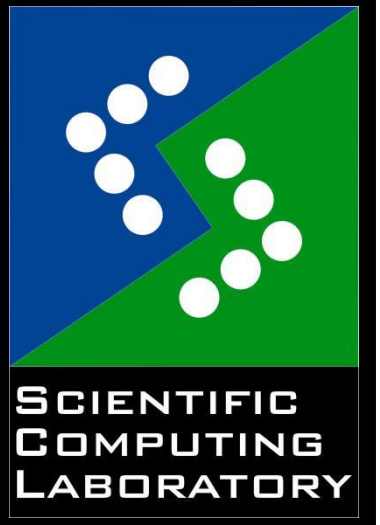


Institute of Physics, Belgrade
Scientific Computing Laboratory

PATH INTEGRALS AT WARP SPEED: REPORTING TO MY CAPTAIN FOR QUARTER-CENTURY

Danica Stojiljković

Belgrade,
11.06.2026.

In memory of Antun Balaž - insights into complex systems

Overview

- Path integrals for n00bs
- Do it smarter – make it faster:
  - Accelerating Path integral calculations
- Use it or Lose it: calculation of energy spectra
- Further expeditions at warp speed
- Open Source Black box: SPEEDUP code package

Based on:

- Bogojević, Balaž, Belić, PRL 94, 180403 (2005)

  "Systematically Accelerated Convergence of Path Integrals"

- Stojiljković, Bogojević, Balaž, PLA 360 (2006)

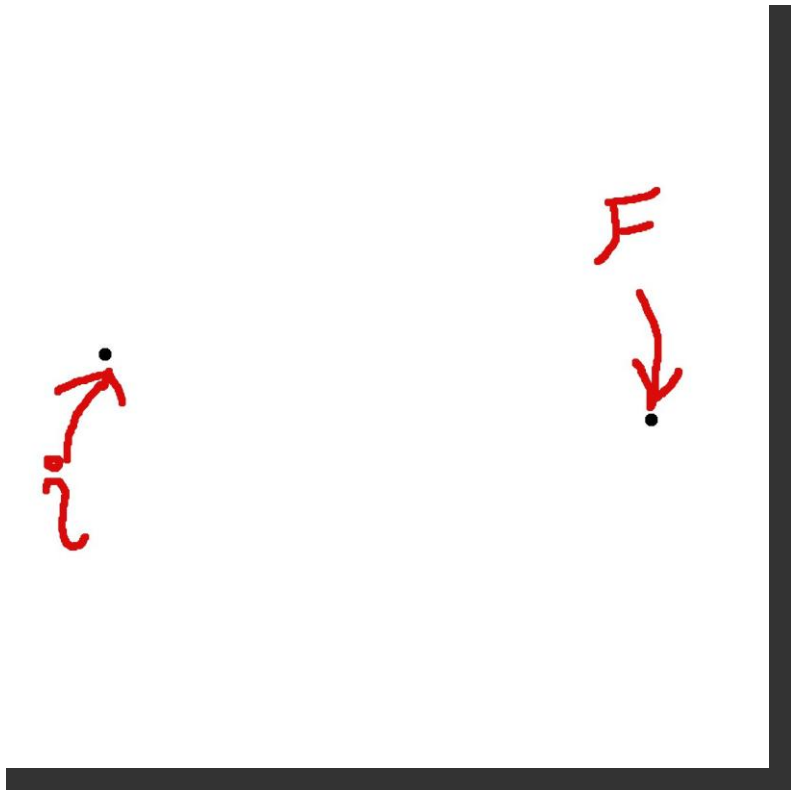
  "Efficient Calculation of Energy Spectra Using Path Integrals“

- Stojiljković et al., JPCS 8 (2008)
- Balaž et al., CiCP 11 (2012)

Brief History of Path Integrals

- R. P. Feynman introduced path integral formulation of QM
- It replaces the traditional operator-based mathematics with infinite-dimensional integration over variables or classical paths.
- different problems are treated in the same manner
- enabled us to treat problems that were unavailable before

