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$O(6)$ algebraic approach to three bound identical particles in the hyperspherical adiabatic representation

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ABSTRACT

We construct the three-body permutation symmetric $O(6)$ hyperspherical harmonics and use them to solve the non-relativistic three-body Schrödinger equation in three spatial dimensions. We label the states with eigenvalues of the $U(1) \otimes SO(3)_{rot} \subset U(3) \subset O(6)$ chain of algebras, and we present the $K \leq 4$ harmonics and tables of their matrix elements. That leads to closed algebraic form of low-K energy spectra in the adiabatic approximation for factorizable potentials with square-integrable hyper-angular parts. This includes homogeneous pairwise potentials of degree $\alpha \geq -1$. More generally, a simplification is achieved in numerical calculations of non-adiabatic approximations to non-factorizable potentials by using our harmonics.

1. Introduction

The three-body bound-state problem has been addressed by a huge literature, see e.g. Refs. [1–7], in which the hyperspherical harmonics (H.H.) provide one of the most firmly established theoretical tools. All three-body calculations conducted thus far have been numerical, suggesting that perhaps there are no quantum-mechanical three-body bound state problems that can be solved in closed form.

Very little is known about the general structure of the three-body bound-state spectrum, such as the ordering of states, even in the (simplest) normal case of three identical particles interacting with a two-body interaction strong enough to bind two particles, i.e., in the non-Borromean regime. In comparison, the two-body bound state problem is much better understood, see Refs. [8–11], where theorems controlling the ordering of bound states in convex two-body potentials were proven more than 30 years ago. In this paper we make the first significant advance in the problem of three-body bound state ordering after the 1990 paper by Taxil & Richard, Ref. [12].

The basic difficulty lay in the absence of a systematic construction of permutation-symmetric three-body wave functions. Classification of wave functions into distinct classes under permutation symmetry in the three-body system, should be a matter of course, and yet permutation symmetric three-body hyperspherical harmonics in three dimensions were known explicitly only in a few special cases, such as those with total orbital angular momentum $L = 0$, see Refs. [5,13]. Instead, mathematically unjustified bases for hyperspherical harmonics were routinely used in the literature, thus leading to significant computational difficulties. This is reflected already at the level of quantum numbers used for labelling of the harmonics, that often feature two sets, (l_ρ, m_ρ) and (l_λ, m_λ), of $SO(3)$ quantum numbers, related to separate rotations of the two Jacobi vectors, $\boldsymbol{\lambda}$ and $\boldsymbol{\rho}$, e.g. Refs. [3,4,6].[1]

The main goal of this paper is to point out the recent progress in the construction and application of permutation symmetric three-body hyperspherical harmonics [14,15]. Rather than going into the technical details of the construction of these harmonics, we here restrict ourselves to simply listing their explicit forms for $K \leq 4$ in Ref. [14] and concentrate on their application to the quantum mechanical three-body problem.

The hyperspherical harmonics we use are permutation-symmetric three-body $O(6)$ HH based on the $U(1) \otimes SO(3)_{rot} \subset U(3) \subset O(6)$ chain of algebras, where $U(1)$ is the "democracy transformation", or "kinematic rotation" group for three particles, $SO(3)_{rot}$ is the 3D rotation group, and $U(3), O(6)$ are the usual Lie groups. This particular chain was recently suggested in Ref. [18], but also by the previous discovery of the dynamical $O(2)$ symmetry of the Y-string potential, Ref. [19]: this $O(2) = U(1)$ symmetry has the permutation group $S_3 \subset O(2)$ as its (discrete) subgroup. The close

[1] Permutation symmetric N-body (with $N \geq 4$) hyperspherical harmonics had only been constructed by means of a numerical recursive procedure that symmetrizes non-permutation-symmetric hyperspherical harmonics, see Refs. [16,17], which, to our knowledge, has not been applied to the three-body problem.

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relation of $U(1)$ kinematic rotations to permutations, on one hand, and the fact that this is the only subgroup of the full $O(6)$ hyperspherical symmetry that commutes with rotations, on the other, imply that the corresponding quantum number must appear in any mathematically justified and permutationally symmetric basis of hyperspherical harmonics.

In two-dimensional space, this requirement strongly suggested an $O(4)$ algebraic approach, Ref. [20] to solve the three-body bound state problem. An independent study of "universal states" using $O(4)$ permutation-symmetric three-body harmonics in two dimensions has appeared recently, Ref. [21]. In three dimensions (3D) the (maximal) hyperspherical symmetry is $O(6)$, however, and thus requires a new set of permutation-symmetric three-body hyperspherical harmonics, that were lacking hitherto, and which we present here.

Then, we apply the new harmonics to the three-identical-particles Schrödinger equation, as written in the so-called hyperspherical adiabatic representation, defined in Refs. [21–24] which simplifies the resulting equations significantly, especially in the case of factorizable (in the hyper-radius and hyper-angles) three-body potentials. Factorizable potentials, see Sect. 3.3.2, include homogeneous potentials, which, in turn, include pairwise sums of two-body power-law potentials, such as the Coulomb one, and the confining "Δ-string", as well as the genuinely three-body "Y-string" potential and Refs. [19,20].

In the adiabatic approximation to the Schrödinger equation with this class of potentials, the energy spectra can be evaluated in closed form, for sufficiently small ($K \leq 7$) values of the grand angular momentum K. Inhomogeneous potentials, and non-adiabatic approximations can only be treated numerically, yet significant simplifications appear there, too, in our method, due to the maximal/optimal sparseness of the adiabatic potential matrix in the permutation-symmetric basis.

In this paper, we shall show: 1) the properties of permutation-symmetric three-body $O(6)$ hyperspherical harmonics; 2) how the Schrödinger equation for three identical particles can be reduced to a set of ordinary differential equations with coefficients determined by $O(6)$ symmetric matrix elements; 3) how, in homogeneous three-body potentials, this set of coupled equations for three identical particles reduces to a set of single decoupled differential equation with coupling strengths determined by $O(6)$ algebra; 4) that our method allows closed-form ("analytical") results in this class of potentials, for sufficiently small values (i.e. for $K \leq 7$) of the grand angular momentum K.

Our work is based on the recent advances in the construction of three-body wave functions with well-defined permutation symmetry, see Sects. 2.1, 2.3, and Ref. [14].

2. Three-body problem in hyper-spherical coordinates

The three-body wave function $\Psi(\boldsymbol{\rho}, \boldsymbol{\lambda})$ can be transcribed from the Euclidean relative position (Jacobi) vectors $\boldsymbol{\rho} = \frac{1}{\sqrt{2}}(\mathbf{x_1} - \mathbf{x_2})$, $\boldsymbol{\lambda} = \frac{1}{\sqrt{6}}(\mathbf{x_1} + \mathbf{x_2} - 2\mathbf{x_3})$, into hyper-spherical coordinates as $\Psi(R, \Omega_5)$, where $R = \sqrt{\boldsymbol{\rho}^2 + \boldsymbol{\lambda}^2}$ is the hyper-radius, and five angles Ω_5 that parametrize a hyper-sphere in the six-dimensional Euclidean space. Three (Φ_i; $i = 1, 2, 3$) of these five angles (Ω_5) are just the Euler angles associated with the orientation in a three-dimensional space of a spatial reference frame defined by the (plane of) three bodies; the remaining two hyper-angles describe the shape of the triangle subtended by three bodies; they are functions of three independent scalar three-body variables, e.g. $\boldsymbol{\rho} \cdot \boldsymbol{\lambda}$, $\boldsymbol{\rho}^2$, and $\boldsymbol{\lambda}^2$. As we saw above, one linear combination of the two variables $\boldsymbol{\rho}^2$, and $\boldsymbol{\lambda}^2$, is already taken by the hyper-radius R, so the shape-space is two-dimensional, and topologically equivalent to the surface of a three-dimensional sphere.

