aging and the probability of failure of supercomputing nodes [16], we have decided to write restarts after given number of simulations defined by the user, so that the calculation can continue from the last stored state.

VII. Conclusion

In this work we have presented the basics of the paralellization techniques that can be applied to the structure of a simplicial complex, which underlies a host of research problems in theoretical physics (see also our accompanying paper [17]). These problems tend to be computationally extremely expensive, and the common underlying software that enables parallelization at the level of the basic data structure can possibly go a long way towards optimization of code for numerical study using heavily parallel hardware platforms such as HPC clusters. In particular, the simplicial complex naturally allows for various aspects of parallelization, and we have described the basic classes, corresponding MPI communication infrastructure, supporting functions and the dataflow paradigm employed for the construction.

One should note that our work represents just a first step towards a full working software implementation, and much more effort is needed to properly implement, optimize and test the resulting code in real world environments. All that is the topic for future work. In particular, the data regarding the experimental evaluation, which would compare the proposed parallelization method to ordinary sequential methods still needs to be gathered and analyzed. Nevertheless, this first step is fundamental, and it is conceptually important since it represents a paradigm in which parallelization is implemented dominantly at the level of the simplicial complex as the underlying data structure, rather than at the level of the particular algorithm that aims to solve some particular problem using these data structures.

Finally, we note that our code, once properly developed, may possibly find applications not just in theoretical physics, but also in other disciplines of science, technology and engineering.

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Infrastructure for Simulating n-Dimensional Simplicial Complexes

Dušan Cvijetić, Nenad Korolija, and Marko Vojinović

***Abstract*—We present an infrastructure for simulating simplicial comple es. The classes for storing the structure of simplicial comple es and simplices are e plained in detail, for arbitrary dimension.**

The implementation is tested using functions for seeding simplicial comple es and for printing them on the screen. eside these functions, the supporting classes and the function for assigning unique identifiers and screen coordinates is also e plained.

esults of simulation show that there are potentials for the simulator to be used for big data problems, although appropriate e perimental results are still being collected. uture wor includes parallelizing the e ecution of the simulator using supercomputing architectures.

***Index Terms*— implicial comple ; triangulation; manifold; algebraic topology.**

I. Introduction

A manifold is one of the fundamental concepts in mathematics [1], and its importance in applications in physics, technology and engineering cannot be overstated. Virtually all modern physics describes the world using *field theory* [2], in which all physical quantities (fields) are represented as functions over some manifold (for example, spacetime). In technology, manifolds appear in all forms and guises, whenever one needs to deal with curved surfaces --- from civil engineering to graphics in video games.

While most of the interest in science and engineering revolves around *smooth* manifolds, for the purpose of studying manifolds using numerical techniques, the attention focuses on the so called *piecewise-linear* manifolds [3], which can intuitively be imagined as a structure made out of small flat cells called *simplices,* arranged like bricks into a structure which models a manifold. The procedure of approximating a smooth manifold with a piecewise-linear one is commonly called *triangulation,* see Fig. 1.

Within the framework of algebraic topology, the formal mathematical structure which describes piecewise-linear manifolds is called a *simplicial comple* . For the purpose of this article, we provide an informal descriptive definition of a simplicial complex, without mathematical rigour. A simplicial complex is a combinatorial structure, containing the information about *simplices* of various dimensions that make up a complex, and the information about how simplices are connected to each other. A *k-simple* is an elementary building block of a simplicial complex. It is an elementary geometrical "cell" of dimension k, which is being used to build simplices of higher dimension, and the entire simplicial complex. For k = 0, the simplex is called a *erte* , it is represented geometrically as a single point, and has no internal structure. The k = 1 simplex is called an *edge,* geometrically represented as a single straight line, having two vertices at its boundary. For k = 2, the simplex is a *triangle,* having three boundary edges and three vertices. The case k = 3 describes a *tetrahedron*, having four boundary triangles, six edges and four vertices. One can go further into higher dimensions: k = 4 represents a simplex called *pentachoron* – it is a 4-dimensional figure, having five boundary tetrahedra, 10 triangles, 10 edges and five vertices. In general, one can introduce a k-simplex for arbitrary dimension k, also called *le el.*

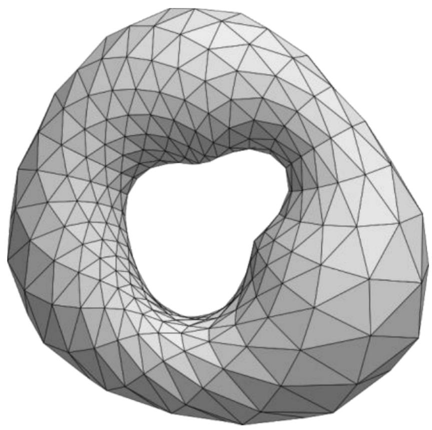

Fig. 1. Simplicial complex of a torus (source: Wikipedia).

Given a set of simplices, one can "glue them up" into a bigger geometrical structure, called simplicial complex. In order to describe a manifold of dimension D, a simplicial complex is constructed by gluing a set of D-simplices by identifying their common boundary (D-1)-simplices. Naturally, this implies the identification of all corresponding sub-simplices of level k < D-1 as well. The resulting simplicial complex is homeomorphic to a piecewise-linear manifold of dimension D.

The most important information about the simplicial complex, aside from its dimension D, is the data that tells one

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which simplices are glued to which. This gives rise to a notion of a *neighborhood* of a k-simplex, which is a set of all simplices which contain a given simplex as its sub-simplex (called super-neighbors) and simplices which are contained in a given simplex (called sub-neighbors). Each k-simplex (for $0 \leq k \leq D$) in the complex has its set of neighbors, where by definition a simplex is not a neighbor of itself (this is convenient to avoid infinite loops when traversing a complex). The neighborhood structure of the entire complex determines the *topology* of the corresponding manifold.

While manifolds of various topologies are important in their own right in mathematics, the applications in physics and engineering typically introduce functions over manifolds, such as distances, areas and volumes, temperature, electric and magnetic fields, etc. In the language of simplicial complexes, these functions are commonly called *colors*, and are assigned to simplices of various level k within the complex. Given a k-simplex, one can assign to it multiple colors, representing the value of a given function when evaluated on the k-simplex. A prototype example of colors is the geometry of a simplicial complex: each k-simplex is assigned its “size” according to its geometry --- each 1-simplex (an edge) is assigned a real number representing its length, each 2-simplex (a triangle) is assigned a real number representing its area, tetrahedra are assigned volumes, and so on. Other examples are abound --- vertices can be assigned a temperature, edges can be assigned vectors of electric field, and so on. Depending on the problem at hand, one may or may not impose relationships between various colors, such as that the area of a triangle is consistent with the length of its edges, or similar. These relationships are collectively called *constraints*.

In most everyday applications, one is interested in manifolds of dimension 1 and 2 (curves and surfaces). However, within the context of theoretical physics, one often needs to deal with manifolds of higher dimension – most commonly 3, 4, 5, 10, 11 and 26, while more sporadically anything in between and above. One of the typical scenarios is *uantum gra ity* [4,5], a vast research area of fundamental theoretical physics, where the notion of spacetime is described as a piecewise-linear manifold of dimension D=4 or higher [6,7]. In order to apply numerical techniques to study the manifolds in such research disciplines, it is necessary to formulate and implement structures and algorithms which describe colored simplicial complexes of arbitrarily large dimension, in a uniform and optimal way. In what follows, we describe one such implementation, which is purposefully designed to mimic the mathematical structure of a simplicial complex as close as possible, while simultaneously providing efficient numerical techniques for the manipulation and study of such structures.

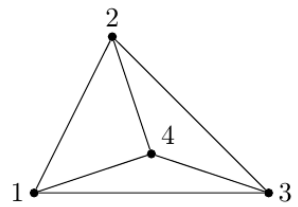
I. N-Dimensional Simplicial Complexes

This section describes the structure of simplicial complexes, and explains an example C++ implementation of classes for storing simplicial complexes.

Simplicial complexes consist of k-simplices at different levels. Given a simplicial complexes of dimension D, these elements include k-simplices for each level from zero to D. Elements at level zero are vertices, elements at level one are edges, elements on level two are triangles, etc. Finally, there are elements of highest level D. The representative source code of class for simplicial complexes is given in Algorithm 3 from the Appendix. The source code is pruned from comments and unnecessary functionalities for the presentation of the simulator.

K-simplex stores the level it has, the dimension of the simplicial complex it belongs to, neighboring elements and colors assigned to it.

Neighboring elements of a k-simplex are defined as k-simplices that this k-simplex is touching. Since these can be on various levels, the structure of neighbors is the same as for the simplicial complex. Therefore, the two main classes are mutually connected.




```
Printing SimpComp tetrahedron, D = 3
Simplices k = 0:
1, 2, 3, 4
Simplices k = 1:
(1-2), (1-3), (1-4), (2-4), (2-3), (3-4)
Simplices k = 2:
(1-2-3), (1-3-4), (1-2-4), (2-3-4)
Simplices k = 3:
(1-2-3-4)
```

Fig. 2. Tetrahedron and a corresponding output of the simplicial complexes simulator.

One possible implementation of the neighboring elements is to store only neighbors from one level above, and one level beneath (first sub-neighbors and first super-neighbors). The lower- and higher-level neighbors can be deduced following the structure of the first neighbors. However, we have opted for storing neighbors from all levels, giving us the opportunity to divide the structure onto multiple computing nodes and run the code in parallel. At current state, the simulator is running on a single CPU.

The instructions a CPU is executing are repeated over and over again, which makes this simulator suitable for acceleration using the dataflow paradigm [8,9]. The effort required for programming such architectures is higher than for conventional von Neumann architectures [10], but the simulator is suitable for transforming the C++ source code automatically [11]. Executing multiple simplicial complex operations in parallel requires appropriate scheduling

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techniques [12].

Each k-simplex (including all vertices, edges, triangles, etc.) can be colored with different types of color. Example colors include:

- k-simplex name,
- unique identifier of k-simplex,
- boundary color of k-simplex,
- screen coordinates.

These colors are included in our simplicial complex simulator, but the structure of the simulator allows adding additional user defined colors.

The representative source code of the class for k-simplices is given in Algorithm 4 from the Appendix. Just like it is the case with simplicial complexes, this source code is pruned for better clarity.

For simulation purposes, we have developed functions for seeding simplicial complexes at various levels, as it will be explained in the following section. In addition, coloring and printing simplicial complexes is also implemented. Pretty printing (or compact printing) prints k-simplices at all levels, where k-simplices of level higher than zero are printed as tuples consisting of unique identifiers (IDs) of their vertices. Fig. 2 shows an example tetrahedron (i.e. simplicial complex of dimension D = 3 consisting of a single 3-simplex and its sub-simplices) whose vertices are colored with unique identifiers that auto-increment after each assignment of the unique color to a vertex. Details of the implementation of compact printing is also explained in this manuscript.

Screen coordinates can be attached to vertices of the tetrahedron. Therefore, it can be drawn on the screen. However, there is no need to assign coordinates. They are just a convenient way to show an object on a screen. Similarly, there is no need to assign unique ID to any vertex. In the previous example, if a vertex with unique ID four would not have a unique ID assigned to it, the tetrahedron could still be printed out, but with word "Simplex" being printed out in place of number four.

II. Seeding Simplicial Complexes

This section describes seeding simplicial complexes using C++ implementation of function *seed single edge* . The example source code for seeding a single edge is used for demonstrating purposes.

The process of seeding simplicial complexes will be explained using the source code shown in Algorithm 1. The source code is pruned from comments and unnecessary statements. Seeding a simplicial complex consists of the following steps, and statements in Algorithm 1 follow the same principle in the same order:

- creating an empty simplicial complex of given dimension,
- creating k-simplices for storing vertices and simplices of higher levels,
- connecting vertices at each level with vertices on higher and lower levels.

Adding a neighbor to a k-simplex is a symmetric operation. This means that both k-simplices (the calling one and the one given as an argument) are neighbors to each other. All functions of the simulator are written in a robust manner, checking the validity of input parameters.

Note that multiple colors can be assigned to each k-simplex, which is left out of consideration in this algorithm for better clarity.

III. Coloring and Pretty Printing K-simplices

This section describes coloring and pretty printing simplicial complexes. These functions might work in pair, but are not necessarily connected.

A. Coloring -simplices

Coloring k-simplices will be explained using Algorithm 2 by coloring vertices of an edge with boundary colors. First, vertices have to be created as k-simplices of level zero. Then, colors have to be created for all vertices. Finally, colors need to be pushed back to the vector of colors that each k-simplex has.

Algorithm 1: Seeding a single edge.

```
SimpComp* seed_single_edge(string name){
    SimpComp *edge = new SimpComp(
            name, 1);
    KSimplex *v1 =
            edge->create_ksimplex(0);
    KSimplex *v2 =
            edge->create_ksimplex(0);
    KSimplex *e1 =
            edge->create_ksimplex(1);
    v1->add_neighbor(e1);
    v2->add_neighbor(e1);
    return edge;
}
```

Algorithm 2: Coloring vertices with boundary color.

```
KSimplex *v1 =
        edge->create_ksimplex(0);
KSimplex *v2 =
        edge->create_ksimplex(0);
Color *c1 = new BoundaryColor(true);
Color *c2 = new BoundaryColor(true);
v1->colors.push_back(c1);
v2->colors.push_back(c2);
```

Following colors are currently available:

- unique ID colors
- boundary colors
- screen coordinate colors.

Additionally, user is allowed to construct a custom color and use it within the simulator. The source code of the simulator is organized as a library, and user is allowed to extend it by using the library.

Unique ID colors are predominantly used for pretty printing simplicial complexes. They are implemented by a class inherited from the basic color class. Two main fields include

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static integer number, and an integer number. The first represents the current maximum of a unique color ID that is in use, and the second one is the color of a given k-simplex.

Unlike unique ID colors, boundary colors have special meaning. Each k-simplex may contain boundary color, but it does not have to. A simplicial complex can have boundaries on k-simplices of one level lower than the dimension of the simplicial complex. For example, a triangle can have edges as boundaries.

Screen coordinate colors are used for drawing simplicial complexes on a screen. The basic graphical user interface is under development.

B. Pretty Printing -simplices

Printing k-simplices includes printing of all of the fields that *Simple* class contains. This includes printing all of the neighborhood elements the k-simplex has. This is usually overwhelming for a user. Therefore, pretty printing is designed to print unique ID colors of each k-simplex in most readable way authors could think of.

Function *Simple print compact* is responsible for pretty printing. It assigns to the pointer to the unique ID a value returned by a function *get uni ueI* that returns either nullptr if a k-simplex doesn't have a unique ID, or a pointer to the color.

If there is no unique ID color assigned to a k-simplex, the output consists solely of word "Simplex". Otherwise, *print compact* function is called for a color that the pointer points to. Further, the following procedure is repeated, if level k is greater than zero and there are neighboring elements for all neighbors. A set of integer values is constructed, and then function *print ertices in parentheses s* is called for neighbors, adding unique IDs to the set. This way, printing sorted values is achieved, along with avoiding duplicate values. Sample output of a simplicial complex pretty printing is shown in Fig. 1.

IV. CONCLUSION

We have demonstrated how one can implement in code the structure of a simplicial complex of arbitrary dimension, in a way that is faithful to its combinatorial definition, and perform the most basic operations on it, like instantiating, coloring and printing.

The implementation of the basic classes of the code described in this work represents a fundamental basic building block for a more versatile software collection that aims to construct, manipulate and study the properties of simplicial complexes of arbitrary dimension. Future extensions of the software library will include the functions which implement attaching additional simplices to a boundary of a complex, performing Pachner moves [13] which transform a given complex into a different one without changing its topology, and functions for manipulating the colors and evaluating various mathematical constructions that include them. Note that the experimental data regarding the parallelization is yet to be collected (see the accompanying paper [14]).