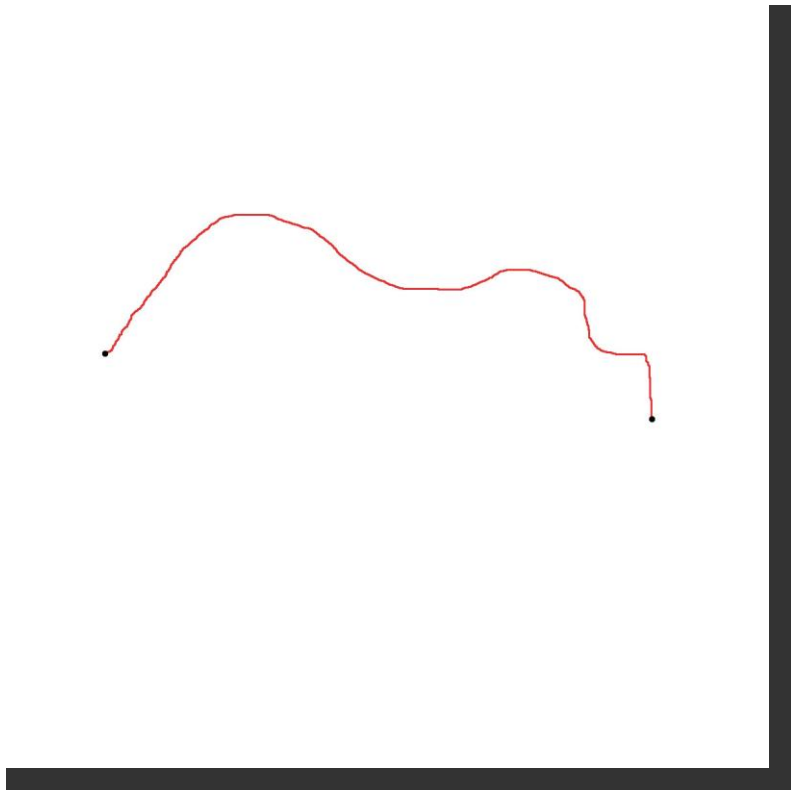
When to use path integral?



- Calculating a transition amplitude for a particle propagation from an initial to a final point in time β

$$A(q_i, q_f; \beta)$$

How to calculate path integral? Three rules



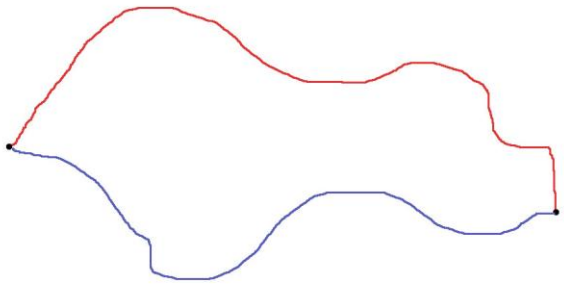
- First rule: single path contribution is

$$\sim e^{-S(a)}$$

- $S(a)$ is action for path a

$$S(a) = \int_0^{\beta} \mathcal{L}\big(q(\tau)\big)\, d\tau$$

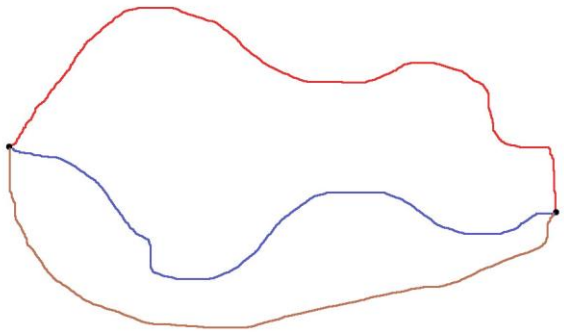
How to calculate path integral? Three rules