There are two traditional ways of parameterizing this sphere: 1) the standard Delves choice, [3], of hyper-angles (χ, θ), that somewhat obscures the full S_3 permutation symmetry of the problem; 2) the Iwai, Ref. [7], hyper-angles (α, ϕ): $(\sin\alpha)^2 = 1 - \left(\frac{2\boldsymbol{\rho}\times\boldsymbol{\lambda}}{R^2}\right)^2$, $\tan\phi = \left(\frac{2\boldsymbol{\rho}\cdot\boldsymbol{\lambda}}{\boldsymbol{\rho}^2 - \boldsymbol{\lambda}^2}\right)$, reveal the full S_3 permutation symmetry of the problem: the angle α does not change under permutations, so that all permutation properties are encoded in the ϕ-dependence of the wave functions. We shall use the latter choice, as it leads to permutation-symmetric hyperspherical harmonics, as explained in Sects. 2.1, 2.3. Specific hyperspherical harmonics with $K \leq 4$ are displayed in Ref. [14].

2.1. $O(6)$ Symmetry of the hyper-spherical approach

The decomposition of the three-body spatial wave functions in terms of the $O(6)$ "grand angular momentum" $K_{\mu\nu}$ eigenfunctions, or hyperspherical harmonics, is based on the fact that the equal-mass three-body kinetic energy T is $O(6)$ invariant and can be written as

$$T = \frac{m}{2}\dot{R}^2 + \frac{K_{\mu\nu}^2}{2mR^2} \tag{1}$$

where the "grand angular" momentum tensor $K_{\mu\nu}$, $(\mu, \nu = 1, 2, \ldots, 6)$

$$\begin{aligned} K_{\mu\nu} &= m\left(\mathbf{x}_\mu \dot{\mathbf{x}}_\nu - \mathbf{x}_\nu \dot{\mathbf{x}}_\mu\right) \\ &= \left(\mathbf{x}_\mu \mathbf{p}_\nu - \mathbf{x}_\nu \mathbf{p}_\mu\right) \end{aligned} \tag{2}$$

and $x_\mu = (\boldsymbol{\lambda}, \boldsymbol{\rho})$. $K_{\mu\nu}$ has 15 linearly independent components, that contain, among themselves three components of the "ordinary" orbital angular momentum: $\mathbf{L} = \mathbf{l}_\rho + \mathbf{l}_\lambda = m\left(\boldsymbol{\rho} \times \dot{\boldsymbol{\rho}} + \boldsymbol{\lambda} \times \dot{\boldsymbol{\lambda}}\right)$.

Apart from the hyperangular momentum K, which labels the $O(6)$ irreducible representation, all hyperspherical harmonics must carry additional labels specifying the transformation properties of the harmonic with respect to (w.r.t.) certain subgroups of the orthogonal group. The symmetries of most three-body potentials, including the three-quark confinement ones, are: parity, rotations and permutations (spatial exchange of particles).

Therefore, the three-body hyperspherical harmonics ought to have definite transformation properties w.r.t. to these three symmetries. Parity is the simplest one to implement, as it is directly related to K: $P = (-1)^K$. The rotation symmetry implies that the hyperspherical harmonics must carry quantum numbers L and m associated with the rotational subgroup $SO(3)_{rot}$.

2.2. Permutation-symmetric three-body hyper-spherical harmonics

We introduce the complex coordinates:

$$X_i^{\pm} = \lambda_i \pm i\rho_i, \quad i = 1, 2, 3. \tag{3}$$

Nine of 15 hermitian $SO(6)$ generators $K_{\mu\nu}$ in these new coordinates become

$$iL_{ij} \equiv X_i^+ \frac{\partial}{\partial X_j^+} + X_i^- \frac{\partial}{\partial X_j^-} - X_j^+ \frac{\partial}{\partial X_i^+} - X_j^- \frac{\partial}{\partial X_i^-}, \tag{4}$$

$$2Q_{ij} \equiv X_i^+ \frac{\partial}{\partial X_j^+} - X_i^- \frac{\partial}{\partial X_j^-} + X_j^+ \frac{\partial}{\partial X_i^+} - X_j^- \frac{\partial}{\partial X_i^-}. \tag{5}$$

Of these, L_{ij} is an antisymmetric tensor, with three components, corresponds to the physical angular momentum vector $\mathbf{L}$, and the symmetric tensor Q_{ij} decomposes as (5) + (1) w.r.t. rotations. The trace:

$$Q \equiv Q_{ii} = \sum_{i=1}^{3} X_i^+ \frac{\partial}{\partial X_i^+} - \sum_{i=1}^{3} X_i^- \frac{\partial}{\partial X_i^-} \tag{6}$$

is the only scalar under rotations, and generates so-called democracy transformations, a special case of which are the cyclic permutations, so its eigenvalue is a natural choice for an additional label of permutation-symmetric hyperspherical harmonics. The remaining five components of the symmetric tensor Q_{ij}, together with three antisymmetric tensors L_{ij} generate the $SU(3)$ Lie algebra, which together with the single scalar Q form an $U(3)$ algebra, Ref. [18].

Therefore, labelling of the $O(6)$ hyper-spherical harmonics with labels K, Q, L and m corresponds to the subgroup chain $U(1) \otimes SO(3)_{rot} \subset U(3) \subset SO(6)$. Yet, these four quantum numbers are in general insufficient to uniquely specify an $SO(6)$ hyper-spherical harmonic: it is well known that $SU(3)$ representations in general have nontrivial multiplicity w.r.t. decomposition into $SO(3)$ subgroup representations, and such a multiplicity also appears here. In this context the operator:

$$\mathcal{V}_{LQL} \equiv \sum_{ij} L_i Q_{ij} L_j \tag{7}$$

(where $L_i = \frac{1}{2}\varepsilon_{ijk} L_{jk}$ and Q_{ij} is given by Eq. (5)) has often been used in the literature, to label the multiplicity of SU(3) states. This operator commutes both with the angular momentum L_i, and with the "democracy rotation" generator Q:

$$\left[\mathcal{V}_{LQL}, L_i\right] = 0; \quad \left[\mathcal{V}_{LQL}, Q\right] = 0$$

Therefore we demand that the hyperspherical harmonics be eigenstates of this operator:

$$\mathcal{V}_{LQL} \mathcal{Y}^{KQ\nu}_{L,m} = \nu \mathcal{Y}^{KQ\nu}_{L,m}.$$

Thus, ν will be the fifth label of the hyper-spherical harmonics, beside the (K, Q, L, m).

2.3. Permutation properties of $O(6)$ hyper-spherical harmonics

We seek hyperspherical harmonics with well-defined values of parity $P = (-1)^K$, rotation-group quantum numbers (L, m), and permutation symmetry, such as the M (mixed), S (symmetric), and A (antisymmetric) ones. In the mixed (M) symmetry representation of the S_3 permutation group being two-dimensional, there are two different H.H. (state vectors) in each mixed permutation symmetry multiplet, usually denoted by M_ρ and M_λ.