The resulting software collection will feature the generality and versatility that aim for applications both in pure mathematics (algebraic topology research) and theoretical physics (quantum gravity, field theory), but also with potential applications in other disciplines of engineering and industry, wherever the analysis and the study of geometry of manifolds and curved surfaces may be relevant.

APPENDIX

Algorithm 3: Declaration of SimpComp class.

```
class SimpComp{
public:
    SimpComp(int dim);
    SimpComp(string s, int dim);
    ~SimpComp();
    int count_number_of_simplexes(
            int level);
    void print(string space = "");
    bool all_uniqueID(int level);
    void collect_vertices(set<int> &s);
    void print_set(set<int> &s);
    void print_vertices_in_parentheses(
            set<int> &s);
    void print_compact();
    // Creating new KSimplex at level k:
    KSimplex* create_ksimplex(int k);
    void print_sizes();

    string name;
    int D;
    // An element at each level
    // is a list or vector
    // of KSimplex pointers
    // to KSimplex on that level:
    vector< vector<KSimplex *> >
            elements;
};
```

Algorithm 4: Declaration of KSimplex class.

```
class KSimplex{
public:
    KSimplex();
    KSimplex(int k, int D);
    ~KSimplex();
    bool find_neighbor(KSimplex *k1);
    void add_neighbor(KSimplex *k1);
    void print(string space = "");
    UniqueIDColor* get_uniqueID();
    void print_compact();

    int k; // level
    int D; // dimension
    SimpComp *neighbors;
    vector<Color *> colors;
};
```

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Construction and examples of higher gauge theories*

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Abstract

We provide several examples of higher gauge theories, constructed as generalizations of a BF model to $2BF$ and $3BF$ models with constraints. Using the framework of higher category theory, we introduce appropriate 2-groups and 3-groups, and construct the actions for the corresponding constrained $2BF$ and $3BF$ theories. In this way, we can construct actions which describe the correct dynamics of Yang-Mills, Klein-Gordon, Dirac, Weyl, and Majorana fields coupled to Einstein-Cartan gravity. Each action is naturally split into a topological sector and a sector with simplicity constraints. The properties of the higher gauge group structure opens up a possibility of a nontrivial unification of all fields.

1. Introduction

The quantization of the gravitational field is one of the fundamental open problems in modern physics. There are various approaches to this problem, some of which have developed into vast research frameworks. One of such frameworks is the Loop Quantum Gravity approach, which aims to establish a nonperturbative quantization of gravity, both canonically and covariantly [1, 2, 3]. The covariant approach is slightly more general, and

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focuses on providing a possible rigorous definition of the path integral for the gravitational field,

$$Z = \int \mathcal{D}g \, e^{iS[g]} \,. \tag{1}$$

This is done by considering a triangulation of a spacetime manifold, and defining the path integral as a discrete state sum of the gravitational field configurations living on the simplices in the triangulation. This quantization technique is known as the *spinfoam* quantization method, and is performed via the following three steps:

(1) one writes the classical action $S[g]$ as a constrained BF action;

(2) one uses the Lie group structure, underlying the topological sector of the action, to define a triangulation-independent state sum Z;

(3) one imposes the simplicity constraints on the state sum, promoting it into a triangulation-dependent state sum, which serves as a definition for the path integral (1).

So far, this quantization prescription has been implemented for various choices of the gravitational action, of the Lie group, and of the spacetime dimension. For example, in 3 dimensions, historically the first spinfoam model is known as the Ponzano-Regge model [4]. In 4 dimensions there are multiple models, depending on the choice of the Lie group and the way one imposes the simplicity constraints [5, 6, 7, 8, 9]. While these models do give a definition for the gravitational path integral, none of them are able to consistently include matter fields. Including the matter fields has so far had limited success [10], mainly due to the absence of the tetrad fields from the topological sector of the theory.

In order to resolve this issue, a new approach has been developed, using the framework of *higher gauge theory* (see [11] for a review). In particular, one uses the idea of a *categorical ladder* to generalize the BF action (based on a Lie group) into a $2BF$ action (based on the so-called 2-group structure). A suitable choice of the *Poincaré 2-group* introduces the needed tetrad fields into the topological sector of the action [12]. While this result opened up a possibility to couple matter fields to gravity, the matter fields could not be naturally expressed using the underlying algebraic structure of a 2-group, rendering the spinfoam quantization method inapplicable. Namely, the matter sector could indeed be added to the classical action, but could not be expressed itself as a constrained $2BF$ theory, which means that the steps 1–3 above could not be performed for the matter sector of the action, but only for gravity.

This final issue has recently been resolved in [13], by passing from the 2-group structure to the 3-group structure, generalizing the action one step further in the categorical ladder. This generalization naturally gives rise to the so-called $3BF$ action, which turns out to be suitable for a unified description of both gravity and matter fields. The steps of the categorical ladder and their corresponding structures are summarized as follows:

categorical structure	algebraic structure	linear structure	topological action	degrees of freedom
Lie group	Lie group	Lie algebra	BF theory	gauge fields
Lie 2-group	Lie crossed module	differential Lie crossed module	$2BF$ theory	tetrad fields
Lie 3-group	Lie 2-crossed module	differential Lie 2-crossed module	$3BF$ theory	scalar and fermion fields

The purpose of this paper is to give a systematic overview of the constructions of classical BF, $2BF$ and $3BF$ actions, both pure and constrained, in order to demonstrate the categorical ladder procedure and the construction of higher gauge theories. In other words, we focus on the step 1 of the spinfoam quantization programme.

The layout of the paper is as follows. Section 2 deals with models based on a BF theory. First we discuss the pure, topological BF theory, and then pass on to the the physically more interesting Yang-Mills theory in Minkowski spacetime and the Plebanski formulation of general relativity. In Section 3 we study the first step in the categorical ladder, namely models based on the $2BF$ theory. After introducing the pure $2BF$ theory, we study the relevant formulation of general relativity [12], and then the coupled Einstein-Yang-Mills theory. Then, in Section 4 we perform the second step in the categorical ladder, passing on to models based on the $3BF$ theory. After the introduction of the pure $3BF$ model, we construct constrained $3BF$ actions for the cases of Klein-Gordon, Dirac, Weyl and Majorana fields, all coupled to the Einstein-Cartan gravity in the standard way. As we shall see, the scalar and fermion fields will be *naturally associated to a new gauge group*, generalizing the purpose of a gauge group in the Yang-Mills theory, which opens up a possibility of an algebraic classification of matter fields. Finally, Section 5 contains a discussion and conclusions.

The notation and conventions are as follows. The local Lorentz indices are denoted by the Latin letters $a, b, c, \dots$, take values $0, 1, 2, 3$, and are raised and lowered using the Minkowski metric η_{ab} with signature $(-,+,+,+)$. Spacetime indices are denoted by the Greek letters $\mu, \nu, \dots$, and are raised and lowered by the spacetime metric $g_{\mu\nu} = \eta_{ab} e^a{}_\mu e^b{}_\nu$, where $e^a{}_\mu$ are the tetrad fields. The inverse tetrad is denoted as $e^\mu{}_a$. All other indices that appear in the paper are dependent on the context, and their usage is explicitly defined in the text where they appear. We work in the natural system of units where $c = \hbar = 1$, and $G = l_p^2$, where l_p is the Planck length.

2. BF theory

We begin with a short review of BF theories. See [14, 15, 16] for additional information.

2.1. Pure BF theory

Given a Lie group G, and denoting its corresponding Lie algebra as $\mathfrak{g}$, one introduces the pure BF action as follows (we limit ourselves to the physically relevant case of 4-dimensional spacetime manifolds $\mathcal{M}_4$):

$$S_{BF} = \int_{\mathcal{M}_4} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} \,. \qquad (2)$$

Here, $\mathcal{F} \equiv \mathrm{d}\alpha + \alpha \wedge \alpha$ is the curvature 2-form for the algebra-valued connection 1-form $\alpha \in \mathcal{A}^1(\mathcal{M}_4 \,, \mathfrak{g})$, and $B \in \mathcal{A}^2(\mathcal{M}_4 \,, \mathfrak{g})$ is a Lagrange multiplier 2-form, while $\langle \_ \,, \_ \rangle_{\mathfrak{g}}$ denotes a G-invariant bilinear symmetric nondegenerate form.

One can see from (2) that the action is diffeomorphism invariant, and it is also gauge invariant with respect to G, provided that B transforms as a scalar with respect to G.

Varying the action (2) with respect to B^β and α^β, where the index β is the group G index (which counts the generators of $\mathfrak{g}$), one obtains the following equations of motion,

$$\mathcal{F}^\beta = 0 \,, \qquad \nabla B^\beta \equiv \mathrm{d}B^\beta + f_{\gamma\delta}{}^\beta \alpha^\gamma \wedge B^\delta = 0 \,, \qquad (3)$$

where $f_{\gamma\delta}{}^\beta$ are the structure constants of the Lie group G. From the first equation of motion, one immediately sees that α is a flat connection, meaning that $\alpha = 0$ up to gauge transformations. Given this, the second equation of motion implies that B is constant. Therefore, there are no local propagating degrees of freedom, and the theory is called *topological*.

2.2. Yang-Mills theory

In physics one is usually interested in theories which are not topological, i.e., which have local propagating degrees of freedom. As a rule of thumb, one recognizes that the theory does have local propagating degrees of freedom if one of the equations of motion is a second-order partial differential equation, usually featuring a D'Alambertian operator $\Box$ in some form. In order to transform the pure BF action into such a theory, one adds an additional term to the action, commonly called the *simplicity constraint*. The resulting action is called a *constrained BF theory*. A nice example is the Yang-Mills theory for the $SU(N)$ group in Minkowski spacetime, which can be rewritten as a constrained BF theory in the following way:

$$\begin{aligned} S \;=\; & \int B_I \wedge F^I + \lambda^I \wedge \Big(B_I - \frac{12}{g} M_{abI} \delta^a \wedge \delta^b \Big) \\ & + \zeta^{abI} \Big(M_{abI} \varepsilon_{cdef} \delta^c \wedge \delta^d \wedge \delta^e \wedge \delta^f - g_{IJ} F^J \wedge \delta_a \wedge \delta_b \Big) \,. \end{aligned} \qquad (4)$$

Here $F \equiv \mathrm{d}A + A \wedge A$ is again the curvature 2-form for the connection $A \in \mathcal{A}^1(\mathcal{M}_4 \,, \mathfrak{su}(N))$, and $B \in \mathcal{A}^2(\mathcal{M}_4 \,, \mathfrak{su}(N))$ is the Lagrange multiplier

2-form. The Killing form $g_{IJ} \equiv \langle \tau_I \,, \tau_J \rangle_{\mathfrak{su}(N)} \propto f_{IK}{}^L f_{JL}{}^K$ is used to raise and lower the indices $I, J, \dots$ which count the generators of $SU(N)$, while $f_{IJ}{}^K$ are the structure constants for the $\mathfrak{su}(N)$ algebra. In addition to the topological $B \wedge F$ term, there are also two simplicity constraint terms present, featuring two Lagrange multipliers, a 2-form λ^I and a 0-form ζ^{abI}. The 0-form M_{abI} is also a Lagrange multiplier, while g is the coupling constant for the Yang-Mills theory.

Finally, δ^a is a nondynamical 1-form, such that there exists a global coordinate frame in which its components are equal to the Kronecker symbol $\delta^a{}_\mu$ (hence the notation δ^a). The 1-form δ^a plays the role of a background field, and defines the global spacetime metric, via the equation

$$\eta_{\mu\nu} = \eta_{ab} \delta^a{}_\mu \delta^b{}_\nu \,, \tag{5}$$

where $\eta_{ab} \equiv \text{diag}(-1, +1, +1, +1)$ is the Minkowski metric. Since the coordinate system is global, the spacetime manifold $\mathcal{M}_4$ is understood to be flat. The indices $a, b, \dots$ are local Lorentz indices, taking values $0, \dots, 3$. Note that the field δ^a has all the properties of the tetrad 1-form e^a in the flat Minkowski spacetime. Also note that the action (4) is manifestly diffeomorphism invariant and gauge invariant with respect to $SU(N)$, but not background independent, due to the presence of δ^a.

Varying the action (4) with respect to the variables ζ^{abI}, M_{abI}, A^I, B_I, and λ^I, respectively (but not with respect to the background field δ^a), we obtain the equations of motion:

$$M_{abI} \varepsilon_{cdef} \delta^c \wedge \delta^d \wedge \delta^e \wedge \delta^f - F_I \wedge \delta_a \wedge \delta_b = 0 \,, \tag{6}$$

$$-\frac{12}{g} \lambda^I \wedge \delta^a \wedge \delta^b + \zeta^{abI} \varepsilon_{cdef} \delta^c \wedge \delta^d \wedge \delta^e \wedge \delta^f = 0 \,, \tag{7}$$

$$-\mathrm{d}B_I + f_{JI}{}^K B_K \wedge A^J + \mathrm{d}(\zeta^{ab}{}_I \delta_a \wedge \delta_b) - f_{JI}{}^K \zeta^{ab}{}_K \delta_a \wedge \delta_b \wedge A^J = 0 \,, \tag{8}$$

$$F_I + \lambda_I = 0 \,, \tag{9}$$

$$B_I - \frac{12}{g} M_{abI} \delta^a \wedge \delta^b = 0 \,, \tag{10}$$

From the equations (6), (7), (9) and (10) one obtains the multipliers as algebraic functions of the field strength $F^I{}_{\mu\nu}$ for the dynamical field A^I:

$$\begin{aligned} M_{abI} &= \frac{1}{48} \varepsilon_{abcd} F_I{}^{cd} \,, \qquad & \zeta^{abI} &= \frac{1}{4g} \varepsilon^{abcd} F^I{}_{cd} \,, \\ \lambda_{Iab} &= F_{Iab} \,, & B_{Iab} &= \frac{1}{2g} \varepsilon_{abcd} F_I{}^{cd} \,. \end{aligned} \tag{11}$$

Here we used the notation $F_{Iab} = F_{I\mu\nu}\delta_a{}^\mu\delta_b{}^\nu$, and similarly for other variables, where we exploited the fact that $\delta^a{}_\mu$ is invertible. Using these equations and the differential equation (8) one obtains the equation of motion for gauge field $A^I{}_\mu$,

$$\nabla_\rho F^{I\rho\mu} \equiv \partial_\rho F^{I\rho\mu} + f_{JK}{}^I A^J{}_\rho F^{K\rho\mu} = 0\,. \tag{12}$$

This is precisely the classical equation of motion for the free Yang-Mills theory. Note that this is a second-order partial differential equation for the field $A^I{}_\mu$, and moreover contains the $\Box$ operator in the first term.

In addition to the Yang-Mills theory, one can easily extend the action (4) in order to describe the massive vector field and obtain the Proca equation of motion. This is done by adding a mass term

$$-\frac{1}{4!}m^2 A_{I\mu}A^I{}_\nu\eta^{\mu\nu}\varepsilon_{abcd}\delta^a\wedge\delta^b\wedge\delta^c\wedge\delta^d \tag{13}$$

to the action (4). Of course, this term explicitly breaks the $SU(N)$ gauge symmetry of the action.