- Second rule: linearity - path contributions add up

$$\sim e^{-S(a)} + e^{-S(b)}$$

How to calculate path integral? Three rules



- Third rule: all paths matter

$$\sim e^{-S(a)} + e^{-S(b)} + e^{-S(c)} + \ldots$$

How to calculate path integral? Three rules

- Single path contribution is

$$\sim e^{-S(a)}$$

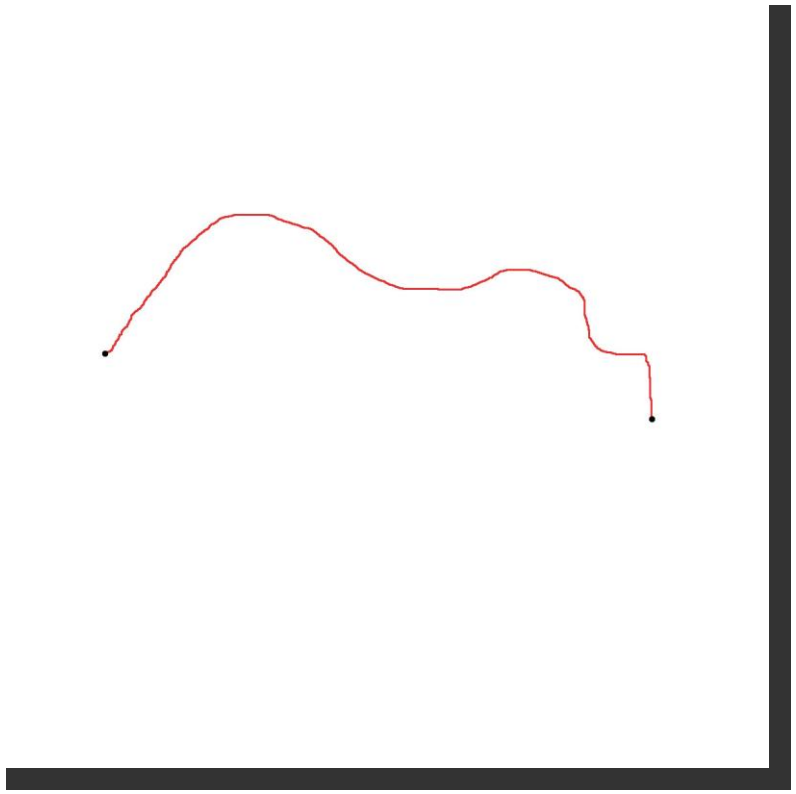
- Linearity: path contributions add up

$$\sim e^{-S(a)}+e^{-S(b)}$$

- All paths matter

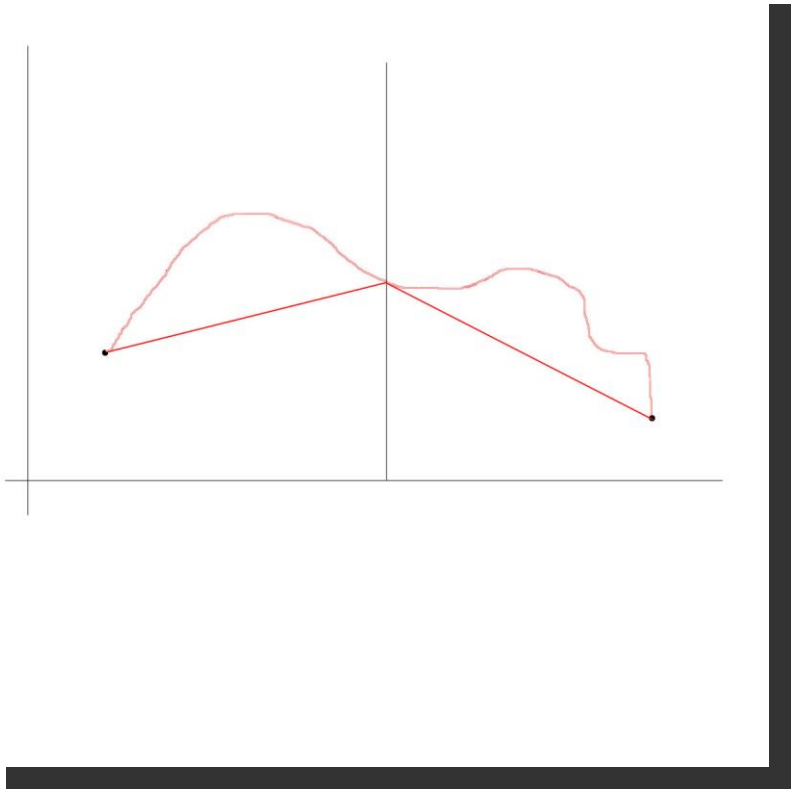
$$\sim e^{-S(a)}+e^{-S(b)}+e^{-S(c)}+\ldots$$