Two- and three-particle permutation properties of H.H. $\mathcal{Y}^{KQ\nu}_{J,m}(\boldsymbol{\lambda}, \boldsymbol{\rho})$ can be inferred from the transformation properties of the coordinates $X^{\pm}_i$, as follows. Under the two-body permutations $\{\mathcal{T}_{12}, \mathcal{T}_{23}, \mathcal{T}_{31}\}$ of pairs of particles (1,2), (2,3) and (3,1), the Jacobi vectors $\boldsymbol{\rho}, \boldsymbol{\lambda}$ transform as:

$$\begin{aligned}
\mathcal{T}_{12}: &\quad \boldsymbol{\lambda} \to \boldsymbol{\lambda}, \quad \boldsymbol{\rho} \to -\boldsymbol{\rho}, \\
\mathcal{T}_{23}: &\quad \boldsymbol{\lambda} \to -\frac{1}{2}\boldsymbol{\lambda} + \frac{\sqrt{3}}{2}\boldsymbol{\rho}, \quad \boldsymbol{\rho} \to \frac{1}{2}\boldsymbol{\rho} + \frac{\sqrt{3}}{2}\boldsymbol{\lambda}, \\
\mathcal{T}_{31}: &\quad \boldsymbol{\lambda} \to -\frac{1}{2}\boldsymbol{\lambda} - \frac{\sqrt{3}}{2}\boldsymbol{\rho}, \quad \boldsymbol{\rho} \to \frac{1}{2}\boldsymbol{\rho} - \frac{\sqrt{3}}{2}\boldsymbol{\lambda}.
\end{aligned} \tag{8}$$

This induces the following transformations of complex vectors $X^{\pm}_i$:

$$\begin{aligned}
\mathcal{T}_{12}: &\quad X^{\pm}_i \to X^{\mp}_i, \\
\mathcal{T}_{23}: &\quad X^{\pm}_i \to e^{\pm\frac{2i\pi}{3}} X^{\mp}_i, \\
\mathcal{T}_{31}: &\quad X^{\pm}_i \to e^{\mp\frac{2i\pi}{3}} X^{\mp}_i.
\end{aligned} \tag{9}$$

The quantum numbers K, L and m do not change under permutations of two particles, whereas the values of the "democracy label" Q and multiplicity label ν are inverted under transpositions: $Q \to -Q, \nu \to -\nu$.

In addition to the changes of labels, transpositions of two particles generally also result in the appearance of an additional phase factor multiplying the hyper-spherical harmonic. For multiplicity-free values of K, Q, L and m, the following transformation properties of H.H. hold under (two-particle) particle transpositions:

$$\begin{aligned}
\mathcal{T}_{12}: &\quad \mathcal{Y}^{KQ\nu}_{L,m} \to (-1)^{K-J} \mathcal{Y}^{K,-Q,-\nu}_{L,m}, \\
\mathcal{T}_{23}: &\quad \mathcal{Y}^{KQ\nu}_{L,m} \to (-1)^{K-L} e^{\frac{2Qi\pi}{3}} \mathcal{Y}^{K,-Q,-\nu}_{L,m}, \\
\mathcal{T}_{31}: &\quad \mathcal{Y}^{KQ\nu}_{L,m} \to (-1)^{K-L} e^{-\frac{2Qi\pi}{3}} \mathcal{Y}^{K,-Q,-\nu}_{L,m}.
\end{aligned} \tag{10}$$

In order to determine which representation of the S_3 permutation group any particular H.H. $\mathcal{Y}^{KQ\nu}_{L,m}$ belongs to, one has to consider various cases, with and without multiplicity. The following linear combinations of the H.H.

$$\mathcal{Y}^{K|Q|\nu}_{L,m,\pm} \equiv \frac{1}{\sqrt{2}} \left(\mathcal{Y}^{K|Q|\nu}_{L,m} \pm (-1)^{K-L} \mathcal{Y}^{K,-|Q|,-\nu}_{L,m} \right) \tag{11}$$

are no longer eigenfunctions of Q operator but are eigenfunctions of the transposition $\mathcal{T}_{12}$ instead:

$$\mathcal{T}_{12}: \mathcal{Y}^{K|Q|\nu}_{L,m,\pm} \to \pm \mathcal{Y}^{K|Q|\nu}_{L,m,\pm}.$$

They are the appropriate H.H. with well-defined permutation properties:

1. $Q \not\equiv 0 \pmod 3$: the H.H. $\mathcal{Y}^{K|Q|\nu}_{L,m,\pm}$ belongs to the mixed representation M, where the $\pm$ sign determines which of the two components it is, M_ρ, M_λ.
2. $Q \equiv 0 \pmod 3$: the H.H. $\mathcal{Y}^{K|Q|\nu}_{L,m,+}$ belongs to the symmetric representation S and $\mathcal{Y}^{K|Q|\nu}_{L,m,-}$ belongs to the antisymmetric representation A.

The above rules define the permutation-group representation for any given H.H.

2.3.1. Labels of $K \leq 4$ $O(6)$ hyper-spherical harmonics

As an illustration, in Table 1 we give the values of "$O(6)$ indices" Q, L, m, ν for the lowest $K \leq 4$ permutation-symmetric hyperspherical harmonics. The corresponding h.s. harmonics, as well as their hyper-angular matrix elements can be found in Ref. [14].

The $K \geq 4$ h.s. harmonics and the corresponding $O(6)$ matrix elements can be readily evaluated using our code written in a commercially available symbolic manipulation language, Ref. [14].

Note that only in the $K = 4$ shell there appear (at most) two multiplets with equal permutation properties and equal (L, m) labels that may mix: a) the $\mathcal{Y}^{4,\pm2,\pm2}_{2,m} \simeq |[70, 2^+]\rangle$ and $\mathcal{Y}^{4,\pm4,\pm3}_{2,m} \simeq |[70', 2^+]\rangle$; and b) the $\mathcal{Y}^{4,\mp2,\pm5}_{4,m} \simeq |[70, 4^+]\rangle$ and $\mathcal{Y}^{4,\mp4,\pm10}_{4,m} \simeq |[70', 4^+]\rangle$. Note, moreover, that both of these have orbital angular momenta $L \geq 2$, as this is required for multiplicity to occur.

3. The three-body Schrödinger equation

First, we briefly explain the adiabatic hyperspherical representation of the three-body Schrödinger equation. Then, we apply the permutation-symmetric h.s. harmonics to this problem, and solve the adiabatic approximation to Schrödinger equation with homogeneous potentials.

3.1. Adiabatic hyperspherical representation

Here we follow the standard derivation of the adiabatic hyperspherical representation, Refs. [23,24]. The three-body Schrödinger equation in 3D for the scaled wave function $\psi = R^{5/2}\Psi$,

Table 1
The labels of distinct $K \leq 4$ h.s. harmonics $\mathcal{Y}^{K,Q,\nu}_{L,m}$ (three-body states, with allowed orbital angular momentum value L; only $L = m$ labels are shown). The correspondence between the S_3 permutation group irreps. and $SU(6)_{FS}$ symmetry multiplets of the three-quark system: $S \leftrightarrow 56$, $A \leftrightarrow 20$ and $M \leftrightarrow 70$.

K	(K, Q, L, m, ν)	$[SU(6), L^P]$	S_3 irrep.
0	$(0, 0, 0, 0, 0)$	$[56, 0^+]$	S
1	$(1, \pm 1, 1, 1, \mp 1)$	$[70, 1^-]$	M
2	$(2, \pm 2, 0, 0, 0)$	$[70, 0^+]$	M
2	$(2, 0, 2, 2, 0)$	$[56, 2^+]$	S
2	$(2, \mp 2, 2, 2, \pm 3)$	$[70, 2^+]$	M
2	$(2, 0, 1, 1, 0)$	$[20, 1^+]$	A
3	$(3, \mp 3, 1, 1, \pm 1)$	$[20, 1^-]$	A
3	$(3, \mp 3, 1, 1, \pm 1)$	$[56, 1^-]$	S
3	$(3, \pm 1, 1, 1, \pm 3)$	$[70, 1^-]$	M
3	$(3, \mp 1, 2, 2, \pm 5)$	$[70, 2^-]$	M
3	$(3, \mp 1, 3, 3, \pm 2)$	$[70, 3^-]$	M
3	$(3, \pm 3, 3, 3, \mp 6)$	$[56, 3^-]$	S
3	$(3, \pm 3, 3, 3, \mp 6)$	$[20, 3^-]$	A
4	$(4, \pm 4, 0, 0, 0)$	$[70, 0^+]$	M
4	$(4, 0, 0, 0, 0)$	$[56, 0^+]$	S
4	$(4, \pm 2, 1, 1, \pm 2)$	$[70, 1^+]$	M
4	$(4, 0, 2, 2, \mp\sqrt{105})$	$[56, 2^+]$	S
4	$(4, 0, 2, 2, \mp\sqrt{105})$	$[20, 2^+]$	A
4	$(4, \pm 2, 2, 2, \pm 2)$	$[70, 2^+]$	M
4	$(4, \pm 4, 2, 2, \mp 3)$	$[70', 2^+]$	M
4	$(4, \mp 2, 3, 3, \pm 13)$	$[70, 3^+]$	M
4	$(4, 0, 3, 3, 0)$	$[20, 3^+]$	A
4	$(4, 0, 4, 4, 0)$	$[56, 4^+]$	S
4	$(4, \mp 2, 4, 4, \pm 5)$	$[70, 4^+]$	M
4	$(4, \mp 4, 4, 4, \pm 10)$	$[70', 4^+]$	M