2.3. Plebanski general relativity

The second example of the constrained BF theory is the Plebanski action for general relativity [16, 14]. Using the Lorentz group $SO(3,1)$ as a gauge group, one constructs a constrained BF action as

$$S = \int_{\mathcal{M}_4} B_{ab}\wedge R^{ab} + \phi_{abcd}B^{ab}\wedge B^{cd}\,. \tag{14}$$

Here R^{ab} is the curvature 2-form for the spin connection ω^{ab}, B_{ab} is the usual Lagrange multiplier 2-form, while ϕ_{abcd} is the additional Lagrange multiplier 0-form multiplying the term $B^{ab}\wedge B^{cd}$ to form a simplicity constraint. It can be shown that the variation of this action with respect to B_{ab}, ω^{ab} and ϕ_{abcd} gives rise to the equations of motion of vacuum general relativity. However, in this model the tetrad fields appear only as a solution of the simplicity constraint equation of motion $B^{ab}\wedge B^{cd} = 0$. Therefore, being intrinsically on-shell objects, the tetrad fields are not present in the action itself and cannot be quantized. This renders the Plebanski model unsuitable for coupling of matter fields to gravity [10, 12, 20]. Nevertheless, regarded as a model for pure gravity, the Plebanski model has been successfully quantized in the context of spinfoam models [8, 9, 1, 2].

3. $2BF$ theory

In this section we perform the first step of the *categorical ladder*, generalizing the algebraic notion of a group to the notion of a 2-group. This leads to the generalization of the BF theory to the $2BF$ theory, also sometimes called $BFCG$ theory [11, 17, 18, 19].

3.1. Pure $2BF$ theory

In order to circumvent the issue of tetrad fields not being present in the Plebanski action, in the context of higher category theory [11] a recent promising approach has been developed [12, 21, 22, 23, 20, 24]. As an essential ingredient, let us first give a short review of the 2-group formalism.

Within the framework of category theory, the group as an algebraic structure can be understood as a category with only one object and invertible morphisms [11]. Additionally, the notion of a category can be generalized to the so-called *higher categories*, which have not only objects and morphisms, but also 2-morphisms (morphisms between morphisms), and so on. This process of generalization is called the *categorical ladder*. Using this process, one can introduce the notion of a 2*-group* as a 2-category consisting of only one object, where all the morphisms and all 2-morphisms are invertible. It has been shown that every strict 2-group is equivalent to a *crossed module* $(H \stackrel{\partial}{\to} G\,,\triangleright)$, see [13] for detailed definitions. Here G and H are groups, ∂ is a homomorphism from H to G, while $\triangleright : G \times H \to H$ is an action of G on H.

Similarly to the case of an ordinary Lie group G which has a naturally associated notion of a connection α, giving rise to a BF theory, the 2-group structure has a naturally associated notion of a 2-connection $(\alpha\,,\beta)$, described by the usual $\mathfrak{g}$-valued 1-form $\alpha \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{g})$ and an $\mathfrak{h}$-valued 2-form $\beta \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{h})$, where $\mathfrak{h}$ is a Lie algebra of the Lie group H. The 2-connection gives rise to the so-called *fake* 2*-curvature* $(\mathcal{F},\mathcal{G})$, given as

$$\mathcal{F} = \mathrm{d}\alpha + \alpha\wedge\alpha - \partial\beta\,, \qquad \mathcal{G} = d\beta + \alpha\wedge^{\triangleright}\beta\,. \tag{15}$$

Here $\alpha\wedge^{\triangleright}\beta$ means that α and β are multiplied as forms using $\wedge$, and simultaneously multiplied as algebra elements using $\triangleright$, see [13]. The curvature pair $(\mathcal{F},\mathcal{G})$ is called "fake" because of the presence of the additional term $\partial\beta$ in the definition of $\mathcal{F}$ [11].

Using the structure of a 2-group, or equivalently the crossed module, one can generalize the BF action to the so-called $2BF$ action, defined as follows [17, 18]:

$$S_{2BF} = \int_{\mathcal{M}_4} \langle B\wedge\mathcal{F}\rangle_{\mathfrak{g}} + \langle C\wedge\mathcal{G}\rangle_{\mathfrak{h}}\,. \tag{16}$$

Here the 2-form $B \in \mathcal{A}^2(\mathcal{M}_4\,,\mathfrak{g})$ and the 1-form $C \in \mathcal{A}^1(\mathcal{M}_4\,,\mathfrak{h})$ are Lagrange multipliers. Also, $\langle\_\,,\_\rangle_{\mathfrak{g}}$ and $\langle\_\,,\_\rangle_{\mathfrak{h}}$ denote the G-invariant bilinear symmetric nondegenerate forms for the algebras $\mathfrak{g}$ and $\mathfrak{h}$, respectively. As a consequence of the axiomatic structure of a crossed module (see [13]), the bilinear form $\langle\_\,,\_\rangle_{\mathfrak{h}}$ is H-invariant as well. See [17, 18] for review and references.

Similarly to the BF action, the $2BF$ action is also topological, which can be seen from equations of motion. Varying with respect to B^α and C^a one obtains

$$\mathcal{F}^\alpha = 0\,, \qquad \mathcal{G}^a = 0\,, \tag{17}$$

where indices a count the generators of the group H. Varying with respect to α^α and β^a one obtains the equations for the multipliers,

$$\mathrm{d}B_\alpha + f_{\alpha\beta}{}^\gamma B_\gamma \wedge \alpha^\beta - \rhd_{\alpha a}{}^b C_b \wedge \beta^a = 0\,, \tag{18}$$

$$\mathrm{d}C_a - \partial_a{}^\alpha B_\alpha + \rhd_{\alpha a}{}^b C_b \wedge \alpha^\alpha = 0\,. \tag{19}$$

We can again see that the equations of motion are only first-order and have only very simple solutions (note that this is not a sufficient argument for the absence of local propagating degrees of freedom — a counterexample is the Dirac equation, being a first-order partial differential equation which *does* have propagating degrees of freedom). One can additionally use the Hamiltonian analysis to rigorously demonstrate that there are no local propagating degrees of freedom [22, 23]. Thus the $2BF$ theory is also topological.

3.2. General relativity

An important example of a crossed module structure is a vector space V equipped with an isometry group O. Namely, V can be regarded as an Abelian Lie group with addition as a group operation, so that a representation of O on V is an action $\rhd$ of O on the group V, giving rise to the crossed module $(V \xrightarrow{\partial} O\,, \rhd)$, where the homomorphism ∂ is chosen to be trivial (it maps every element of V into a unit of O).

We can employ this construction to introduce the *Poincaré 2-group*. One constructs a crossed module by choosing

$$G = SO(3,1)\,, \qquad H = \mathbb{R}^4\,. \tag{20}$$

The map ∂ is trivial, while $\rhd$ is a natural action of $SO(3,1)$ on $\mathbb{R}^4$, defined by the equation

$$M_{ab} \rhd P_c = \eta_{[bc}P_{a]}\,, \tag{21}$$

where M_{ab} and P_a are the generators of groups $SO(3,1)$ and $\mathbb{R}^4$, respectively. The action $\rhd$ of $SO(3,1)$ on itself is given via conjugation. At the level of the algebra, conjugation reduces to the action via the adjoint representation, so that

$$M_{ab} \rhd M_{cd} = [\,M_{ab}\,,\, M_{cd}\,] \equiv \eta_{ad}M_{bc} - \eta_{ac}M_{bd} + \eta_{bc}M_{ad} - \eta_{bd}M_{ac}\,. \tag{22}$$

The 2-connection (α, β) is given by the algebra-valued differential forms

$$\alpha = \omega^{ab}M_{ab}\,, \qquad \beta = \beta^a P_a\,, \tag{23}$$

where ω^{ab} is called the spin connection. The corresponding 2-curvature in this case is given by

$$\begin{aligned} \mathcal{F} &= (\mathrm{d}\omega^{ab} + \omega^a{}_c \wedge \omega^{cb})M_{ab} &&\equiv R^{ab}M_{ab}\,, \\ \mathcal{G} &= (\mathrm{d}\beta^a + \omega^a{}_b \wedge \beta^b)P_a &&\equiv \nabla\beta^a P_a \equiv G^a P_a\,, \end{aligned} \tag{24}$$

Note that, since ∂ is trivial, the fake curvature is the same as ordinary curvature. Introducing the bilinear forms

$$\langle M_{ab}\,, M_{cd}\rangle_{\mathfrak{g}} = \eta_{a[c}\eta_{bd]}\,, \qquad \langle P_a\,, P_b\rangle_{\mathfrak{h}} = \eta_{ab}\,, \tag{25}$$

one can show that 1-forms C^a transform in the same way as the tetrad 1-forms e^a under the Lorentz transformations and diffeomorphisms, so the fields C^a can be identified with the tetrads. Then one can rewrite the pure $2BF$ action (16) for the Poincaré 2-group as

$$S_{2BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla\beta^a\,. \tag{26}$$

Note that the above step of recognizing that $C^a \equiv e^a$ was crucial, since we now see that the tetrad fields are explicitly present in the $2BF$ action for the Poincaré 2-group.

In order to promote (26) to an action for general relativity, we add a convenient simplicity constraint term:

$$S = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla\beta^a - \lambda_{ab} \wedge \Big(B^{ab} - \frac{1}{16\pi l_p^2}\varepsilon^{abcd} e_c \wedge e_d\Big)\,. \tag{27}$$

Here λ_{ab} is a Lagrange multiplier 2-form associated to the simplicity constraint term, and l_p is the Planck length. Note that the term "simplicity constraint" derives its name from the fact that the constraint imposes the property of *simplicity* on B^{ab} — a 2-form is said to be *simple* if it can be written as an exterior product of two 1-forms.

Varying the action (27) with respect to B_{ab}, e_a, ω_{ab}, β_a and λ_{ab}, we obtain the following equations of motion:

$$R_{ab} - \lambda_{ab} = 0\,, \tag{28}$$

$$\nabla\beta_a + \frac{1}{8\pi l_p^2}\varepsilon_{abcd}\lambda^{bc} \wedge e^d = 0\,, \tag{29}$$

$$\nabla B_{ab} - e_{[a} \wedge \beta_{b]} = 0\,, \tag{30}$$

$$\nabla e_a = 0\,, \tag{31}$$

$$B^{ab} - \frac{1}{16\pi l_p^2}\varepsilon^{abcd} e_c \wedge e_d = 0\,. \tag{32}$$

Given this system of equations, all fields can be algebraically determined in terms of the tetrads ${e^a}_\mu$, as follows. From the equations (31) and (32) we obtain that $\nabla B^{ab} = 0$, from which it follows, using the equation (30), that

$e_{[a} \wedge \beta_{b]} = 0$. Assuming that the tetrads are nondegenerate, $e \equiv \det(e^a{}_\mu) \neq 0$, it can be shown that this is equivalent to $\beta^a = 0$ [12]. Therefore, from the equations (28), (30), (31) and (32) we obtain

$$\lambda^{ab}{}_{\mu\nu} = R^{ab}{}_{\mu\nu}\,, \quad \beta^a{}_{\mu\nu} = 0\,, \quad B_{ab\mu\nu} = \frac{1}{8\pi l_p^2}\varepsilon_{abcd}e^c{}_\mu e^d{}_\nu\,, \quad \omega^{ab}{}_\mu = \triangle^{ab}{}_\mu\,. \tag{33}$$

Here the Ricci rotation coefficients are defined as

$$\triangle^{ab}{}_\mu \equiv \frac{1}{2}(c^{abc} - c^{cab} + c^{bca})e_{c\mu}\,, \tag{34}$$

where

$$c^{abc} = e^\mu{}_b e^\nu{}_c \left(\partial_\mu e^a{}_\nu - \partial_\nu e^a{}_\mu\right)\,. \tag{35}$$

The last equation establishes that the spin connection 1-form ω^{ab} is expressed as a function of the tetrads, which then implies the same for the curvature 2-form R^{ab}. Finally, the remaining equation (29) then reduces to

$$\varepsilon_{abcd}R^{bc} \wedge e^d = 0\,, \tag{36}$$

which is nothing but the vacuum Einstein field equation,

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = 0\,.$$

Therefore, the action (27) is classically equivalent to general relativity.

3.3. Einstein-Yang-Mills theory

As we have already mentioned above, the main advantage of the action (27) over the Plebanski model lies in the fact that the tetrad fields are explicitly present in the topological sector of the action. This allows one to couple matter fields in a straightforward way [12]. However, one can do even more [13], and couple the $SU(N)$ Yang-Mills fields to gravity within a unified framework of 2-group formalism.

Namely, we can modify the Poincaré 2-group structure to include the $SU(N)$ gauge group, as follows. We choose the two Lie groups as

$$G = SO(3,1) \times SU(N)\,, \qquad H = \mathbb{R}^4\,, \tag{37}$$

and we define the action $\triangleright$ of the group G in the following fashion. As in the case of the Poincaré 2-group, it acts on itself via conjugation. Next, it acts on H such that the $SO(3,1)$ subgroup acts on $\mathbb{R}^4$ via the vector representation (21), while the action of the $SU(N)$ subgroup is trivial,

$$\tau_I \triangleright P_a = 0\,, \tag{38}$$

where τ_I are the $SU(N)$ generators. The map ∂ also remains trivial, as before. The form of the 2-connection (α, β) now reflects the structure of the group G,

$$\alpha = \omega^{ab} M_{ab} + A^I \tau_I \,, \qquad \beta = \beta^a P_a \,, \tag{39}$$

where A^I is the gauge connection 1-form. Next, the curvature for α then becomes

$$\mathcal{F} = R^{ab} M_{ab} + F^I \tau_I \,, \qquad F^I \equiv \mathrm{d}A^I + f_{JK}{}^I A^J \wedge A^K \,. \tag{40}$$

The curvature for β remains the same as before, because of (38). Finally, the product structure of the group G implies that its Killing form $\langle \_ , \_ \rangle_{\mathfrak{g}}$ reduces to the Killing forms for the $SO(3,1)$ and $SU(N)$, along with the identity $\langle M_{ab} \,, \tau_I \rangle_{\mathfrak{g}} = 0$.

Given a crossed module defined in this way, its corresponding pure $2BF$ action (16) becomes

$$S_{2BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + B^I \wedge F_I + e_a \wedge \nabla \beta^a \,, \tag{41}$$

where $B^I \in \mathcal{A}^2(\mathcal{M}_4 \,, \mathfrak{su}(N))$ is the new Lagrange multiplier. The action (41) is topological, and again we add appropriate simplicity constraint terms, in order to transform it into action with nontrivial dynamics. The constraint giving rise to gravity is the same as in (27), while the constraint for the gauge fields is given as in the action (4) with the substitution $\delta^a \to e^a$. Putting everything together, we obtain:

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + B^I \wedge F_I + e_a \wedge \nabla \beta^a \\ & - \lambda_{ab} \wedge \Big(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \Big) + \lambda^I \wedge \Big(B_I - \frac{12}{g} M_{abI} e^a \wedge e^b \Big) \\ & + \zeta^{abI} \Big(M_{abI} \varepsilon_{cdef} e^c \wedge e^d \wedge e^e \wedge e^f - g_{IJ} F^J \wedge e_a \wedge e_b \Big) \,. \end{aligned} \tag{42}$$

It is crucial to note that the Yang-Mills simplicity constraints in (42) are obtained from the Yang-Mills action (4) by substituting the nondynamical background field δ^a from (4) with a dynamical field e^a. The relationship between these fields has already been hinted at in the equation (5), which describes the connection between δ^a and the flat spacetime metric $\eta_{\mu\nu}$. Once promoted to e^a, this field becomes dynamical due to the presence of gravitational terms, while the equation (5) becomes the usual relation between the tetrad and the metric,

$$g_{\mu\nu} = \eta_{ab} e^a{}_\mu e^b{}_\nu \,, \tag{43}$$

further confirming the identification $C^a = e^a$. Moreover, the total action (42) now becomes background independent, as expected in general relativity. All this is a consequence of the fact that the tetrad field is explicitly present in the topological sector of the action (27), and represents a clear improvement over the Plebanski model.