Numerical calculation of path integrals



- Continuous paths are approximated by discretized paths

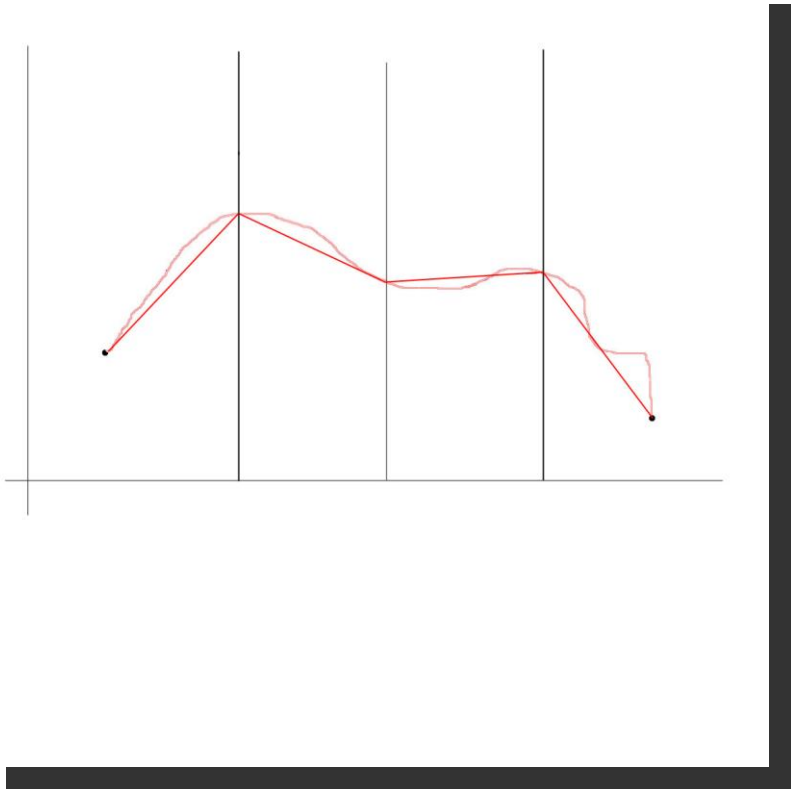
Numerical calculation of path integrals



- two propagation steps

$\sim A_2$

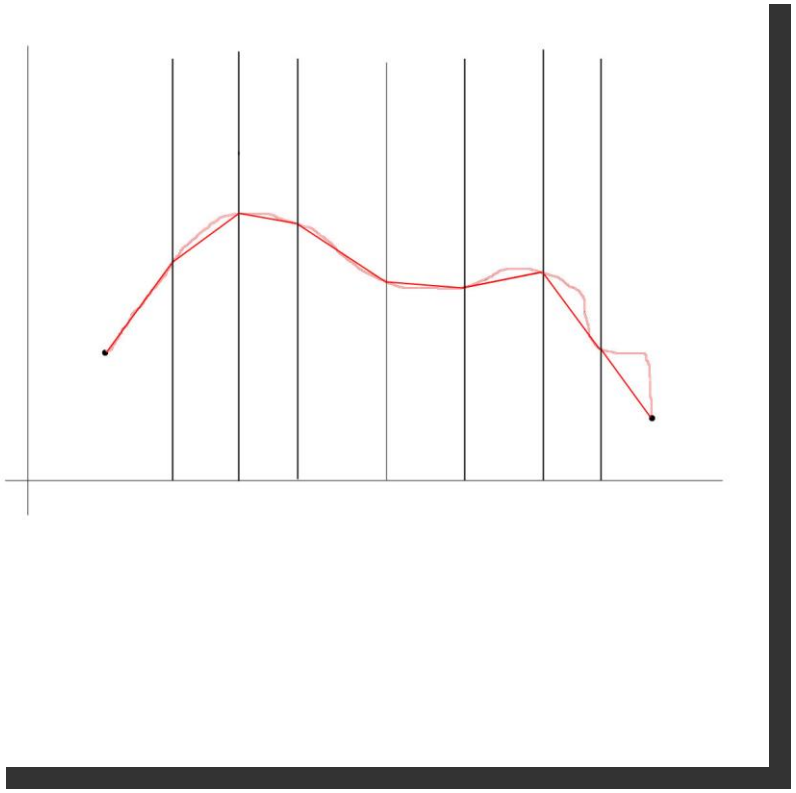
Numerical calculation of path integrals



- four propagation steps

$\sim A_4$

Numerical calculation of path integrals



- Eight propagation steps

$\sim A_8$

Numerical calculation of path integrals

- By continuing procedure, we get series that converge to its continuum limit:

$$A_1 \to A_2 \to A_4 \to A_8 \to \cdots \to A_\infty =< A >$$

- Convergence speed: $A_\infty - A_N \sim 1/N$
  - Slow and CPU demanding
  - Expensive
  - Sometimes insufficiently accurate

Systematically accelerated convergence of path integrals

A. Bogojevic, A. Balaz, and A. Belic, *Phys. Rev. Lett. 94, 180403 (2005)*

- Convergence can be accelerated by different choice of the action
- New Method for constructing hierarchy of effective action for general theory in QM is developed and tested

$$S^{(1)} \rightarrow S^{(2)} \rightarrow S^{(3)} \rightarrow \cdots \rightarrow S^{*}$$