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial R^2} + H_{\rm ad}(R;\Omega_5)\right]\psi_E(R;\Omega_5) = E\psi_E(R;\Omega_5), \tag{12}$$

can be (re)formulated as an algebraic (matrix) eigenvalue problem for the "adiabatic Hamiltonian" $H_{\rm ad}(R;\Omega_5)$

$$H_{\rm ad}(R;\Omega_5) = \frac{K^2_{\mu\nu}(\Omega_5) - 1/4}{2mR^2} + V(R,\alpha,\phi), \tag{13}$$

where $K^2_{\mu\nu}(\Omega_5)$ is the grand angular momentum squared, i.e., the hyper-angular part of the kinetic energy, $V(R,\alpha,\phi)$ is the interparticle interaction potential, E is the total energy and $\Omega_5 \equiv (\gamma,\alpha,\phi)$ denotes the set of three Euler (γ) and two hyper-angles (α,ϕ). The shift of $K^2_{\mu\nu}(\Omega_5)$ by 1/4 in Eq. (13), as compared with Eq. (1), is due to the rescaling $\Psi \to \psi/R^{5/2}$ of the wave function that was implemented in order to eliminate the first derivative in R term from Eq. (12).

In the adiabatic hyperspherical representation, the scaled three-body wave function $\psi_E(R;\Omega_5)$ is expanded in terms of the "channel functions" $\Phi_\mu(R;\Omega_5)$,

$$\psi_E(R;\Omega_5) = \sum_\mu F_{\mu E}(R)\Phi_\mu(R;\Omega_5), \tag{14}$$

Here $F_{\mu E}(R)$ are the hyper-radial wave functions and the channel functions $\Phi_\mu(R;\Omega_5)$ form a complete set of orthonormal functions at each value of R being the eigenfunctions of $H_{\rm ad}$,

$$H_{\rm ad}(R;\Omega_5)\Phi_\mu(R;\Omega_5) = U_\mu(R)\Phi_\mu(R;\Omega_5) \tag{15}$$

The "channel index" μ,[2] represents all quantum numbers necessary to specify each channel and "may serve to identify new sets of approximate quantum numbers", Ref. [23]. The eigenvalue problem Eq. (15) is (still) an infinite-dimensional one (in spite of absence of hyper-radial derivatives): $H_{\rm ad}(R;\Omega_5)$ is a linear Hermitian differential operator in the hyper-angles Ω_5. In general Eq. (15) cannot be solved exactly, so that approximate and/or numerical solutions must be sought.

The eigenvalues $U_\mu(R)$ correspond to the three-body potentials in the channel specified by the set of quantum numbers μ. From the eigenvalues $U_\mu(R)$ one can define the effective three-body potentials for the hyper-radial motion in those channels.

The basic idea of the adiabatic representation/expansion, is that the "channel functions" $\Phi_\mu(R;\Omega_5)$ vary smoothly with R except in localized regions of avoided crossings. The simplest approximation is to ignore the coupling of different channels – this is called the adiabatic approximation.[3] The energies obtained by solving two slightly different adiabatic approximations form an upper- and a lower bound on the true eigenenergy, Refs. [22,24].

3.2. $O(6)$ *reduction*

The presence of the hyper-angular momentum squared, $K^2_{\mu\nu}(\Omega_5)$ in $H_{\rm ad}(R;\Omega_5)$, immediately suggests the $O(6)$ hyperspherical harmonics as the basis vectors in three-body systems. Thus we employ hyperspherical harmonics to solving the channel eigenvalue equation (15), and hence decompose the channel functions $\Phi_\nu(R;\Omega_5)$ as

$$\Phi_\mu(R;\Omega_5) = \sum_{K,[m]} f^K_{[m]}(R)\mathcal{Y}^K_{[m]}(\Omega_5),$$

where [m] denotes all the labels of hyperspherical harmonics apart from K. After projecting out the $\mathcal{Y}^{K'}_{[m']}$ component, Eq. (15) becomes

$$\left[\frac{K(K+4) - 1/4}{2mR^2} - U^K_\mu(R)\right] f^K_{[m]}(R) + \\ + \sum_{K',[m']} V^{K\,K'}_{[m][m']}(R) f^{K'}_{[m']}(R) = 0, \tag{16}$$

where

$$V^{K\,K'}_{[m][m']}(R) = \left\langle\!\!\left\langle \mathcal{Y}^K_{[m]} \middle| V(R,\alpha,\phi) \middle| \mathcal{Y}^{K'}_{[m']} \right\rangle\!\!\right\rangle. \tag{17}$$

The double-bracket matrix element signifies that integrations are carried out only over the angular coordinates Ω_5. Eq. (16) is the (final) result of the $O(6)$ reduction of the eigenvalue equation (15) – it turns into an eigenvalue problem for an infinite-dimensional, hyper-radius dependent matrix. For arbitrary potentials it can only be solved numerically, but there are special cases, such as factorizable potentials and/or dominantly hyper-radially dependent potentials, that can be treated (semi)analytically, see below.

It is immediately clear, however, that the application of the permutation-symmetric hyperspherical harmonics simplifies this

[2] Not to be confused with the reduced mass μ, nor with the index of the grand angular momentum tensor $K_{\mu\nu}$, Eq. (2).

[3] The name is apparently due to the formal similarity to the adiabatic approximation, where solving the time-dependent Schrödinger equation is separated into two steps: first solve the ("quasi-static") eigenvalue problem (without the partial derivative in time) at each moment in time; and then insert these eigenvalue solutions into the full Schrödinger equation including the partial derivative in time and solve it, Ref. [35]. The validity of the conventional (time-dependent) "adiabatic approximation" depends on just how slowly the potential changes with time: the slower, the better. Here, we have made a similar separation, albeit with an eigenvalue problem Eq. (15), which contains no partial derivatives in the hyper-radius R. Its solutions are then "fed" into the full Schrödinger equation (12) that contains the partial derivative(s) in hyper-radius R. The name (hyper-radial) "adiabatic approximation" is a misnomer here, because the eigenvalue problem Eq. (15) always contains the $\frac{K^2_{\mu\nu}(\Omega_5)-1/4}{2mR^2}$ term, with its strong R dependence, no matter how the potential $V(R,\alpha,\phi)$ depends on R. Indeed, the only non-trivial case when this approximation is exact is with the $-1/R^2$ potential, which changes rather rapidly in R!

matrix eigenproblem substantially, as the matrix then turns into a block-diagonal form, with block sub-matrices corresponding to labels from the set [m] that are preserved by the symmetries of the potential, *viz.* rotational numbers L and m, parity P, and permutation symmetry labels A, S, M. Consequently, the channel functions $\Phi_\mu(R;\Omega_5)$ must be labelled by these four good quantum numbers, i.e., the channel index $\mu = (L^P, m, Q)$ must consist of at least these four good quantum numbers.[4]

Apart from the case of hyper-radial potentials, matrix elements Eq. (17) may be nonzero when $K \neq K'$ (i.e. the level crossing $\Delta K \neq 0$ transitions may exist), meaning that K is not a good quantum number for labelling of the channels in general. Nevertheless, the breaking of $O(6)$ symmetry by permutation-symmetric homogeneous potentials is sufficiently small, see Table 2, so as to allow a systematic approximation scheme based on $O(6)$ symmetry.[5] Thus, in the following, K may be treated as an approximate quantum number.