Taking the variations of the action (42) with respect to the variables B_{ab}, ω_{ab}, β_a, λ_{ab}, ζ^{abI}, M_{abI}, B_I, λ^I, A^I, and e^a, we obtain equations of motion. Similarly as before, all variables can be algebraically expressed as functions of A^I and e^a and their derivatives:

$$\begin{gathered}
\lambda_{ab\mu\nu} = R_{ab\mu\nu}\,, \qquad \beta_{a\mu\nu} = 0\,, \qquad \omega_{ab\mu} = \triangle_{ab\mu}\,, \qquad \lambda_{abI} = F_{abI}\,, \\
B_{\mu\nu I} = -\frac{e}{2g}\varepsilon_{\mu\nu\rho\sigma}F^{\rho\sigma}{}_I\,, \qquad B_{ab\mu\nu} = \frac{1}{8\pi l_p^2}\varepsilon_{abcd}e^c{}_\mu e^d{}_\nu\,, \\
M_{abI} = -\frac{1}{4eg}\varepsilon^{\mu\nu\rho\sigma}F_{\mu\nu}{}^I e^a{}_\rho e^b{}_\sigma\,, \qquad \zeta^{abI} = \frac{1}{4eg}\varepsilon^{\mu\nu\rho\sigma}F_{\mu\nu}{}^I e^a{}_\rho e^b{}_\sigma\,.
\end{gathered} \tag{44}$$

In addition, we obtain two differential equations — An equation for A^I,

$$\nabla_\rho F^{I\rho\mu} \equiv \partial_\rho F^{I\rho\mu} + \Gamma^\rho{}_{\lambda\rho}F^{I\lambda\mu} + f_{JK}{}^I A^J{}_\rho F^{K\rho\mu} = 0\,, \tag{45}$$

where $\Gamma^\lambda{}_{\mu\nu}$ is the standard Levi-Civita connection, and an equation for e^a,

$$R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R = 8\pi l_p^2\, T^{\mu\nu}\,, \tag{46}$$

where

$$T^{\mu\nu} \equiv -\frac{1}{4g}\left(F_{\rho\sigma}{}^I F^{\rho\sigma}{}_I g^{\mu\nu} + 4F^{\mu\rho}{}_I F_\rho{}^{\nu I}\right)\,. \tag{47}$$

In this way, we see that both gravity and gauge fields can be successfully represented within a unified framework of higher gauge theory, based on a 2-group structure. A generalization from $SU(N)$ Yang-Mills case to more complicated cases such as $SU(3)\times SU(2)\times U(1)$ is completely straightforward.

4. $3BF$ theory

While the structure of a 2-group can successfully describe both gravitational and gauge fields, unfortunately it cannot accommodate other matter fields, such as scalars or fermions. In order to remedy this drawback, we make one further step in the categorical ladder, passing from the notion of a 2-group to the notion of a 3-group. As it turns out, the 3-group structure is excellent for the description of all fields that are present in the Standard Model, coupled to gravity. Moreover, a 3-group contains one more gauge group, which is novel and corresponds to the choice of the scalar and fermion fields present in the theory. This is an unexpected and beautiful result, not present in ordinary gauge theory.

As before, we will begin by introducing the notion of a 3-group, and constructing the corresponding $3BF$ action. Afterwards, we will modify this action by adding appropriate simplicity constraints, giving rise to theories with expected nontrivial dynamics. Along the way, we shall see that scalar and fermion fields are being treated pretty much on an equal footing with gravity and gauge fields.

4.1. Pure $3BF$ theory

Similarly to the concepts of a group and a 2-group, one can introduce the notion of a 3-group in the framework of higher category theory, as a 3-category with only one object where all the morphisms, 2-morphisms and 3-morphisms are invertible. Also, in the same way as a 2-group is equivalent to a crossed module, it was proved that a strict 3-group is equivalent to a 2-*crossed module* [25].

A Lie 2-crossed module, denoted as $(L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G\,, \triangleright\,, \{\_\,,\_\})$, is an algebraic structure specified by three Lie groups G, H and L, together with the homomorphisms δ and ∂, an action $\triangleright$ of the group G on all three groups, and a G-equivariant map

$$\{\_\,,\_\} : H \times H \to L\,.$$

called the Peiffer lifting. The maps ∂, δ, $\triangleright$ and the Peiffer lifting satisfy certain axioms, so that the resulting structure is equivalent to a 3-group [13].

Like in the cases of BF and $2BF$ actions, we can introduce a gauge invariant topological $3BF$ action over the manifold $\mathcal{M}_4$ for a given 2-crossed module $(L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G\,, \triangleright\,, \{\_\,,\_\})$. Denoting $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{l}$ as Lie algebras corresponding to the groups G, H and L, respectively, one can introduce a 3-connection (α, β, γ) given by the algebra-valued differential forms $\alpha \in \mathcal{A}^1(\mathcal{M}_4\,, \mathfrak{g})$, $\beta \in \mathcal{A}^2(\mathcal{M}_4\,, \mathfrak{h})$ and $\gamma \in \mathcal{A}^3(\mathcal{M}_4\,, \mathfrak{l})$. The corresponding fake 3-curvature $(\mathcal{F}\,, \mathcal{G}\,, \mathcal{H})$ is then defined as

$$\begin{gathered} \mathcal{F} = \mathrm{d}\alpha + \alpha \wedge \alpha - \partial\beta\,, \qquad \mathcal{G} = \mathrm{d}\beta + \alpha \wedge^{\triangleright} \beta - \delta\gamma\,, \\ \mathcal{H} = \mathrm{d}\gamma + \alpha \wedge^{\triangleright} \gamma + \{\beta \wedge \beta\}\,, \end{gathered} \tag{48}$$

see [25, 26] for details. Note that γ is a 3-form, while its corresponding field strength $\mathcal{H}$ is a 4-form, necessitating that the spacetime manifold be at least 4-dimensional. Then, a $3BF$ action is defined as

$$S_{3BF} = \int_{\mathcal{M}_4} \langle B \wedge \mathcal{F} \rangle_{\mathfrak{g}} + \langle C \wedge \mathcal{G} \rangle_{\mathfrak{h}} + \langle D \wedge \mathcal{H} \rangle_{\mathfrak{l}}\,, \tag{49}$$

where $B \in \mathcal{A}^2(\mathcal{M}_4, \mathfrak{g})$, $C \in \mathcal{A}^1(\mathcal{M}_4, \mathfrak{h})$ and $D \in \mathcal{A}^0(\mathcal{M}_4, \mathfrak{l})$ are Lagrange multipliers. Note that in precisely 4 spacetime dimensions the Lagrange multiplier D corresponding to $\mathcal{H}$ is a 0-form, i.e. a scalar function. The functionals $\langle \_ , \_ \rangle_{\mathfrak{g}}$, $\langle \_ , \_ \rangle_{\mathfrak{h}}$ and $\langle \_ , \_ \rangle_{\mathfrak{l}}$ are G-invariant bilinear symmetric nondegenerate forms on $\mathfrak{g}$, $\mathfrak{h}$ and $\mathfrak{l}$, respectively. Under certain conditions, the forms $\langle \_ , \_ \rangle_{\mathfrak{h}}$ and $\langle \_ , \_ \rangle_{\mathfrak{l}}$ are also H-invariant and L-invariant.

One can see that varying the action with respect to the variables B^α, C^a and D^A (where indices A count the generators of the group L), one obtains the equations of motion

$$\mathcal{F}^\alpha = 0\,, \qquad \mathcal{G}^a = 0\,, \qquad \mathcal{H}^A = 0\,, \tag{50}$$

while varying with respect to α^α, β^a, γ^A one obtains

$$\mathrm{d}B_\alpha + f_{\alpha\beta}{}^\gamma B_\gamma \wedge \alpha^\beta - \rhd_{\alpha a}{}^b C_b \wedge \beta^a + \rhd_{\alpha B}{}^A D_A \wedge \gamma^B = 0\,, \tag{51}$$

$$\mathrm{d}C_a - \partial_a{}^\alpha B_\alpha + \rhd_{\alpha a}{}^b C_b \wedge \alpha^\alpha + 2X_{\{ab\}}{}^A D_A \wedge \beta^b = 0\,, \tag{52}$$

$$\mathrm{d}D_A - \rhd_{\alpha A}{}^B D_B \wedge \alpha^\alpha + \delta_A{}^a C_a = 0\,. \tag{53}$$

4.2. Klein-Gordon theory

Now we proceed to demonstrate that one can use the 3-group structure and the corresponding $3BF$ theory to describe the Klein-Gordon field coupled to general relativity. We begin by specifying a 2-crossed module, which is used to construct the topological $3BF$ theory, and then we impose appropriate simplicity constraints to obtain the desired equations of motion.

We specify a 2-crossed module $(L \xrightarrow{\delta} H \xrightarrow{\partial} G\,, \rhd\,, \{\_ , \_\})$, as follows. The groups are given as

$$G = SO(3,1)\,, \qquad H = \mathbb{R}^4\,, \qquad L = \mathbb{R}\,. \tag{54}$$

The group G acts on itself via conjugation, on H via the vector representation, and on L via the trivial representation. This specifies the definition of the action $\rhd$. The map ∂ is chosen to be trivial, as before. The map δ is also trivial, that is, every element of L is mapped to the identity element of H. Finally, the Peiffer lifting is trivial as well, mapping every ordered pair of elements in H to an identity element in L. This specifies one concrete 2-crossed module which, as we shall see below, corresponds to gravity and one real scalar field.

Given this choice of a 2-crossed module, the 3-connection $(\alpha\,, \beta\,, \gamma)$ takes the form

$$\alpha = \omega^{ab} M_{ab}\,, \qquad \beta = \beta^a P_a\,, \qquad \gamma = \gamma \mathbb{I}\,, \tag{55}$$

where $\mathbb{I}$ is the sole generator of the Lie group $\mathbb{R}$. Since the homomorphisms ∂ and δ are trivial, as well as the Peiffer lifting, the fake 3-curvature (48) reduces to the ordinary 3-curvature,

$$\mathcal{F} = R^{ab} M_{ab}\,, \qquad \mathcal{G} = \nabla \beta^a P_a\,, \qquad \mathcal{H} = \mathrm{d}\gamma\,, \tag{56}$$

where we used the fact that G acts trivially on L, that is, $M_{ab} \triangleright \mathbb{I} = 0$. This means that the 3-form γ transforms as a scalar with respect to Lorentz symmetry. Consequently, its Lagrange multiplier D also transforms as a scalar, since it also belongs to the algebra $\mathfrak{l}$. Since D is also a 0-form, it transforms as a scalar with respect to diffeomorphisms as well. In other words, D completely behaves as a real scalar field, so we relabel it into more traditional notation, $D \equiv \phi$, and write the pure $3BF$ action (49) as:

$$S_{3BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a + \phi \, \mathrm{d}\gamma \,, \tag{57}$$

where the bilinear form for L is $\langle \mathbb{I} , \mathbb{I} \rangle_{\mathfrak{l}} = 1$.

The existence of a scalar field in the $3BF$ action is a crucial property of a 3-group in a 4-dimensional spacetime, just like identifying the Lagrange multiplier C^a with a tetrad field e^a was a crucial property of the $2BF$ action and the Poincaré 2-group. We can also see that the choice of the third gauge group, L, dictates the number and the structure of the matter fields present in the action. In this case, $L = \mathbb{R}$ implies that we have only one real scalar field, corresponding to a single generator $\mathbb{I}$ of $\mathbb{R}$. The trivial nature of the action $\triangleright$ of $SO(3,1)$ on $\mathbb{R}$ implies that ϕ transforms as a scalar field. Finally, the scalar field appears in the topological sector of the action, making the quantization procedure feasible.

As in the case of BF and $2BF$ theories, we need to add appropriate simplicity constraints to the action (57). In order to obtain the Klein-Gordon field ϕ of mass m coupled to gravity in the standard way, the action takes the form:

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a + \phi \, \mathrm{d}\gamma \\ & - \lambda_{ab} \wedge \Big(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \Big) \\ & + \lambda \wedge \Big(\gamma - \frac{1}{2} H_{abc} e^a \wedge e^b \wedge e^c \Big) \\ & + \Lambda^{ab} \wedge \Big(H_{abc} \varepsilon^{cdef} e_d \wedge e_e \wedge e_f - \mathrm{d}\phi \wedge e_a \wedge e_b \Big) \\ & - \frac{1}{2 \cdot 4!} m^2 \phi^2 \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d \,. \end{aligned} \tag{58}$$

The first row is the topological sector (57), the second row is the familiar simplicity constraint for gravity from the action (27), the third and fourth rows contain the new simplicity constraints featuring the Lagrange multiplier 1-forms λ and Λ^{ab} and the 0-form H_{abc}, while the fifth row is the mass term for the scalar field.

The variation of (58) with respect to the variables B_{ab}, ω_{ab}, β_a, λ_{ab}, Λ_{ab}, γ, λ, H_{abc}, ϕ and e^a gives us the equations of motion. As before, all variables can be algebraically expressed in terms of the tetrads e^a and the scalar field ϕ:

$$\begin{gathered}
\lambda_{ab\mu\nu} = R_{ab\mu\nu}\,, \qquad \omega^{ab}{}_{\mu} = \triangle^{ab}{}_{\mu}\,, \qquad \gamma_{\mu\nu\rho} = -\frac{e}{2}\varepsilon_{\mu\nu\rho\sigma}\partial^\sigma\phi\,, \\
\beta^a{}_{\mu\nu} = 0\,, \qquad \Lambda^{ab}{}_{\mu} = \frac{1}{12e}g_{\mu\lambda}\varepsilon^{\lambda\nu\rho\sigma}\partial_\nu\phi e^a{}_\rho e^b{}_\sigma\,, \qquad \lambda_\mu = \partial_\mu\phi\,, \\
H^{abc} = \frac{1}{6e}\varepsilon^{\mu\nu\rho\sigma}\partial_\mu\phi e^a{}_\nu e^b{}_\rho e^c{}_\sigma\,, \qquad B_{ab\mu\nu} = \frac{1}{8\pi l_p^2}\varepsilon_{abcd}e^c{}_\mu e^d{}_\nu\,.
\end{gathered} \tag{59}$$

The equations of motion for e^a and ϕ, however, are differential equations. The equation for the scalar field becomes the covariant Klein-Gordon equation,

$$\left(\nabla_\mu\nabla^\mu - m^2\right)\phi = 0\,, \tag{60}$$

while the equation for the tetrads is

$$R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R = 8\pi l_p^2\, T^{\mu\nu}\,, \tag{61}$$

where

$$T^{\mu\nu} \equiv \partial^\mu\phi\partial^\nu\phi - \frac{1}{2}g^{\mu\nu}\left(\partial_\rho\phi\partial^\rho\phi + m^2\phi^2\right) \tag{62}$$

is the stress-energy tensor for a single real scalar field.

4.3. Einstein-Cartan-Dirac theory

In order to describe the Dirac field coupled to Einstein-Cartan gravity, we follow the same procedure as for the case of the scalar field, but now we choose the 2-crossed module $(L \overset{\delta}{\to} H \overset{\partial}{\to} G\,, \triangleright\,, \{\_\,,\_\})$ in a different way, as follows. The groups are:

$$G = SO(3,1)\,, \qquad H = \mathbb{R}^4\,, \qquad L = \mathbb{R}^8(\mathbb{G})\,, \tag{63}$$

where $\mathbb{G}$ is the algebra of complex Grassmann numbers. The maps ∂, δ and the Peiffer lifting are trivial, as before. The action of the group G on itself is given via conjugation, on H via vector representation, and on L via spinor representation, in the following way. Denoting the 8 generators of the Lie group $\mathbb{R}^8(\mathbb{G})$ as P_α and P^α, where the index α takes the values $1,\dots,4$, the action $\triangleright$ of G on L is thus given explicitly as

$$M_{ab} \triangleright P_\alpha = \frac{1}{2}(\sigma_{ab})^\beta{}_\alpha P_\beta\,, \qquad M_{ab} \triangleright P^\alpha = -\frac{1}{2}(\sigma_{ab})^\alpha{}_\beta P^\beta\,, \tag{64}$$

where $\sigma_{ab} = \frac{1}{4}[\gamma_a, \gamma_b]$, and γ_a are the usual Dirac matrices, satisfying the anticommutation rule $\{\gamma_a\,, \gamma_b\} = -2\eta_{ab}$.

As in the case of the scalar field, the choice of the group L dictates the matter content of the theory, while the action $\triangleright$ of G on L specifies its transformation properties.

Let us now proceed to construct the $3BF$ action. The 3-connection $(\alpha\,,\beta\,,\gamma)$ takes the form

$$\alpha = \omega^{ab} M_{ab}\,, \qquad \beta = \beta^a P_a\,, \qquad \gamma = \gamma^\alpha P_\alpha + \bar{\gamma}_\alpha P^\alpha\,, \tag{65}$$

while the 3-curvature $(\mathcal{F}\,,\mathcal{G}\,,\mathcal{H})$ is given as

$$\begin{aligned} &\mathcal{F} = R^{ab} M_{ab}\,, \qquad \mathcal{G} = \nabla\beta^a P_a\,, \\ \mathcal{H} &= \Big(\mathrm{d}\gamma^\alpha + \frac{1}{2}\omega^{ab}(\sigma_{ab})^\alpha{}_\beta \gamma^\beta\Big) P_\alpha + \Big(\mathrm{d}\bar{\gamma}_\alpha - \frac{1}{2}\omega^{ab}\bar{\gamma}_\beta(\sigma_{ab})^\beta{}_\alpha\Big) P^\alpha \\ &\equiv (\overset{\rightarrow}{\nabla}\gamma)^\alpha P_\alpha + (\bar{\gamma}\overset{\leftarrow}{\nabla})_\alpha P^\alpha\,, \end{aligned} \tag{66}$$

where we have used (64). The bilinear form $\langle\_\,,\_\rangle_{\mathfrak{l}}$ is defined via its action on the generators:

$$\begin{aligned} \langle P_\alpha\,, P_\beta\rangle_{\mathfrak{l}} = 0\,, &\qquad \langle P^\alpha\,, P^\beta\rangle_{\mathfrak{l}} = 0\,, \\ \langle P_\alpha\,, P^\beta\rangle_{\mathfrak{l}} = -\delta_\alpha^\beta\,, &\qquad \langle P^\alpha\,, P_\beta\rangle_{\mathfrak{l}} = \delta^\alpha_\beta\,. \end{aligned} \tag{67}$$

Note that the bilinear form defined in this way is antisymmetric, rather than symmetric, when it acts on the generators. The reason for this is the following. For general $A, B \in \mathfrak{l}$, we want the bilinear form to be symmetric. Expanding A and B into components, we can write

$$\langle A\,, B\rangle_{\mathfrak{l}} = A^I B^J g_{IJ}\,, \qquad \langle B\,, A\rangle_{\mathfrak{l}} = B^J A^I g_{JI}\,. \tag{68}$$

Since we require the bilinear form to be symmetric, the two expressions must be equal. However, since the coefficients in $\mathfrak{l}$ are Grassmann numbers, we have $A^I B^J = -B^J A^I$, so it follows that $g_{IJ} = -g_{JI}$. Hence the antisymmetry of (67) — it compensates for the anticommutativity property of the Grassman coefficients, making the bilinear form symmetric for general algebra elements $A, B \in \mathfrak{l}$.

Now we employ the action $\triangleright$ of G on L to determine the transformation properties of the Lagrange multiplier D in (49). Indeed, the choice of the group L dictates that D contains 8 independent complex Grassmannian matter fields as its components. Moreover, due to the fact that D is a 0-form and that it transforms according to the spinorial representation of $SO(3,1)$, we can identify its components with the Dirac bispinor fields, and write

$$D = \psi^\alpha P_\alpha + \bar{\psi}_\alpha P^\alpha\,. \tag{69}$$

This is again an illustration of the fact that information about the structure of the matter sector in the theory is specified by the choice of the group L

in the 2-crossed module, and its transformation properties with respect to the Lorentz group are fixed by the action $\triangleright$.

Given all of the above, we write the corresponding pure $3BF$ action as:

$$S_{3BF} = \int_{\mathcal{M}_4} B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a + (\bar{\gamma}\overleftarrow{\nabla})_\alpha \psi^\alpha + \bar{\psi}_\alpha (\overrightarrow{\nabla}\gamma)^\alpha \,. \tag{70}$$

In order to obtain the action that gives us the dynamics of Einstein-Cartan theory of gravity coupled to a Dirac field, we add the following simplicity constraints:

$$\begin{aligned} S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a + (\bar{\gamma}\overleftarrow{\nabla})_\alpha \psi^\alpha + \bar{\psi}_\alpha (\overrightarrow{\nabla}\gamma)^\alpha \\ & - \lambda_{ab} \wedge \left(B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d \right) \\ & - \lambda^\alpha \wedge \left(\bar{\gamma}_\alpha - \frac{i}{6} \varepsilon_{abcd} e^a \wedge e^b \wedge e^c (\bar{\psi}\gamma^d)_\alpha \right) \\ & + \bar{\lambda}_\alpha \wedge \left(\gamma^\alpha + \frac{i}{6} \varepsilon_{abcd} e^a \wedge e^b \wedge e^c (\gamma^d \psi)^\alpha \right) \\ & - \frac{1}{12} m \, \bar{\psi}\psi \, \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d + 2\pi i l_p^2 \, \bar{\psi}\gamma_5 \gamma^a \psi \, \varepsilon_{abcd} e^b \wedge e^c \wedge \beta^d . \end{aligned} \tag{71}$$

Similarly to the previous case of the scalar field, we recognize the topological sector in the first row, the gravitational simplicity constraint in the second row, while the third and fourth rows contain the new simplicity constraints for the Dirac field, featuring the Lagrange multiplier 1-forms λ^α and $\bar{\lambda}_\alpha$. The fifth row contains the mass term for the Dirac field, and a term which ensures the correct coupling between the torsion and the spin of the Dirac field. In particular, we want to obtain

$$T_a \equiv \nabla e_a = 2\pi l_p^2 s_a \,, \tag{72}$$

as one of the equations of motion, where

$$s_a = i \varepsilon_{abcd} e^b \wedge e^c \bar{\psi} \gamma_5 \gamma^d \psi \tag{73}$$

is the Dirac spin 2-form. Of course, other alternative coupling choices are possible, but we choose this one since this is the traditional coupling most often discussed in textbooks.

The variation of the action (71) with respect to B_{ab}, λ^{ab}, $\bar{\gamma}_\alpha$, γ^α, λ^α, $\bar{\lambda}_\alpha$, $\bar{\psi}_\alpha$, ψ^α, e^a, β^a and ω^{ab}, again gives us equations of motion, which can be algebraically solved for all fields as functions of e^a, ψ and $\bar{\psi}$:

$$B_{ab\mu\nu} = \frac{1}{8\pi l_p^2}\varepsilon_{abcd}e^c{}_\mu e^d{}_\nu\,, \qquad \lambda^\alpha{}_\mu = (\overrightarrow{\nabla}_\mu\psi)^\alpha\,, \qquad \bar{\lambda}_{\alpha\mu} = (\bar{\psi}\overleftarrow{\nabla}_\mu)_\alpha\,,$$
$$\bar{\gamma}_{\alpha\mu\nu\rho} = i\varepsilon_{abcd}e^a{}_\mu e^b{}_\nu e^c{}_\rho(\bar{\psi}\gamma^d)_\alpha\,, \qquad \gamma^\alpha{}_{\mu\nu\rho} = -i\varepsilon_{abcd}e^a{}_\mu e^b{}_\nu e^c{}_\rho(\gamma^d\psi)^\alpha\,,$$
$$\beta^a{}_{\mu\nu} = 0\,, \qquad \lambda_{ab\mu\nu} = R_{ab\mu\nu}\,, \qquad \omega^{ab}{}_\mu = \triangle^{ab}{}_\mu + K^{ab}{}_\mu\,. \tag{74}$$

Here $K^{ab}{}_\mu$ is the contorsion tensor, constructed in the standard way from the torsion tensor. In addition, we also obtain

$$T_a \equiv \nabla e_a = 2\pi l_p^2 s_a\,, \tag{75}$$

which is precisely the desired equation (72) for the torsion. Finally, the differential equations of motion for ψ and $\bar{\psi}$ are the standard covariant Dirac equation,

$$(i\gamma^a e^\mu{}_a\overrightarrow{\nabla}_\mu - m)\psi = 0\,, \tag{76}$$

and its conjugate,

$$\bar{\psi}(i\overleftarrow{\nabla}_\mu e^\mu{}_a\gamma^a + m) = 0\,, \tag{77}$$

where $e^\mu{}_a$ is the inverse tetrad. The differential equation of motion for e^a is

$$R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R = 8\pi l_p^2\, T^{\mu\nu}\,, \tag{78}$$

where

$$T^{\mu\nu} \equiv \frac{i}{2}\bar{\psi}\gamma^a\overleftrightarrow{\nabla}^\nu e^\mu{}_a\psi - \frac{1}{2}g^{\mu\nu}\bar{\psi}\Big(i\gamma^a\overleftrightarrow{\nabla}_\rho e^\rho{}_a - 2m\Big)\psi\,, \tag{79}$$

Here, we used the notation $\overleftrightarrow{\nabla} = \overrightarrow{\nabla} - \overleftarrow{\nabla}$. As expected, the equations of motion (75), (76), (77) and (78) are precisely the equations of motion of the Einstein-Cartan-Dirac theory.

4.4. Weyl and Majorana fields coupled to Einstein-Cartan gravity

As is well known, the Dirac fermions are not an irreducible representation of the Lorentz group, and one can rewrite them as left-chiral and right-chiral irreducible Weyl fermion fields. Hence, it is useful to construct the 2-crossed module and a constrained $3BF$ action for left and right Weyl spinors. For simplicity, we will discuss only the left-chiral spinor field (the right-chiral can be studied analogously). Additionally, we can also describe Majorana fermions using the same formalism, the only difference being the presence of an additional mass term in the Majorana action.

We soecify a 2-crossed module $(L \stackrel{\delta}{\to} H \stackrel{\partial}{\to} G\,, \triangleright\,, \{\_\,,\_\})$, in a way similar to the Dirac case, as follows. The groups are:

$$G = SO(3,1)\,, \qquad H = \mathbb{R}^4\,, \qquad L = \mathbb{R}^4(\mathbb{G})\,. \tag{80}$$

The maps ∂, δ and the Peiffer lifting are trivial. The action $\triangleright$ of the group G on G, H and L is given in the same way as for the Dirac case, whereas the spinorial representation reduces to

$$M_{ab} \triangleright P^\alpha = \frac{1}{2}(\sigma_{ab})^\alpha{}_\beta P^\beta\,, \qquad M_{ab} \triangleright P_{\dot\alpha} = \frac{1}{2}(\bar\sigma_{ab})^{\dot\beta}{}_{\dot\alpha} P_{\dot\beta}\,, \tag{81}$$

where $\sigma^{ab} = -\bar\sigma^{ab} = \frac{1}{4}(\sigma^a\bar\sigma^b - \sigma^b\bar\sigma^a)$, for $\sigma^a = (1,\vec\sigma)$ and $\bar\sigma^a = (1,-\vec\sigma)$, in which $\vec\sigma$ denotes the set of three Pauli matrices. The four generators of the group L are denoted as P^α and $P_{\dot\alpha}$, where the Weyl indices $\alpha, \dot\alpha$ take values $1,2$.

The 3-connection $(\alpha\,,\beta\,,\gamma)$ takes the form

$$\alpha = \omega^{ab} M_{ab}\,, \qquad \beta = \beta^a P_a\,, \qquad \gamma = \gamma_\alpha P^\alpha + \bar\gamma^{\dot\alpha} P_{\dot\alpha}\,, \tag{82}$$

while the 3-curvature $(\mathcal{F}\,,\mathcal{G}\,,\mathcal{H})$ is

$$\begin{aligned} \mathcal{F} &= R^{ab} M_{ab}\,, \qquad \mathcal{G} = \nabla\beta^a P_a\,, \\ \mathcal{H} &= \big(\mathrm{d}\gamma_\alpha + \frac{1}{2}\omega^{ab}(\sigma^{ab})^\beta{}_\alpha\gamma_\beta\big)P^\alpha + \big(\mathrm{d}\bar\gamma^{\dot\alpha} + \frac{1}{2}\omega_{ab}(\bar\sigma^{ab})^{\dot\alpha}{}_{\dot\beta}\bar\gamma^{\dot\beta}\big)P_{\dot\alpha} \\ &\equiv (\overrightarrow{\nabla}\gamma)_\alpha P^\alpha + (\bar\gamma\overleftarrow{\nabla})^{\dot\alpha} P_{\dot\alpha}\,. \end{aligned} \tag{83}$$

The Lagrange multiplier D now contains as coefficients the spinor fields ψ_α and $\bar\psi^{\dot\alpha}$,

$$D = \psi_\alpha P^\alpha + \bar\psi^{\dot\alpha} P_{\dot\alpha}\,, \tag{84}$$

and the bilinear form $\langle\_\,,\_\rangle_{\mathfrak{l}}$ for the group L is

$$\begin{aligned} \langle P^\alpha\,, P^\beta\rangle_{\mathfrak{l}} &= \varepsilon^{\alpha\beta}\,, \qquad \langle P_{\dot\alpha}\,, P_{\dot\beta}\rangle_{\mathfrak{l}} = \varepsilon_{\dot\alpha\dot\beta}\,, \\ \langle P^\alpha\,, P_{\dot\beta}\rangle_{\mathfrak{l}} &= 0\,, \qquad \langle P_{\dot\alpha}\,, P^\beta\rangle_{\mathfrak{l}} = 0\,, \end{aligned} \tag{85}$$

where $\varepsilon^{\alpha\beta}$ and $\varepsilon_{\dot\alpha\dot\beta}$ are the usual two-dimensional antisymmetric Levi-Civita symbols.