3.3. Potential matrix elements

3.3.1. Hyperspherical expansion of three-body potentials

As the spatial part of any spin-independent three-body interaction potential must be invariant under overall ("ordinary $O(3)$") rotations, it is a scalar, or equivalently, it contains only the zero-angular momentum $L = m = 0$ hyperspherical components. Of course, this holds for both the permutation-symmetric and unsymmetrized hyperspherical harmonics.

So far, we have eschewed specifying the h.s. harmonics used in Sect. 3.2. Next we show the substantial advantages/simplifications in the form of the hyperspherical expansion of the three-body potential, and in the evaluation of hyper-angular matrix elements, gained by using the permutation-symmetric set.

This means choosing the set $[m] = [L^P, L_z = m, Q, \nu]$ that consists of parity P, the (total orbital) angular momentum L, its projection on the z-axis $L_z = m$, the Abelian hyper-angular momentum quantum number Q conjugated with the Iwai angle ϕ, and the multiplicity label ν that distinguishes between hyperspherical harmonics with remaining four quantum numbers that are identical.

The three-body potential $V(R,\alpha,\phi)$ can be expanded in terms of $O(6)$ hyper-spherical harmonics with zero angular momenta $L = m = 0$ (due to the rotational invariance of the potential),

$$V(R,\alpha,\phi) = \sum_{K,Q}^{\infty} v_{K,Q}^{\text{3-body}}(R)\mathcal{Y}_{00}^{KQ\,\nu}(\alpha,\phi) \tag{18}$$

In the present case of three identical particles (and therefore also of permutation symmetric potential) the sum runs only over double-even-order ($K = 0, 4, \ldots$) $O(6)$ hyper-spherical harmonics with zero value of the democracy quantum number $G_3 = Q = 0$, as well as over $K = 6, 12, 18\ldots$ $O(6)$ hyper-spherical harmonics with democracy quantum number $G_3 \equiv Q \equiv 0 \pmod 6$, always with vanishing angular momentum $L = m = 0$. There is no summation over the multiplicity index in Eq. (18), because no multiplicity arises for harmonics with $L < 2$.

Here $v_{KQ}^{\text{3-body}}$ are defined as

$$v_{K,Q}^{\text{3-body}}(R) = \int \mathcal{Y}_{0,0}^{K,Q,\nu *}(\Omega_5)\, V_{\text{3-body}}(R,\alpha,\phi)\, d\Omega_5. \tag{19}$$

Table 2
Non-vanishing expansion coefficients v_{KQ} of the Y- and Δ-string and the QCD Coulomb potentials in terms of $O(6)$ hyper-spherical harmonics $\mathcal{Y}_{0,0}^{K,0,0}$, for $K = 0$, 4, 8, respectively, and of the hyper-spherical harmonics $\mathcal{Y}_{0,0}^{6,\pm 6,0}$, for $K \leq 11$. The last row gives the percentage of the "Parseval unity" for the potential that is accounted for by its expansion into these five harmonics, calculated as $\sum (v_{K,Q}^{\text{3-body}})^2 / (\int (V_{\text{3-body}})^2\, d\Omega_5)$.

(K, Q)	v_{KQ}^{Y}	v_{KQ}^{Δ}	v_{KQ}^{Coulomb}
(0,0)	8.18	16.04	20.04
(4,0)	−0.44	−0.44	2.95
(6,±6)	0	−0.14	1.88
(8,0)	−0.09	−0.06	1.49
$\frac{\sum (v_{K,Q}^{\text{3-body}})^2}{\int (V_{\text{3-body}})^2\, d\Omega_5}$	99%	99%	94%

In the special case of a factorizable three-body potential, see below, the $v_{KQ}^{\text{3-body}}$ coefficients do not depend on the hyper-radius R; these coefficients are determined by the hyper-angular part $V(\alpha,\phi)$ of the potential.

The numerical values for the first four allowed (non-vanishing) $v_{K,Q}^{\text{3-body}}$ coefficients for $K \leq 11$, in the Y- and Δ-string and Coulomb potential's hyperspherical expansions are tabulated in Table 2, together with a check to which extent Parseval's identity Eq. (20) is fulfilled by the truncation of the sum. All other coefficients must vanish for $K < 12$. Vanishing of the coefficient $v_{6,\pm 6}^{Y} = 0$ indicates (an additional) dynamical symmetry of the Y-string potential.

Note that Parseval's theorem

$$\sum_{K,Q}^{\infty} |v_{K,Q}^{\text{3-body}}|^2 = \int |V_{\text{3-body}}|^2\, d\Omega_5\,, \tag{20}$$

requires square integrability of the potential at each value of the hyper-radius R, i.e., finiteness of the right-hand side of Eq. (20), regardless of the kind of h.s. harmonics that were used. The requirement of square integrability also holds for any expansion of the potential in terms of a complete set of basis functions, whether $O(6)$ harmonics, or not.

This condition (of square integrability) eliminates all sums of two-body power-law potentials $\sum_{i>j=1}^{3} |\mathbf{x}_i - \mathbf{x}_j|^\alpha$, with powers $\alpha < -1$, as well as other singular potentials, such as the Dirac δ-function one. Thus, it poses a strong restriction on the class of three-body potentials that can be treated in this manner, that has not been considered so far: in particular, potentials such as the Lennard-Jones, v.d. Waals and Morse ones will have to be examined individually.

3.3.2. Factorizable potentials

Factorizable potentials satisfy

$$V(R,\alpha,\phi) = V(R)V(\alpha,\phi),$$

and form a non-negligible class that contains homogeneous potentials,[6] such as: 1) the Δ-string, $V_\Delta = \sigma_\Delta \sum_{i>j=1}^{3} |\mathbf{x}_i - \mathbf{x}_j|$; 2) the Y-string, $V_Y = \sigma_Y \min_{\mathbf{x}_0} \sum_{i=1}^{3} |\mathbf{x}_i - \mathbf{x}_0|$; and 3) the QCD Coulomb $V_{\text{Coulomb}} = -\alpha_C \sum_{i>j=1}^{3} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}$.

Then Eq. (17) factors into a common hyper-radial part $V(R)$ and the hyper-angular matrix $C_{[m][m']}^{K\ K'}$:

$$V_{[m][m']}^{K\ K'}(R) = V(R)\langle \mathcal{Y}_{[m]}^{K}(\Omega_5)|V(\alpha,\phi)|\mathcal{Y}_{[m']}^{K'}(\Omega_5)\rangle \equiv V(R)\, C_{[m][m']}^{K\ K'}. \tag{21}$$

[4] There may be additional, approximate quantum numbers, however, depending on the specific dynamics.

[5] In exceptional cases, such as the Coulombic, or the harmonic oscillator ones, where the dynamical symmetry of the problem is larger than $O(6)$, K is not the principal quantum number; rather it is some other integer N, and K appears as the label of degenerate states within an N-multiplet, i.e., $\nu = [N, K, [m]]$.

[6] Of course, this class does not include many of the realistic potentials in molecular and nuclear physics, such as the Lennard-Jones, Morse, v.d. Waals and Yukawa potentials.