The pure $3BF$ action (49) now becomes

$$S_{3BF} = \int_{\mathcal{M}_4} B^{ab}\wedge R_{ab} + e_a \wedge \nabla\beta^a + \psi^\alpha \wedge (\overrightarrow{\nabla}\gamma)_\alpha + \bar\psi_{\dot\alpha}\wedge(\bar\gamma\overleftarrow{\nabla})^{\dot\alpha}\,. \tag{86}$$

In order to obtain the suitable equations of motion for the Weyl spinors, we again introduce appropriate simplicity constraints, to obtain:

$$
\begin{aligned}
S = \int_{\mathcal{M}_4} & B^{ab} \wedge R_{ab} + e_a \wedge \nabla \beta^a + \psi^\alpha \wedge (\overrightarrow{\nabla}\gamma)_\alpha + \bar{\psi}_{\dot{\alpha}} \wedge (\bar{\gamma}\overleftarrow{\nabla})^{\dot{\alpha}} \\
& - \lambda_{ab} \wedge (B^{ab} - \frac{1}{16\pi l_p^2} \varepsilon^{abcd} e_c \wedge e_d) \\
& - \lambda^\alpha \wedge (\gamma_\alpha + \frac{i}{6} \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \sigma^d{}_{\alpha\dot{\beta}} \bar{\psi}^{\dot{\beta}}) \\
& - \bar{\lambda}_{\dot{\alpha}} \wedge (\bar{\gamma}^{\dot{\alpha}} + \frac{i}{6} \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \bar{\sigma}^{d\dot{\alpha}\beta} \psi_\beta) \\
& - 4\pi l_p^2 \varepsilon_{abcd} e^a \wedge e^b \wedge \beta^c (\bar{\psi}_{\dot{\alpha}} \bar{\sigma}^{d\dot{\alpha}\beta} \psi_\beta) \,.
\end{aligned}
\tag{87}
$$

The new simplicity constraints, in the third and fourth rows, feature the Lagrange multiplier 1-forms λ_α and $\bar{\lambda}^{\dot{\alpha}}$. Also, in analogy to the coupling between the spin and the torsion in Einstein-Cartan-Dirac theory, the term in the fifth row is chosen to ensure that the coupling between the Weyl spin tensor

$$
s_a \equiv i \varepsilon_{abcd} e^b \wedge e^c \; \psi^\alpha \sigma^d{}_{\alpha\dot{\beta}} \bar{\psi}^{\dot{\beta}} \tag{88}
$$

and torsion is given as:

$$
T_a = 4\pi l_p^2 s_a \,. \tag{89}
$$

The action for the Majorana field is precisely the same, but for an additional mass term in the action:

$$
-\frac{1}{12} m \varepsilon_{abcd} e^a \wedge e^b \wedge e^c \wedge e^d (\psi^\alpha \psi_\alpha + \bar{\psi}_{\dot{\alpha}} \bar{\psi}^{\dot{\alpha}}) \,. \tag{90}
$$

The variation of the action (87) with respect to the variables B_{ab}, λ^{ab}, γ_α, $\bar{\gamma}^{\dot{\alpha}}$, λ_α, $\bar{\lambda}^{\dot{\alpha}}$, ψ_α, $\bar{\psi}^{\dot{\alpha}}$, e^a, β^a and ω^{ab} gives us the equations of motion, which can be algebraically solved for all variables as functions of ψ_α, $\bar{\psi}^{\dot{\alpha}}$ and e^a:

$$
\begin{gathered}
\beta^a{}_{\mu\nu} = 0 \,, \quad \lambda^{ab}{}_{\mu\nu} = R^{ab}{}_{\mu\nu} \,, \quad \lambda_{\alpha\mu} = \nabla_\mu \psi_\alpha \,, \quad \bar{\lambda}^{\dot{\alpha}}{}_\mu = \nabla_\mu \bar{\psi}^{\dot{\alpha}} \,, \\
B_{ab\mu\nu} = \frac{1}{8\pi l_p^2} \varepsilon_{abcd} e^c{}_\mu e^d{}_\nu \,, \quad \omega_{ab\mu} = \triangle_{ab\mu} + K_{ab\mu} \,, \\
\gamma_{\alpha\mu\nu\rho} = i \varepsilon_{abcd} e^a{}_\mu e^b{}_\nu e^c{}_\rho \sigma^d{}_{\alpha\dot{\beta}} \bar{\psi}^{\dot{\beta}} \,, \quad \bar{\gamma}^{\dot{\alpha}}{}_{\mu\nu\rho} = i \varepsilon_{abcd} e^a{}_\mu e^b{}_\nu e^c{}_\rho \bar{\sigma}^{d\dot{\alpha}\beta} \psi_\beta \,.
\end{gathered}
\tag{91}
$$

In addition, one also obtains (89). Finally, the differential equations of motion for the spinor and tetrad fields are

$$
\bar{\sigma}^{a\dot{\alpha}\beta} e^\mu{}_a \nabla_\mu \psi_\beta = 0 \,, \qquad \sigma^a{}_{\alpha\dot{\beta}} e^\mu{}_a \nabla_\mu \bar{\psi}^{\dot{\beta}} = 0 \,, \tag{92}
$$

and

$$R^{\mu\nu} - \frac{1}{2} g^{\mu\nu} R = 8\pi l_p^2 \, T^{\mu\nu} \,, \tag{93}$$

where

$$\begin{aligned} T^{\mu\nu} \;\; \equiv \;\; & \frac{i}{2}\bar{\psi}\bar{\sigma}^b e^\nu{}_b \nabla^\mu \psi + \frac{i}{2}\psi\sigma^b e^\nu{}_b \nabla^\mu \bar{\psi} \\ & -\frac{1}{2} g^{\mu\nu} \Big(i\bar{\psi}\bar{\sigma}^a e^\lambda{}_a \nabla_\lambda \psi + i\psi\sigma^a e^\lambda{}_a \nabla_\lambda \bar{\psi} \Big) \,. \end{aligned} \tag{94}$$

Here we have suppressed the spinor indices, for simplicity. In the case of the Majorana field, the equations of motion (91) remain the same. The equations of motion for ψ_α and $\bar{\psi}^{\dot\alpha}$ obtain the additional mass term,

$$i\sigma^a{}_{\alpha\dot\beta} e^\mu{}_a \nabla_\mu \bar{\psi}^{\dot\beta} - m\psi_\alpha = 0 \,, \qquad i\bar{\sigma}^{a\dot\alpha\beta} e^\mu{}_a \nabla_\mu \psi_\beta - m\bar{\psi}^{\dot\alpha} = 0 \,, \tag{95}$$

while the stress-energy tensor becomes

$$\begin{aligned} T^{\mu\nu} \;\; \equiv \;\; & \frac{i}{2}\bar{\psi}\bar{\sigma}^b e^\nu{}_b \nabla^\mu \psi + \frac{i}{2}\psi\sigma^b e^\nu{}_b \nabla^\mu \bar{\psi} \\ & -g^{\mu\nu} \frac{1}{2} \left[i\bar{\psi}\bar{\sigma}^a e^\lambda{}_a \nabla_\lambda \psi + i\psi\sigma^a e^\lambda{}_a \nabla_\lambda \bar{\psi} - \frac{1}{2} m \left(\psi\psi + \bar{\psi}\bar{\psi} \right) \right] \,. \end{aligned} \tag{96}$$

5. Conclusions

Let us summarize the results of the paper. In Section 2 we have introduced the BF theory and discussed models based on constrained BF action, in particular the Yang-Mills theory in Minkowski spacetime and the Plebanski formulation of general relativity. Section 3 was devoted to the first step in the categorical ladder and the $2BF$ theory. After introducing the notions of a 2-group, a crossed module, and the corresponding $2BF$ theory, we have studied the $2BF$ formulation of general relativity and the Einstein-Yang-Mills theory. Then, in Section 4 we have performed one more step in the categorical ladder, and introduced the notions of a 3-group, 2-crossed module, and the $3BF$ theory. This structure was employed to construct the constrained $3BF$ actions for the cases of Klein-Gordon, Dirac, Weyl and Majorana fields, each coupled to the Einstein-Cartan gravity in the standard way. In those descriptions, it turned out that the scalar and fermion fields are associated to a *new gauge group*, similar to the gauge fields being associated to a gauge group in the Yang-Mills theory. This opens up a possibility of a classification of matter fields based on an algebraic structure of a 3-group.

All the obtained results serve to complete the first step of the spinfoam quantization programme, as outlined in the Introduction. This paves the way to the study of steps 2 and 3 of the programme. Namely, the full action for gravity, gauge fields and matter is written completely in the langulage of differential forms, which can be easily adapted to a triangulated spacetime manifold, in the sense of Regge calculus. This can be seen in the following table:

d	triangulation	dual triangulation	form	fields	field strengths
0	vertex	4-polytope	0-form	ϕ, $\psi_{\tilde{\alpha}}$, $\bar{\psi}^{\tilde{\alpha}}$	
1	edge	3-polyhedron	1-form	ω^{ab}, A^I, e^a	
2	triangle	face	2-form	β^a, B^{ab}	R^{ab}, F^I, T^a
3	tetrahedron	edge	3-form	γ, $\gamma_{\tilde{\alpha}}$, $\bar{\gamma}^{\tilde{\alpha}}$	$\mathcal{G}^a$
4	4-simplex	vertex	4-form		$\mathcal{H}$, $\mathcal{H}_{\tilde{\alpha}}$, $\bar{\mathcal{H}}^{\tilde{\alpha}}$

This data can be utilized to construct a Regge-discretized topological $3BF$ action, and from that a state sum Z, giving rise to a rigorous definition of the path integral

$$Z = \int \mathcal{D}g \int \mathcal{D}\phi \; e^{iS[g,\phi]} \,, \tag{97}$$

which is a generalization of (1) in the sense that it adds matter fields (including the gauge boson sector) to gravity at the quantum level. Being a topological theory, and given the underlying structure of the 3-group, a pure $3BF$ action ought to ensure the topological invariance of the state sum Z, i.e., Z should be triangulation independent. This step, however, requires the generalizations of the Peter-Weyl and Plancharel theorems to 2-groups and 3-groups, which are unfortunately still missing (though there are some attempts to circumvent them at least in the 2-group case [27, 28]). Namely, the purpose of the Peter-Weyl and Plancharel theorems is to provide a decomposition of a function on a group into a sum over the corresponding irreducible representations, which then specifies the spectrum of labels for the simplices in the triangulation, and fixes the domain of values for the fields living on those simplices. In the absence of the two theorems, one can still try to *guess* the irreducible representations of the 2- and 3-groups, as was done for example in the *spincube model* of quantum gravity [12], or to try to construct the state sum using other techniques, as was done in [27, 28]).

Of course, when building a realistic theory, we are not interested in a topological theory, but instead in one which contains local propagating degrees of freedom. Thus the state sum Z need not be a topological invariant. This is obtained via the step 3 of the spinfoam quantization programme, by imposing the simplicity constraints on Z. The classical actions discussed in this paper manifestly distinguish the topological sector from the simplicity constraints, which have been explicitly determined. Imposing them should thus be a straightforward procedure for a given Z. Completing this programme would ultimately lead us to a tentative state sum describing both gravity and matter at a quantum level, which is a topic for future research.

In addition to the construction of a full quantum theory of gravity, there are also many additional possible studies of the classical constrained $3BF$ action. For example, a Hamiltonian analysis of the theory could be interesting for the canonical quantization programme, and some work has begun in this area [29]. Also, it is worth looking into the idea of imposing the simplicity constraints using a spontaneous symmetry breaking mechanism. Finally, one can also study in more depth the mathematical structure and properties of the simplicity constraints. The list is not conclusive, and there may be many other interesting topics to study.

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Quantum gravity for piecewise flat spacetimes*

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Abstract

We describe a theory of quantum gravity which is based on the assumption that the spacetime structure at small distances is given by a piecewise linear (PL) 4-manifold corresponding to a triangulation of a smooth 4-manifold. The fundamental degrees of freedom are the edge lengths of the triangulation. One can work with finitely many edge lengths, so that the corresponding Regge path integral can be made finite by using an appropriate path-integral measure. The semi-classical limit is computed by using the effective action formalism, and the existence of a semi-classical effective action restricts the choice of the path-integral measure. The classical limit is given by the Regge action, so that one has a quantum gravity theory for a piecewise-flat general relativity. By using the effective action formalism we show that the observed value of the cosmological constant can be recovered from the effective cosmological constant. When the number of 4-simplices in the spacetime triangulation is large, then the PL effective action is well approximated by a quantum field theory effective action with a physical cutoff determined by the smallest edge length.

1. Introduction

The standard approach to the problem of constructing a quantum gravity (QG) theory [1, 2] can be described as the following problem. Let M be a smooth 4-manifold, of topology $\Sigma \times I$, where Σ is a 3-manifold and I an interval from $\mathbf{R}$. Let g be a Minkowski-signature metric on M and Φ a set of matter fields on M. Then the goal is to find a triple $(\hat{g}, \hat{\Phi}, \hat{U})$, where $\hat{g}$ and $\hat{\Phi}$ represent Hermitian operators parametrized by the points of M,

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acting in some Hilbert space $\mathcal{H}$, while $\hat{U}$ is a unitary evolution operator parametrized by I, such that the the classical limit ($\hbar \to 0$) of the quantum time-evolution is equivalent to the Einstein equations.

The best known example of this approach is Loop Quantum Gravity (LQG), see [3] for a recent review and references. In the LQG case, the Hilbert space $\mathcal{H}$ is only known to be a subset of a non-separable Hilbert space and $\hat{U}$ can be constructed only for a triangulation $T(M)$ of M, so that it is not clear what is the classical limit. Note that in the standard QG approach, the structure of M is not changed after the quantization, and it is well known that this is the main source of the difficulties for a quantization of gravity [1, 2]. This leads us to an alternative approach where M is replaced by a quantum spacetime $\widehat{M}$. The obvious choice would be a noncommutative manifold based on M, like in the case of noncommutative geometry (NCG) [4], where the coordinates of M become elements of a noncommutative algebra. Another choice is made in the superstring theory [5], where the coordinates of M become coordinates of the loop manifold $\mathcal{L}M$ and new Grassmann (anticommuting) coordinates are added, so that $\widehat{M}$ is a loop super manifold.

In this paper we would like to present the case when $\widehat{M} = T(M)$, see [12, 13]. This is clearly a much simpler choice for $\widehat{M}$ than the one made in NCG or in the superstring theory, but the price paid is that the spacetime triangulation becomes a physical structure. However, the PL manifold $T(M)$ looks like the smooth manifold M when the number of 4-simplices is large. Also, by using $T(M)$ one reduces the infinite number of the degrees of freedom (DOF) for g and Φ to a finite number, which then simplifies the quantization.

Note that Regge was the first to use $T(M)$ in order to define the path integral for general relativity (GR) [6], see [7] for a modern review. However, in Regge's approach the triangulation was an auxiliary structure and had to be removed via the smooth limit $T(M) \to M$. However, obtaining the smooth limit in the Regge approach is a difficult problem. The same applies to the case of spin-foam models of LQG, which can be only defined when the spacetime is a PL manifold. In causal dynamical triangulations (CDT) approach [8], $T(M)$ is also used to define the path integral, but it is also considered an auxiliary structure. Obtaining the smooth limit in CDT is proposed by performing a sum over the triangulations.

2. PL gravity path integral

Let $T(M)$ be a regular[1] triangulation of a smooth 4-manifold M. We will assign positive numbers L_ϵ to the edges ϵ of $T(M)$. If we think of an L_ϵ as a distance between two vertices of $T(M)$ induced by some metric, then we

[1]Any two k-simplices of $T(M)$ cannot have more than one common $(k-1)$-simplex, where $k = 1, 2, 3, 4$.

can define a constant metric in each 4-simplex σ

$$g_{kl}^{(\sigma)} = \frac{L_{0k}^2 + L_{0l}^2 - L_{kl}^2}{2L_{0k}L_{0l}}\,, \qquad 1 \le k,l \le 4\,, \tag{1}$$

where the indices $0,1,2,3,4$ denote the vertices of a 4-simplex σ. Hence we replace a smooth metric g on M by a PL version (1). We want that the PL metric has the Minkowski signature, and this can be ensured by requiring that L_ϵ satisfy the triangle inequalities for the triangles which belong to one of the tetrahedrons of σ, for example the tetrahedron $(1,2,3,4)$, while the L_ϵ of the triangles $(0,i,j)$ must not satisfy the triangle inequalities.

Having all $L_\epsilon > 0$ means that all triangles in $T(M)$ are spacelike. For $M = \Sigma \times I$ manifolds, this gives an accordion-like triangulation (triangulation of a cylinder). A more natural triangulation is to take a finite number of spacelike slices $T_k(\Sigma)$ which are linked by timelike edges such that each 4-simplex has a spacelike tetrahedron in T_k and a vertex in T_{k-1} or in T_{k+1}. This class of triangulations is used in CDT models [8]. We will then require that the L_ϵ of T_k satisfy the triangle inequalities, while a timelike edge will be assigned an imaginary length iL_ϵ. Hence the labels of the edges of timelike triangles will not satisfy the triangle inequalities and the metric (1) will have the correct signature.

The curvature scalar R will be concentrated on the triangles and R will be given by the deficit angle divided by the area of the dual face. Hence in each σ we have a flat metric (1) so that we can say the corresponding PL metric is a piecewise-flat metric.

Note that an L_ϵ label represents a proper length, so that L_ϵ is invariant under the local Lorentz transformations in each 4-simplex. We will also have $(L_\epsilon)^2 > 0$ for a spacelike edge, while $(L_\epsilon)^2 < 0$ for a timelike edge.

The Einstein-Hilbert action for the PL metric (1) becomes the Regge action

$$S_{Rc} = \frac{1}{G_N}\sum_{\Delta=1}^{F} A_\Delta(L)\theta_\Delta(L) + \Lambda_c V_4(L)\,, \tag{2}$$

where G_N is the Newton constant, $A_\Delta(L)$ is the area of a triangle $\Delta \in T(M)$ and θ_Δ is the deficit angle. Λ_c is the cosmological constant and V_4 is the 4-volume of $T(M)$. See [8] how to define (2) when the timelike triangles are present. Note that the Regge action describes a theory with a finite number of DOF when Σ is compact, while in the case when Σ is non-compact, we can restrict L_ϵ to be non-zero only in a ball $B \subset \Sigma$.

One can also couple the matter fields to a Regge PL metric and the corresponding smooth actions will become the PL actions for a finite number of matter DOF. For example, a scalar field will be defined by the values of the field at the vertices of $T(M)$, which is equivalent to a PL function on the 4-polytopes of the dual triangulation.

In the case of a scalar field matter, the Regge path integral will be given by the following $(E+V)$-dimensional integral

$$Z = \int_{D_E} \mu(L)\, d^E L \int_{\mathbf{R}^V} \prod_{\nu=1}^{V} d\phi_\nu \, e^{i[S_{Rc}(L)+S_m(L,\phi)]/\hbar} \,, \tag{3}$$

where E is the number of the edges in $T(M)$ and V is the number of the vertices in $T(M)$ [13]. S_m is the PL form of the scalar-field action and the integration region D_E is a subset of $\mathbf{R}_+^E$ where the triangle inequalities hold. The measure μ has to be chosen such that it makes Z finite. The matter PI measure is taken to be trivial and we will assume that the matter path integral is finite. This is true, because the matter path integral will be given by a finite product of the integrals of the type

$$I(\alpha,\beta) = \int_{-\infty}^{\infty} dx\, e^{-\alpha x^2 - \beta x^4} \,, \tag{4}$$

where $\alpha, \beta \in \mathbf{C}$. Since I is convergent for $\alpha, \beta > 0$, the analytic continuation $I(i\alpha, i\beta)$ will be finite.

Note that in the standard Regge formulation the spacetime metric is of the Euclidean signature. This was done in analogy to the QFT case where the Euclidean signature improves the convergence of the path integral (3). However, in the QG case this does not help, because the scalar curvature also changes the sign in the Euclidean case and can be unbounded. Actually, the Lorentzian integral has better convergence properties, which can be seen on a toy example $R(x) = \alpha\, x^2$ where $x \in \mathbf{R}_+$ and α is a constant different from zero. Then $Z_E = \int_0^\infty dx\, e^{-R(x)}$ is convergent only for $\alpha > 0$ while $Z_L = \int_0^\infty dx\, e^{iR(x)}$ is convergent for any sign of α. The presence of imaginary edge lengths and imaginary angles in the Lorentzian case is not a problem, since all the geometric quantities can be defined [8].

Finding the smooth limit $T(M) \to M$ for Z is a difficult problem. However, there is a promising approach, based on the Wilson renormalization group [7]. In this approach one considers Z as function of the dimensionless couplings γ e λ

$$\gamma = l_0^2/(G_N \hbar) = l_0^2/l_P^2 \,, \quad \lambda = l_0^4 \Lambda_c/\hbar = l_0^4/(L_c^2 l_P^2) \,,$$

where $L_c^2 = G_N/\Lambda_c$ and l_0 is an arbitrary length. One then looks for a critical point $P_0 = (\gamma_0, \lambda_0)$ where the second derivatives of Z diverge so that there is a second-order phase transition. At the critical point the correlation length diverges, so that a transition to the smooth phase occurs. However, the problem with this approach is that at P_0 the perturbation theory does not apply, so that the calculation has to be done by using numerical methods. Also the semiclassical limit $l_P^2 \to 0$ corresponds to a strong coupling region $\gamma \to \infty$ and $\lambda \to \infty$ so that it is difficult to determine it analytically.

However, the easiest way to determine the semiclassical limit in a QG theory defined by a path integral is to use the effective action, see [9, 10, 11, 12, 13]. Namely, the effective action can be calculated analytically in the $\hbar \to 0$ limit. Also the PI measure $\mu(L)$ has to be such that allows a semiclassical expansion for the effective action for large L_ϵ. This gives us an additional constraint on the choice of $\mu(L)$.

3. Effective action for PL quantum gravity

We will assume that $T(M)$ is the fundamental spacetime structure, i.e. the spacetime is a *piecewise linear* 4-manifold $T(M)$ with a flat metric in each cell (4-simplex σ). If N is the number of cells of $T(M)$, then for $N \gg 1$, $T(M)$ will look like the smooth manifold M on a scale much larger than the maximal edge length.

By an appropriate choice of the measure μ the integral $Z(T(M))$ can be made finite. Since $T(M)$ is the physical spacetime, there is no need to define the smooth limit $T(M) \to M$. Instead, we need a large-N approximation for the observables. This is analogous to the fluid dynamics situation where on the scales much larger than the inter-molecular distance we can approximate the molecular velocities as a smooth field and use the Navier-Stokes equations.

We will determine the semiclassical limit of PL quantum gravity by using the effective action. It can be computed by using the effective action equation in the limit $L_\epsilon \gg l_P = \sqrt{G_N \hbar}$.

Let us recall first the effective action definition from quantum field theory (QFT). Let ϕ be a real scalar field on M and let

$$S(\phi) = \frac{1}{2}\int_M d^4x \sqrt{|g|}\left[g^{\mu\nu}\,\partial_\mu\phi\,\partial_\nu\phi - \frac{1}{2}\omega^2\phi^2 - \lambda\,\phi^4\right],$$

be a flat-spacetime action. The effective action $\Gamma(\phi)$ can be determined from the following integro-differential equation

$$e^{i\Gamma(\phi)/\hbar} = \int \mathcal{D}h \exp\left[\frac{i}{\hbar}S(\phi+h) - \frac{i}{\hbar}\int_M d^4x\,\frac{\delta\Gamma}{\delta\phi(x)}h(x)\right], \tag{5}$$

see [14, 15].

Note that a generic solution $\Gamma(\phi)$ is a function with values in $\mathbf{C}$. The Wick rotation is used to obtain a real-valued function $\Gamma(\phi)$. This is done by solving first the EA equation in the Euclidean spacetime

$$e^{-\Gamma_E(\phi)/\hbar} = \int \mathcal{D}h \exp\left[-\frac{1}{\hbar}S_E(\phi+h) + \frac{1}{\hbar}\int_M d^4x\,\frac{\delta\Gamma_E}{\delta\phi(x)}h(x)\right]. \tag{6}$$

Then $x_0 = -it$ is inserted into a solution $\Gamma_E(\phi)$, where (x_0, x_k) are the spacetime coordinates, so that

$$\Gamma(\phi) = i\Gamma_E(\phi)|_{x_0=-it}\,.$$

However, the Wick rotation cannot be used in quantum gravity, since in many problems of interest, introducing a flat background metric does not make sense. One way to resolve this difficulty is to use the fact that the Wick rotation in QFT is equivalent to

$$\Gamma(\phi) \to Re\,\Gamma(\phi) + Im\,\Gamma(\phi)\,, \tag{7}$$

see [9, 10]. This prescription is convenient for quantum gravity because it does not involve a background metric, nor a system of coordinates.

In the case of PL quantum gravity without matter, the effective action (EA) equation is given by

$$e^{i\Gamma(L)/l_P^2} = \int_{D_E(L)} d^E x\, \mu(L+x) e^{iS_{Rc}(L+x)/l_P^2 - i\sum_{\epsilon=1}^{E} \Gamma'_\epsilon(L) x_\epsilon / l_P^2}\,, \tag{8}$$

where $l_P^2 = G_N \hbar$ and $D_E(L)$ is a subset of $\mathbf{R}^E$ obtained by translating D_E by a vector $-L$ [12]. Note that $D_E(L) \subseteq [-L_1, \infty) \times \cdots \times [-L_E, \infty)$.

We will look for a semiclassical solution

$$\Gamma(L) = S_{Rc}(L) + l_P^2 \Gamma_1(L) + l_P^4 \Gamma_2(L) + \cdots\,,$$

where $L_\epsilon \gg l_P$ and

$$|\Gamma_n(L)| \gg l_P^2 |\Gamma_{n+1}(L)|\,.$$

When $L_\epsilon \to \infty$, then $D_E(L) \to \mathbf{R}^E$ and

$$e^{i\Gamma(L)/l_P^2} \approx \int_{\mathbf{R}^E} d^E x\, \mu(L+x) e^{iS_{Rc}(L+x)/l_P^2 - i\sum_{\epsilon=1}^{E} \Gamma'_\epsilon(L) x_\epsilon / l_P^2}\,. \tag{9}$$

Actually, one can use the equation (9) to determine $\Gamma(L)$ for large L when μ falls off sufficiently quickly [12]. The reason is that

$$D_E(L) \approx [-L_1, \infty) \times \cdots \times [-L_E, \infty)\,,$$

for $L_\epsilon \to \infty$, so that the relevant behaviour is captured by the following one-dimensional integral

$$\int_{-L}^{\infty} dx\, e^{-zx^2/l_P^2 - wx} = \sqrt{\pi}\, l_P \exp\Big[-\frac{1}{2}\log z + l_P^2 \frac{w^2}{4z}$$

$$+ l_P \frac{e^{-z\bar{L}^2/l_P^2}}{2\sqrt{\pi z}\,\bar{L}} \left(1 + O(l_P^2/z\bar{L}^2)\right) \Big]\,,$$

where $\bar{L} = L + l_P^2 \frac{w}{2z}$ and $Re\, z = -(\log\mu)''$. The non-analytic terms in $\hbar$ will be absent if

$$\lim_{L\to\infty} e^{-z\bar{L}^2/l_P^2} = 0 \Leftrightarrow (\log\mu)'' < 0 \text{ for } L \to \infty\,.$$

Hence the perturbative solution exists for the exponentially damped measures and it will be given by the equation (9).

For $D_E(L) = \mathbf{R}^E$ and $\mu(L)$ a constant, the perturbative solution is given by the EA diagrams

$$\Gamma_1 = \frac{i}{2} Tr \log S''_{Rc} \,, \quad \Gamma_2 = \langle S_3^2 G^3 \rangle + \langle S_4 G^2 \rangle \,,$$

and

$$\Gamma_3 = \langle S_3^4 G^6 \rangle + \langle S_3^2 S_4 G^5 \rangle + \langle S_3 S_5 G^4 \rangle + \langle S_4^2 G^4 \rangle + \langle S_6 G^3 \rangle \,, \, ...$$

where $G = i(S''_{Rc})^{-1}$ is the propagator and $S_n = iS^{(n)}_{Rc}/n!$ for $n > 2$, are the vertex weights, see [15, 12]. The contractions $\langle X \cdots Y \rangle$ are the sums over the repeated DOF indices

$$\langle X \cdots Y \rangle = \sum_{k,\dots,l} X_{k\dots l} \cdots Y_{k\dots l} \quad .$$

When $\mu(L)$ is not a constant, then the perturbative solution is given by

$$\Gamma(L) = \bar{S}_{Rc}(L) + l_P^2 \bar{\Gamma}_1(L) + l_P^4 \bar{\Gamma}_2(L) + \cdots \,,$$

where

$$\bar{S}_{Rc} = S_{Rc} - i l_P^2 \log \mu \,,$$

while $\bar{\Gamma}_n$ is given by the sum of n-loop EA diagrams with $\bar{G}$ propagators and $\bar{S}_n$ vertex weights [12].

Therefore

$$\Gamma_1 = -i \log \mu + \frac{i}{2} Tr \log S''_{Rc} \,,$$

$$\Gamma_2 = \langle S_3^2 G^3 \rangle + \langle S_4 G^2 \rangle + Res[l_P^{-4} Tr \log \bar{G}] \,,$$

$$\Gamma_3 = \langle S_3^4 G^6 \rangle + \cdots + \langle S_6 G^3 \rangle + Res[l_P^{-6} Tr \log \bar{G}]$$

$$+ Res[l_P^{-6} \langle \bar{S}_3^2 \bar{G}^3 \rangle] + Res[l_P^{-6} \langle \bar{S}_4 \bar{G}^2 \rangle] \,,$$

see [12].

Since the PI measure μ has to vanish exponentially for large edge lengths, a natural choice is

$$\mu(L) = \exp\left(-V_4(L)/(L_0)^4\right) \,, \tag{10}$$

where L_0 is a length parameter [12]. Since $\log \mu(L) = O\left((L/L_0)^4\right)^2$ then for $L_\epsilon > L_c$ and

$$L_0 > \sqrt{l_P \, L_c} \,, \tag{11}$$

[2] The notation $f(x_1, ..., x_n) = O(x^\alpha)$ means that $f(\lambda x_1, ..., \lambda x_n) = O(\lambda^\alpha)$ for $\lambda \to \infty$.

where $L_c^{-2} = \Lambda_c$, we get the following large-L asymptotics [13, 16]

$$\Gamma_1(L) = O(L^4/L_0^4) + \log O(L^2/L_c^2) + \log\theta(L) + O(L_c^2/L^2) \qquad (12)$$

and

$$\Gamma_{n+1}(L) = O\left((L_c^2/L^4)^n\right) + L_{0c}^{-2n} O\left((L_c^2/L^2)\right) , \qquad (13)$$

where $L_{0c} = L_0^2/L_c$.

4. Effective cosmological constant

The asymptotics (12) and (13) imply that the series

$$\Gamma(L) = \sum_{n\geq 0} (l_P)^{2n} \Gamma_n(L)$$

is semiclassical (SC) for $L_\epsilon \gg l_P$ and $L_0 \gg \sqrt{l_P\, L_c}$.

Let $\Gamma \to \Gamma/G_N$ so that $S_{eff} = (Re\,\Gamma + Im\,\Gamma)/G_N$. The effective action is then given by

$$S_{eff} = \frac{S_{Rc}}{G_N} + \frac{l_P^2}{G_N L_0^4} V_4 + \frac{l_P^2}{2G_N} Tr \log S''_{Rc} + O(l_P^4) ,$$

for $L_\epsilon \gg l_P$. Hence the $O(\hbar)$, or the one-loop, cosmological constant (CC) for pure gravity is given by

$$\Lambda = \Lambda_c + \frac{l_P^2}{L_0^4} = \Lambda_c + \Lambda_{qg} . \qquad (14)$$

One can show that the one-loop cosmological constant is exact because there are no $O(L^4)$ terms beyond the one-loop order [13, 16]. This is a consequence of the large-L asymptotics

$$\log \bar{S}''_{Rc}(L) = \log O(L^2/\bar{L}_c^2) + \log\theta(L) + O(\bar{L}_c^2/L^2)$$

$$\bar{\Gamma}_{n+1}(L) = O\left((\bar{L}_c^2/L^4)^n\right) ,$$

where $\bar{L}_c^2 = L_c^2 \left[1 + i l_P^2 (L_c^2/L_0^4)\right]^{-1/2}$.