For homogeneous potentials $\sim R^\alpha$, with exponent $\alpha = -2$, the eigenvalue equation (16) becomes effectively independent of the hyper-radius R, which leads to conformal symmetry, Refs. [25,26], together with a substantial simplification of the problem.

3.3.3. Selection rules

Plugging the potential decomposition (18) into Eq. (17), or Eq. (21) requires the knowledge of $O(6)$ hyper-angular matrix elements of the form

$$C^{\mathrm{K}'' \ \mathrm{K}'}_{[\mathrm{m}''][\mathrm{m}']} = \sum_{\mathrm{K},Q}^{\infty} v^{3\text{-body}}_{\mathrm{K},Q} \langle \mathcal{Y}^{\mathrm{K}''}_{[\mathrm{m}'']}(\Omega_5) | \mathcal{Y}^{\mathrm{KQ}\,\nu}_{00}(\alpha,\phi) | \mathcal{Y}^{\mathrm{K}'}_{[\mathrm{m}']}(\Omega_5) \rangle$$

The $O(6)$ hyper-angular matrix elements

$$\langle \mathcal{Y}^{\mathrm{K}''}_{[\mathrm{m}'']}(\Omega_5) | \mathcal{Y}^{\mathrm{KQ}\,\nu}_{00}(\alpha,\phi) | \mathcal{Y}^{\mathrm{K}'}_{[\mathrm{m}']}(\Omega_5) \rangle$$

can be evaluated using the permutation-symmetric hyperspherical harmonics obtained in Sect. 2.2, see also Ref. [14].

Generally, the $O(6)$ matrix elements obey the following selection rules that reduce the number of non-zero values: they are subject to the "triangular" conditions $\mathrm{K}' + \mathrm{K}'' \geq \mathrm{K} \geq |\mathrm{K}' - \mathrm{K}''|$ plus the condition that $\mathrm{K}' + \mathrm{K}'' + \mathrm{K} = 0, 2, 4, \ldots$, and the angular momenta satisfy the selection rules: $L' = L''$, $m' = m''$. Moreover, Q is an Abelian (i.e. additive) quantum number that satisfies the simple selection rule: $Q'' = Q' + Q$. All of this reduces the sum in $C^{\mathrm{K}'' \ \mathrm{K}'}_{[\mathrm{m}''][\mathrm{m}']}$ to a finite one, that depends on a finite number of coefficients $v^{3\text{-body}}_{\mathrm{K},Q}$; for small values of K, this number is also small, see Sect. 4.1.

The hyper-angular matrix element

$$\langle \mathcal{Y}^{\mathrm{K}''}_{[\mathrm{m}'']}(\Omega_5) | \mathcal{Y}^{\mathrm{KQ}\,\nu}_{00}(\alpha,\phi) | \mathcal{Y}^{\mathrm{K}'}_{[\mathrm{m}']}(\Omega_5) \rangle$$

is (merely) a product of two $O(6)$ group Clebsch–Gordan coefficients that can be calculated using Ref. [14], and the physics is contained in the three-body potential expansion coefficients $v^{3\text{-body}}_{\mathrm{K},Q}$.

3.3.4. Advantages of the permutation-symmetric basis

Of course, Eq. (16) must also hold with any other complete set of three-body hyperspherical harmonics, including the permutation non-symmetric ones, such as those based on the Delves choice of hyper-angles, see Ref. [34]. Note, however, that the Delves-type h.s. harmonics do not have a well-defined set of labels ("quantum numbers"): besides the three standard/obvious quantum numbers K, L, m there is an ambiguity as to what one ought to use for the rest, see Sects. 2.3.2 and 2.3.3 in Ref. [34] and Sect. 5. in Ref. [18].

The permutation-symmetric basis is the optimal one in so far as it maximally observes the symmetries of the permutation-symmetric three-body problem and leads to a minimal number of h.s. components in the decomposition of the potential and of non-vanishing off-diagonal matrix elements. Using the Table 2 as an example, we note the following: there are overall $(\mathrm{K}+3)!(\mathrm{K}+2)/(12\mathrm{K}!) = 2366$ hyperspherical harmonics in the $\mathrm{K} \leq 11$ shells, and this number is independent of the choice of h.s. basis. However, it is a unique feature of the permutation-symmetric basis that the decomposition of *any* permutation symmetric potential has no more than four distinct nonvanishing coefficients out of 2366 possible ones! This "sparseness" is even more marked when one considers (of the order of) 10^6 off-diagonal $\mathrm{K} \leq 11$ matrix elements, all of which depend only on these four coefficients, see Sect. 4.1.

The sparseness of this matrix suggests that our three-body problem might be diagonalizable, at least in some circumstances – see Sect. 4. The manifest permutation symmetry of our hyperspherical harmonics, together with the complete set of commuting operators, simplifies all subsequent calculations. This simplification becomes increasingly pronounced as the value of K increases, see Ref. [15] where we applied these HH to the problem of three-quark bound states. In that display of utility of our approach, we explicitly calculated the orderings of $\mathrm{K} \leq 4$ states and showed that, thanks to the symmetry properties of our harmonics, these levels' energies can be accurately parameterized by only four potential-dependent constants. Furthermore, as a consequence of the mentioned matrix sparseness, the expressions for the energies in Ref. [15] are given in an analytic form.

Table 3
The values of non-vanishing off-diagonal matrix elements of the hyper-angular part of the three-body potential $\pi\sqrt{\pi}\langle [SU(6)_f, L^P_f] || 2\Re e \mathcal{Y}^{6,\pm 6,0}_{0,0} || [SU(6)_i, L^P_i] \rangle_{\mathrm{ang}}$, for various $\mathrm{K} = 4$ states (for all allowed orbital waves L).

K	$[SU(6)_f, L^P_f]$	$[SU(6)_i, L^P_i]$	$\pi\sqrt{\pi}\langle 2\Re e \mathcal{Y}^{6,\pm 6,0}_{0,0} \rangle_{\mathrm{ang}}$
4	$[70, 2^+]$	$[70', 2^+]$	$\frac{6}{7}\sqrt{\frac{6}{5}}$
4	$[70, 4^+]$	$[70', 4^+]$	$\frac{8}{21}$

Table 4
The values of the off-diagonal matrix elements of the hyper-angular part of the three-body potential $\pi\sqrt{\pi}\langle [SU(6)_f, L^P_f] || \mathcal{Y}^{4,0,0}_{00} || [SU(6)_i, L^P_i] \rangle_{\mathrm{ang}}$, for various $\mathrm{K} = 0$, 2, 4 states (for all allowed orbital waves L).

$(\mathrm{K}_f, [SU(6)_f, L^P_f])$	$(\mathrm{K}_i, [SU(6)_i, L^P_i])$	$\pi\sqrt{\pi}\langle \mathcal{Y}^{4,0,0}_{00} \rangle_{\mathrm{ang}}$
$(0, [56, 0^+])$	$(4, [56, 0^+])$	1
$(2, [70, 2^+])$	$(4, [70, 2^+])$	$\frac{4}{5}\sqrt{\frac{6}{7}}$
$(2, [56, 0^+])$	$(4, [56, 0^+])$	$\frac{4}{5}\sqrt{\frac{2}{7}}$

Table 5
The values of non-vanishing off-diagonal matrix elements of the hyper-angular part of the three-body potential $\pi\sqrt{\pi}\langle [SU(6)_f, L^P_f] || 2\Re e \mathcal{Y}^{6,\pm 6,0}_{0,0} || [SU(6)_i, L^P_i] \rangle_{\mathrm{ang}}$, for various $\mathrm{K} = 4$ states (for all allowed orbital waves L).

$(\mathrm{K}_f, [SU(6)_f, L^P_f])$	$(\mathrm{K}_i, [SU(6)_i, L^P_i])$	$\pi\sqrt{\pi}\langle 2\Re e \mathcal{Y}^{6,\pm 6,0}_{0,0} \rangle_{\mathrm{ang}}$
$(2, [70, 2^+])$	$(4, [70', 2^+])$	$2\sqrt{\frac{3}{35}}$

4. Results

In general, the eigenvalue problem Eq. (16) has to be solved numerically, but its solution is significantly simplified by the use of permutation-symmetric h.s. harmonics basis, as the hyper-angular matrix elements are subject to the selection rules shown in Sect. 3.3.3.

The couplings of lower-K′ states to the higher-K″ ones are proportional to the higher-K valued coefficients $v^{3\text{-body}}_{\mathrm{K},Q}$, due to the $\mathrm{K}' + \mathrm{K}'' \geq \mathrm{K} \geq |\mathrm{K}' - \mathrm{K}''|$ selection rule, which coefficients, in turn, are smaller than the lower-K ones, see Table 2. This reduction becomes increasingly pronounced as the values of $\mathrm{K}', \mathrm{K}''$ increase, see Ref. [15]. That fact leads, in the case of homogeneous potentials, to a clear ordering of off-diagonal matrix elements and allows controllable approximations to the solution, that may even be convergent in some special cases, e.g. with conformal invariance.

4.1. Off-diagonal matrix elements

The non-vanishing single-shell ($\Delta\mathrm{K} = 0$) off-diagonal matrix elements, for $\mathrm{K} = 0, 1, 2, 3, 4$ states, are shown in Table 3.

The non-vanishing two-shell off-diagonal (nonadiabatic) matrix elements, for various $\mathrm{K} = 0, 2, 4$ states, are shown in Tables 4, 5, and for $\mathrm{K} = 1, 3$ states, in Table 6.

4.2. Diagonalization

The sparseness of the hyper-angular coupling coefficients matrix $C^{\mathrm{K}\ \mathrm{K}'}_{[\mathrm{m}][\mathrm{m}']}$ in the permutation-symmetric basis displayed in Sect. 4.1 suggests that we attempt an analytic diagonalization.

Table 6
The values of the off-diagonal matrix elements of the hyper-angular part of the three-body potential $\pi\sqrt{\pi}\langle[SU(6)_f, L_f^P]|\,\mathcal{Y}_{00}^{4,0,0}\,|[SU(6)_i, L_i^P]\rangle_{\rm ang}$, for various K = 1, 3, 5 states (for all allowed orbital waves L).

$(\mathrm{K}_f, [SU(6)_f, L_f^P])$	$(\mathrm{K}_i, [SU(6)_i, L_i^P])$	$\pi\sqrt{\pi}\langle\mathcal{Y}_{00}^{4,0,0}\rangle_{\rm ang}$
$(1, [70, 1^-])$	$(5, [70', 1^-])$	$\sqrt{\frac{2}{3}}$
$(1, [70, 1^-])$	$(3, [70, 1^-])$	$\frac{1}{\sqrt{3}}$

4.2.1. Adiabatic mixing ($\Delta\mathrm{K} = 0$)

Inspection of the Table 2 reveals that all of the potentials considered there have coefficients $v_{00}^{\text{3-body}}$ that are one order of magnitude larger than the rest $v_{\mathrm{K}>0,\mathrm{Q}}^{\text{3-body}}$. This fact justifies taking only the term proportional to $v_{00}^{\text{3-body}}$ in the expansion Eqs. (16), (18) as the zeroth order approximation. To this zeroth order, all the solutions with the same principal number K are degenerate, with $U_\mu(R) = U_{\mathrm{K}}(R) = \frac{\mathrm{K}(\mathrm{K}+4)-1/4}{2mR^2} + v_{00}^{\text{3-body}}(R)$. The first order corrections lift this degeneracy, i.e., that would amount to including all off-diagonal elements within the same K-shell (i.e. those with $\mathrm{K} = \mathrm{K}'$) into Eq. (17).

In a such case, the eigenvalue problem Eq. (16) splits into separate equations for each value of K. For a given K the term in the first line in Eq. (16) is proportional to a unit matrix, so it may be removed from the diagonalization. Therefore, the potential matrix $V_{[\mathrm{m}][\mathrm{m}']}^{\mathrm{K}\ \mathrm{K}'}(R)$ is the only one that needs to be diagonalized; it can be brought into the diagonal form

$$V_{[\mathrm{m}][\mathrm{m}']}^{\mathrm{K}\ \mathrm{K}'}(R) = \delta_{\mathrm{K},\mathrm{K}'}\delta_{[\mathrm{m}],[\mathrm{m}']}V_{[\mathrm{m}]}^{\mathrm{K}}(R),$$

due to its Hermiticity, yielding the eigenvalues of the equation Eq. (16) in the form

$$U_{[\mathrm{m}]}^{\mathrm{K}}(R) = \frac{\mathrm{K}(\mathrm{K}+4)-1/4}{2mR^2} + V_{[\mathrm{m}]}^{\mathrm{K}}(R). \tag{22}$$

The matters simplify further in the case of factorizable potentials, i.e., when $V_{[\mathrm{m}]}^{\mathrm{K}}(R) = V(R)C_{[\mathrm{m}]}^{\mathrm{K}}$. In such a case, the coefficients $f_{[\mathrm{m}]}^{\mathrm{K}}(R)$ form (mutually orthogonal) eigenvectors that effectively do not depend on the hyper-radius R, as we can choose the normalization so that $f_{[\mathrm{m}]}^{\mathrm{K}}(R) = f_{[\mathrm{m}]}^{\mathrm{K}}(0)$. This is so because the matrix $C_{[\mathrm{m}][\mathrm{m}']}^{\mathrm{K}\ \mathrm{K}'}$ that is being diagonalized does not depend on R.

This implies that the non-adiabatic coupling terms, Eq. (3.10) in Ref. [23], or Eqs. (16), (17) in Ref. [21], vanish: $P_{[\mathrm{m}],[\mathrm{m}']}^{\mathrm{K},\mathrm{K}'}(R) = 0$ and $Q_{[\mathrm{m}],[\mathrm{m}']}^{\mathrm{K},\mathrm{K}'}(R) = 0$. In this sense, the single K-shell mixing approximation corresponds to the adiabatic one for factorizable potentials. That, in turn, leads to the explicit solution $V_{\text{eff }[\mathrm{m}]}^{\mathrm{K}}(R) = U_{[\mathrm{m}]}^{\mathrm{K}}(R)$, to the hyper-radial effective potential.

4.2.2. Non-adiabatic mixing ($\Delta\mathrm{K} \neq 0$)

Introducing higher-order corrections to Eq. (17) corresponds to taking into account the inter-shell ($\mathrm{K} \neq \mathrm{K}'$) mixings. It is then no longer possible (in general) to choose $f_{[\mathrm{m}]}^{\mathrm{K}}(R)$ as being independent of hyper-radius R. Note that in the $\mathrm{K}, \mathrm{K}' \leq 4$ shells there is at most two-state mixing, see Tables 4, 5, 6. In such simple cases one can solve for the mixing angle $\Theta(R)$ in closed form.

For (smooth, monotonic) homogeneous potentials $V(R) \sim R^\alpha$, the two-state mixing angle $\Theta(R)$ changes monotonically from $\Theta(0) = 0$ to its asymptotic value $\Theta_{\text{as.}}$, as $R \to \infty$.[7] The "hyper-radial functions" $f_{[\mathrm{m}]}^{\mathrm{K}}(R) \sim \cos\Theta(R)$ lead to non-vanishing non-adiabatic coupling coefficients, Eq. (3.10) in Ref. [23], or Eqs. (16), (17) in Ref. [21], $P_{[\mathrm{m}],[\mathrm{m}']}^{\mathrm{K},\mathrm{K}'}(R) \neq 0$ and $Q_{[\mathrm{m}],[\mathrm{m}']}^{\mathrm{K},\mathrm{K}'}(R) \neq 0$ because $\frac{d\Phi_{[\mathrm{m}]}^{\mathrm{K}}}{dR} \sim \left(\frac{df_{[\mathrm{m}]}^{\mathrm{K}}(R)}{dR}\right) \neq 0$. This leads to a non-vanishing non-adiabatic correction $Q_{[\mathrm{m}],[\mathrm{m}]}^{\mathrm{K},\mathrm{K}}(R) \neq 0$ to the hyper-radial effective potential.