Hence the one-loop formula (14) is exact in the case of pure gravity. If $\Lambda_c = 0$, the observed value of Λ is obtained for $L_0 \approx 10^{-5} m$ so that $l_P^2 \Lambda \approx 10^{-122}$ [12]. Note that $L_0 \approx 10^{-5} m$ is consistent with the requirement that $L_0 \gg l_P$, which replaces the SC condition $L_0 \gg \sqrt{L_c l_P}$ when $\Lambda_c = 0$.

The formula (14) is intriguing but unrealistic, since there is matter in the universe. In order to obtain a realistic expression for the effective CC, we need to study the EA equation with matter. This study also requires the understanding of the emergence of the smooth spacetime from a PL manifold $T(M)$. If $T(M)$ has a large number of the edges ($E \gg 1$) then the following approximations are valid

$$S_R(L) \approx \frac{1}{2}\int_M d^4x\sqrt{|g|}\,R(g)\,, \tag{15}$$

and

$$\Lambda_c V_4(L) \approx \Lambda_c \int_M d^4x\sqrt{|g|} = \Lambda_c\, V_M\,, \tag{16}$$

where $|g| = |\det g|$. These are the standard formulas of the Regge calculus and they nicely illustrate how the PL manifold $T(M)$ with many 4-simplices can be approximated by a smooth manifold M with a smooth (differentiable) metric g.

Similarly, the effective action $\Gamma(L)$ will be approximated by a QFT effective action $\Gamma^*(g)$, where g is a smooth metric on M. Let L_K be a minimal length in a triangulation, so that $L_\epsilon \geq L_K$ and let $L_K \gg l_P$. When $E \gg 1$ the following approximation is valid

$$Tr\log S_R''(L) \approx \int_M d^4x\sqrt{|g|}\left[aR^2 + bR_{\mu\nu}R^{\mu\nu}\right]\log(K/K_0)\,, \tag{17}$$

where $R_{\mu\nu}$ is the Ricci tensor, and a, b, K_0 are some constants.

The formula (17) follows from the fact that a PL function on a lattice with a cell size L_K can be written as a Fourier integral over a compact region $|q| \leq \pi/L_K$ where q is the wave vector[3]. Hence the PL trace-log term can be approximated by using the QFT formulation of GR with a momentum cutoff $K = 2\pi\hbar/L_K$.

The effect of the matter on the CC can be studied by introducing a scalar field on M

$$S_m(g,\phi) = \frac{1}{2}\int_M d^4x\sqrt{|g|}\left[g^{\mu\nu}\,\partial_\mu\phi\,\partial_\nu\phi - U(\phi)\right]\,, \tag{18}$$

where $U = \frac{1}{2}\omega^2\phi^2 + \lambda\,\phi^4$.

On a PL manifold $T(M)$ the action (18) becomes

$$S_m = \frac{1}{2}\sum_\sigma V_\sigma(L)\sum_{k,l} g_\sigma^{kl}(L)\,\phi_k'\,\phi_l' - \frac{1}{2}\sum_p V_p^*(L)\,U(\phi_p)\,,$$

where $\phi_k' = (\phi_k - \phi_0)/L_{0k}$ and $k, l, 0$ are vertices in a 4-simplex σ, p labels the vertices of $T(M)$ and V^* is the volume of the dual cell. Then the total classical action of gravity plus matter on $T(M)$ is given by

$$S(L,\phi) = \frac{1}{G_N}S_{Rc}(L) + S_m(L,\phi)\,.$$

[3]This region is known as the first Brillouin zone.

The corresponding EA equation is given by

$$e^{\frac{i}{l_P^2}\Gamma(L,\phi)} = \int_{D_E(L)} d^E l \int_{\mathbf{R}^V} d^V\chi$$

$$\exp\left[\frac{i}{l_P^2}\left(\bar{S}(L+l,\phi+\chi) - \sum_\epsilon \frac{\partial\Gamma}{\partial L_\epsilon}\, l_\epsilon - \sum_p \frac{\partial\Gamma}{\partial\phi_p}\,\chi_p\right)\right], \quad (19)$$

where $\bar{S} = S_{Rc} - il_P^2\log\mu + G_N S_m$, see [13].

We will look for a perturbative solution

$$\Gamma(L,\phi) = S(L,\phi) + l_P^2\Gamma_1(L,\phi) + l_P^4\Gamma_2(L,\phi) + \cdots ,$$

and require it to be semiclassical for $L_\epsilon \gg l_P$ and $|\sqrt{G_N}\,\phi| \ll 1$. This can be checked on the $E=1$ toy model

$$S(L,\phi) = (L^2 + L^4/L_c^2)\theta(L) + L^2\theta(L)\phi^2(1+\omega^2L^2+\lambda\phi^2L^2)\,,$$

where $\theta(L)$ is a homogeneous function of degree zero.

It is not difficult to see that

$$\Gamma(L,\phi) = \Gamma_g(L) + \Gamma_m(L,\phi)\,,$$

and

$$\Gamma_m(L,\phi) = V_4(L)\,U_{eff}(\phi)$$

for constant ϕ where $U_{eff}(0)=0$. Furthermore,

$$\Gamma_g(L) = \Gamma_{pg}(L) + \Gamma_{mg}(L)\,,$$

where Γ_{pg} is the pure gravity contribution and Γ_{mg} is the matter induced contribution.

In the smooth-manifold approximation one has

$$\Gamma_{mg}(L) \approx \Lambda_m V_M + \Omega_m(R,K)\,,$$

where $K = 2\pi\hbar/L_K$ is the momentum cutoff. One can show that

$$\Omega_m = \Omega_1 l_P^2 + O(l_P^4)$$

and

$$\begin{aligned}\Omega_1(R,K) &= a_1K^2\int_M d^4x\sqrt{|g|}\,R \\ &+ \log(K/\omega)\int_M d^4x\sqrt{|g|}\Big[a_2R^2 + a_3R^{\mu\nu}R_{\mu\nu} \\ &\qquad + a_4R^{\mu\nu\rho\sigma}R_{\mu\nu\rho\sigma} + a_5\nabla^2R\Big] \\ &+ O(1/K^2)\,,\end{aligned} \quad (20)$$

where $R_{\mu\nu\rho\sigma}$ is the Riemann curvature tensor, see [13].

The effective CC will be then given as

$$\Lambda = \Lambda_c + \Lambda_{qg} + \Lambda_m \,,$$

where Λ_{qg} is given by (14). Note that the matter contribution to CC can be approximated by a sum

$$\Lambda_m \approx \sum_\gamma v(\gamma, K) \tag{21}$$

where $v(\gamma, K)$ is a one-particle irreducible vacuum Feynman diagram for the field-theory action S_m in flat spacetime with the cutoff K. One can show that

$$\begin{aligned} \sum_\gamma v(\gamma, K) \quad &\approx \quad l_P^2 K^4 \Big[c_1 \ln(K^2/\omega^2) + \sum_{n\geq 2} c_n (\bar\lambda)^{n-1} (\ln(K^2/\omega^2))^{n-2} \\ &+ \quad \sum_{n\geq 4} d_n (\bar\lambda)^{n-1} (K^2/\omega^2)^{n-3} \Big] \,, \end{aligned} \tag{22}$$

for $K \gg \omega$, where $\bar\lambda = l_P^2 \lambda$, see [16]. Therefore one has a highly divergent sum of matter vacuum-energy contributions to the cosmological constant when $K \to \infty$. This is the famous cosmological constant problem which appears in any QFT formulation of quantum gravity.

However, in the PL formulation of quantum gravity (PLQG), the QFT which produces the infinite sum in (22) is just an approximation. The fundamental theory has finitely many DOF so that the exact solution of the EA equation will give a finite and cutoff-independent value for Λ. Therefore

$$\Lambda_m = V(\omega^2, \lambda, l_P^2) \,, \tag{23}$$

and

$$\Lambda = \pm \frac{1}{L_c^2} + \frac{l_P^2}{2L_0^4} + V(\omega 2, \lambda, l_P^2) \,. \tag{24}$$

The equation (24) can be used to fix the free parameters L_0 and L_c. By equating Λ with the experimentally observed value, we obtain

$$\lambda = x + y + \lambda_m \tag{25}$$

where $\lambda = l_P^2 \Lambda \approx 10^{-122}$, $x = \pm\, l_P^2/L_c^2$, $y = l_P^4/2L_0^4$ and $\lambda_m = l_P^2 V$. The equation (25) has infinitely many solutions, but we also have to impose the condition for the existence of the semi-classical limit (11). This gives the restriction

$$0 < y < 2|x| \,. \tag{26}$$

The value of λ_m is not known, but for any value of λ_m the equation (25) has infinitely many solutions which obey the restriction (26). Note that the solution $x = -\lambda_m$ and $y = \lambda$, which was proposed in [13], will be acceptable if $|\lambda_m| > \lambda/2$. This solution is special because it gives a value for L_0 which is independent of the value of λ_m, $L_0 \approx 10^{-5}$m. This is the same value which was obtained in the case of pure PL gravity without the cosmological constant [12].

5. The CC problem in quantum gravity

The formula (24) for the exact effective cosmological constant is an essential ingredient for the resolution of the CC problem from QFT in the context of a QG theory. The result (24) can be better understood if we recall the definition of the CC problem given by Polchinski [17]. According to this definition, the CC problem in a QG theory has two parts:

1) show that the observed CC value is in the CC spectrum,

2) explain why the CC takes the observed value.

The meaning of the first part (P1) of the CC problem is obvious if the cosmological constant is represented by an operator. In the case when one has a quantum corrected expression of the classical CC value, one has to show that there are values of the free parameters which give the observed CC value. The PLQG theory clearly solves P1, while the second part (P2) of the CC problem cannot be addressed by the current formalism. The reason is that one has to generalise the standard formalism of quantum mechanics in order to provide a mechanism for a selection of a wavefunction of the universe with a particular value of the cosmological constant.

Note that demonstrating P1 is a highly non-trivial task in any QG theory. The problem P1 has been addressed so far only in PLQG theory and in string theory. In the string theory case there are only plausibility arguments that P1 is true [18, 19]. The CC spectrum in string theory is discrete with $O(10^{500})$ values [18]. Although positive CC values are not natural in string theory, a mechanism for their appearance was provided in [19]. Hence it is plausible to assume that the CC spectrum is sufficiently dense around zero such that the observed value is sufficiently close to some CC spectrum value.

The second part of the CC problem has been only addressed in string theory. This is the multiverse proposal, see [21], and the assumption is that there are many universes, each having a fixed CC value from the CC spectrum. We live in the universe with the CC value $\Lambda_c l_P^2 \approx 10^{-122}$, because this is the value that allows formation of galaxies, planets and life, see [20] for the anthropic determination of the CC value.

Note that there are many proposals for P2 which are not derived from a QG theory, but instead it is assumed that a certain effective action exists such that its equations of motion give the required CC value, see for example [22].

6. Conclusions

The PLQG theory is a theory of quantum gravity which has finitely many degrees of freedom and no infinities. The underlying spacetime structure is a PL manifold $T(M)$ and the smooth spacetime M is recovered as an approximation valid when the number of 4-simplices is large and at a length scale much larger than the typical edge length. The smooth spacetime approximation is analogous to the smooth vector field approximation for the molecular velocities in a fluid.

The PLQG theory is defined by the Regge path integral with a non-trivial measure. The measure is chosen such that it gives a finite path integral, and also it has to admit a semi-classical solution of the effective action equation. These criteria select the exponentially vanishing measures for large edge lengths, and a simple and natural choice for the measure is (10). This measure simplifies the analysis of the effective cosmological constant and one can obtain the formula (24) for the exact effective CC, i.e. to all orders in $\hbar$. The two free parameters in (24) can be consistently chosen such that the observed CC value is obtained. This is an important requirement for any QG theory and PLQG is the only existing QG theory where this property has been demonstrated explicitly.

Another nice property of the PLQG theory is that the effective action Γ can be approximated by a QFT effective action Γ^* when the number of 4-simplices in $T(M)$ is large. Γ^* can be calculated by using the perturbative QFT for GR with matter and with a momentum cutoff K, when $L_\epsilon \geq L_K \gg l_P$. Hence the minimal edge length L_K in the triangulation determines the momentum cutoff K and

$$\Gamma(L_1, \cdots, L_E, \phi_1, \cdots, \phi_V) \approx \Gamma^*(g(x), \phi(x), K)\,, \tag{27}$$

for $E \gg 1$ and $V \gg 1$.

The QFT approximation (27) will be still valid for $L_K \leq l_P$, but in this case Γ^* cannot be calculated by the perturbative QFT methods. Instead, one has to use a non-perturbative method to solve the EA equation. The existence of the QFT approximation (27) implies that one can obtain the running of the elementary particle masses and the coupling constants with K, see for example the equation (20).

Note that the effective action only makes sense for the spacetimes which are given by the direct product of a 3-manifold with an interval. In order to study the quantum cosmology questions, one needs to consider 4-manifolds of general topology, which is different from $\Sigma\times I$ topology. When $M \neq \Sigma\times I$, the concept of the effective action cannot be used. However, the Hartle-Hawking (HH) wavefunction [23] can be defined for any $T(M)$ by using the PLQG path integral (3). By choosing a triangulation for a manifold

$$M \cup (\Sigma \times I)\ , \quad \partial M = \Sigma\,,$$

one can describe a Big-Bang quantum cosmology with an initial HH state, which evolves by the evolution operator defined by the PLQG path integral for the $T(\Sigma \times I)$ part of the spacetime. It is then plausible to assume that the effective dynamics which corresponds to the time evolution of the HH state will be given by the PLQG effective action, defined by the equation (19).

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P r o c e e d i n g s

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September 9 – 14, 2019, Belgrade, Serbia

Editors

B. Dragovich, I. Salom and M. Vojinović

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Belgrade, 2020
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P R E F A C E

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The previous nine meetings in this series of schools and conferences on modern mathematical physics were also held in Serbia: Sokobanja 2001, Kopaonik 2002, Zlatibor 2004, Belgrade 2006, 2008, 2010, 2012, 2014, and 2017. The corresponding proceedings of all these meetings were published by the Institute of Physics Belgrade, and are available in the printed form as well as online at the websites. According to an agreement with the journal Symmetry, several papers are published in the special issue "Selected Papers: 10th Mathematical Physics Meeting".

This jubilary tenth meeting took place at two different venues — the opening and the first day of lectures was held in the grand lecture hall of the Serbian Academy of Sciences and Arts, while the lectures for the remaining five days were held at the Mathematical Institute. Both venues are located in Belgrade downtown, across the road of each other. We hope that all attendees of this meeting will recall it as a useful and pleasant event, and will wish to participate again in the future.

We wish to thank all lecturers and other speakers for their interesting and valuable talks. We also thank all participants for their active participation. Financial support of our sponsors, *Ministry of Education, Science and Technological Development of the Republic of Serbia, Belgrade; Telekom Srbija; Open access journal "Symmetry"*, and the support of our media partner, *Open access journal "Entropy"*, were very significant for realization of this activity.

April 2020

E d i t o r s

B. Dragovich
I. Salom
M. Vojinović


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СУВЕНИРИ - SOUVENIRS

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