In general, the problem has to be solved numerically, but solving Eq. (16) is significantly simplified in the permutation-symmetric h.s. harmonics basis, as the hyper-angular matrix elements are subject to the (now familiar) selection rules in Sect. 3.3.3. Couplings to higher-K, K′ shells are proportional to higher values of expansion coefficients $v_{\mathrm{K},\mathrm{Q}}^{\text{3-body}}$, which, in turn, are smaller than the lower ones; this allows a controlled/convergent approximation.

4.3. Homogeneous permutation-symmetric potentials in adiabatic approximation

The adiabatic approximation is obtained by setting the non-adiabatic coefficients equal to zero: $P_{[\mathrm{m}],[\mathrm{m}']}^{\mathrm{K},\mathrm{K}'}(R) = 0$. One can argue that the adiabatic approximation is a reasonable one for confining ($\alpha > 0$) three-body potentials, at least for low values of $\mathrm{K} \leq 4$. In such cases hyper-radial equations decouple, leading to solutions that depend on the (diagonalized values of) quantum numbers $[m]$ and thus lead to (slightly) different eigen-energies within the same K shell.

The ordering of states in each shell depends only on four coefficients $(v_{00}, v_{40}, v_{6\pm6}, v_{80})$, for $\mathrm{K} \leq 5$, and the largest number of states that mix is three, so the eigenvalue equations are at most cubic algebraic ones, with well-known closed form solutions.

Homogeneous confining three-body potentials, such as the Δ-string and the Y-string, have coefficients $v_{00}^{\text{3-body}}$ that are one order of magnitude larger than the rest $v_{\mathrm{K}>0,\mathrm{Q}}^{\text{3-body}}$, see Table I in Ref. [15]. Consequently, the K expansion ought to converge quickly. In Ref. [15] we used the above-described methods to calculate the eigen-energies of various $SU(6)/S_3$ multiplets in the $\mathrm{K} \leq 4$ shells of the Y-, Δ-string potential spectra, with the following results.

The $\mathrm{K} = 2$ shell depends only on two coefficients (v_{00}, v_{40}), so the level splittings depend only on one free parameter (the ratio v_{40}/v_{00}) and the $O(6)$ matrix elements/Clebsch–Gordan coefficients, thus confirming the "universal splitting" result of Refs. [28, 29].

In the $\mathrm{K} = 3$ shell, however, there are three coefficients $(v_{00}, v_{40}, v_{6\pm6})$, leading to two free parameters, the independent ratios v_{40}/v_{00} and $v_{6\pm6}/v_{00}$, which means that the energy splittings depend on the potential, i.e., that they are not "universal".

A clear example of this difference appears between the eigen-energies in the Y-string and the Δ-string potential, as a consequence of $|v_{6\pm6}^{\mathrm{Y}}| \ll |v_{6\pm6}^{\Delta}|$. That is also the first direct consequence of the dynamical $O(2)$ symmetry of the "Y-string" potential. Numerical values of eigen-energies can be obtained from the results in Ref. [15] by using Eqs. (22), (24)–(26) in Sect. 3.3 and Eqs. (C1)–(C8) in App. C; as well as the numerical values shown in Tables 4, 5, 6 in Sect. 4.2 and Table 11 in App. C of Ref. [30]. The $\mathrm{K} = 4$ shell is too complicated to be discussed here; for these results see Ref. [15] – the general conclusions agree with those from $\mathrm{K} = 3$ shell.

The ordering of bound states has its most immediate application in the physics of three confined quarks, where the question was originally raised, Refs. [12,27–29], but, as time passed it has become more of a question in mathematical physics, see Refs. [8,9,11]. The above discussion ought to have made it clear

[7] For (in-homogeneous, smooth) non-monotonic potentials with a hard inner-core, $\alpha < -2$ and/or weak asymptotic tail falling off faster than $1/R^2$, the mixing angle $\Theta(R)$ behaves differently, and its two limits, $R \to \infty$, and $R \to 0$, may be "reversed". For $V(R) \simeq 1/R^2$, $\alpha = -2$, the mixing angle Θ does not depend on R, as the complete R dependence can be factored out of the eigenvalue equation (16). That is a consequence of the scale invariance of $V(R) \simeq 1/R^2$ potentials in non-relativistic dynamics, see Refs. [25,26].

that three-body analogons of two-body state-ordering theorems, Refs. [8,9,11], do not hold for realistic three-body systems at $K > 2$.

5. Summary and conclusions

In summary, we have constructed the three-body permutation-symmetric hyperspherical harmonics and then used them in a permutation symmetric version of the hyperspherical adiabatic representation to reduce the non-relativistic three-body problem to a set of coupled ordinary differential equation for the hyper-radial wave functions with effective potentials that are derived as functions of the three-body potential's hyperspherical harmonics expansion coefficients.

In the adiabatic approximation this set of equations decouples to one ordinary differential equation, that can be solved in the same manner as the one-body radial Schrödinger equation.

This transcription of the three-body problem into hyperspherical variables is possible only for three-body potentials whose hyper-angular dependence is square integrable, however. One such subset are the factorizable potentials, and more specifically homogeneous potentials, such as the pairwise sums of single-power-law terms, with the power larger than -1.

Then, we applied these methods to three homogeneous potentials that satisfy the square integrability condition. The ordering of states ("pattern") in the spectrum depends on the $O(6)$ symmetry-breaking, which in turn is determined by the hyperspherical expansion coefficients of the three-body potential. These coefficients depend on the dynamical "remnant" symmetries of the potential. Thus, for example the so-called Y-string potential has an $O(2)$ dynamical symmetry, Ref. [19], that is absent in potentials that are pairwise sums of single-power-law terms (for powers different than the second one). We used this $O(2)$ dynamical symmetry, of which the permutation group $S_3 \subset O(2)$ is a subgroup, to guide our construction of the permutation symmetric harmonics. In three dimensions (3D) the "hyper-spherical symmetry" is $O(6)$, and the residual dynamical symmetry of the potential is $S_3 \otimes SO(3)_{rot} \subset O(2) \otimes SO(3)_{rot} \subset O(6)$, where $SO(3)_{rot}$ is the rotational symmetry associated with the (total orbital) angular momentum L.

Our $O(6)$ permutation-symmetric three-body hyperspherical harmonics appear to be the first of their kind in the literature. Symmetrized three-body hyper-spherical harmonics have been pursued before, albeit without emphasis on the the "kinematic rotation" $O(2)$ symmetry label. To our knowledge, aside from the special case $L = 0$ results of Simonov, Ref. [5] and $L = 1$ of Barnea and Mandelzweig, Ref. [13], several other attempts, Refs. [6,31–33], some based on so-called "tree pruning" techniques, exist in the literature, beside the recursively symmetrized N-body hyperspherical harmonics of Barnea and Novoselsky, Refs. [16,17]. The latter are based on the $O(3) \otimes S_N \subset O(3N-3)$ chain of algebras, which does not explicitly include the "kinematic rotation"/"democracy" $O(2)$ symmetry.

The method of permutation-symmetric hyperspherical harmonics is not specific to any particular non-relativistic quantum three-body problem, i.e., it should find application in realistic 3D three-body problems in atomic, molecular and Efimov physics, three-quark problem in hadronic physics, as well as in positronium ion $P_s^-(=e^-e^+e^-)$ physics.

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