- Effective action of level p: $S^{(p)}$ have the property

$$A^{(p)}{}_{\infty} - A^{(p)}{}_{N} \sim 1/N^{p}$$

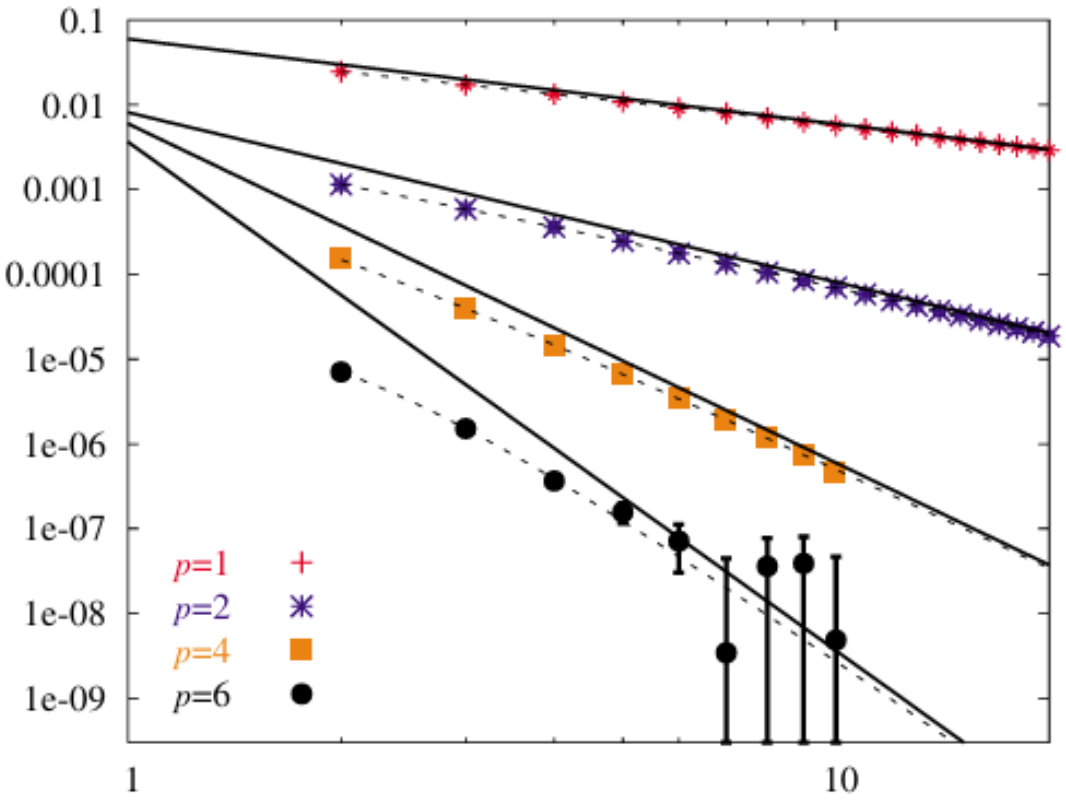
Systematically accelerated convergence of path integrals

A. Bogojevic, A. Balaz, and A. Belic, *Phys. Rev. Lett. 94, 180403 (2005)*

"The increase in speed results from new analytical input that comes from a systematic investigation of the relation between discretizations of different coarseness. We have presented an explicit procedure for obtaining a set of effective actions $S^{(p)}$ that have the same continuum limit as the starting action S, but which approach that limit ever faster."

Systematically accelerated convergence of path integrals

A. Bogojevic, A. Balaz, and A. Belic, *Phys. Rev. Lett. 94, 180403 (2005)*



Deviations from the continuum limit $\left|A_N^{(p)} - A\right|$ as functions of N for p=1, 2, 4, and 6 for an anharmonic oscillator with quadratic coupling $g = 10$, time of propagation T=1 from i=0 to f=1. NMC was 9.2×10^9 for p=1, 2, 9.2×10^{10} for p=4, and 3.68×10^{11} for p=6. Dashed lines correspond to appropriate *1/N* polynomial fits to the data. Solid lines give the leading *1/N* behavior. The level p curve has a $1/N^p$ leading behavior.

Systematically accelerated convergence of path integrals

A. Bogojevic, A. Balaz, and A. Belic, *Phys. Rev. Lett. 94, 180403 (2005)*

"We have found that the growth in complexity of the effective actions with increasing p has little effect on computation time for $p = 4$, while simulations with $p = 9$ are roughly 10 times slower due to this. However, this is an extremely small price to pay for a gain of 9 orders of magnitude in the speed of convergence."

Numerical results - calculating energy spectra

- First few energy levels can be extracted recursively from free energies calculated for a set of temperatures β

$$F(\beta) = -\frac{1}{\beta}\ln\sum_{n=0}^{\infty} e^{-\beta E_n}$$

Numerical results - calculating energy spectra

- Single 1D particle in a quartic potential

$$V(q) = \frac{1}{2}q^2 + \frac{g}{4!}q^4$$

- Free energy is related to partition function:

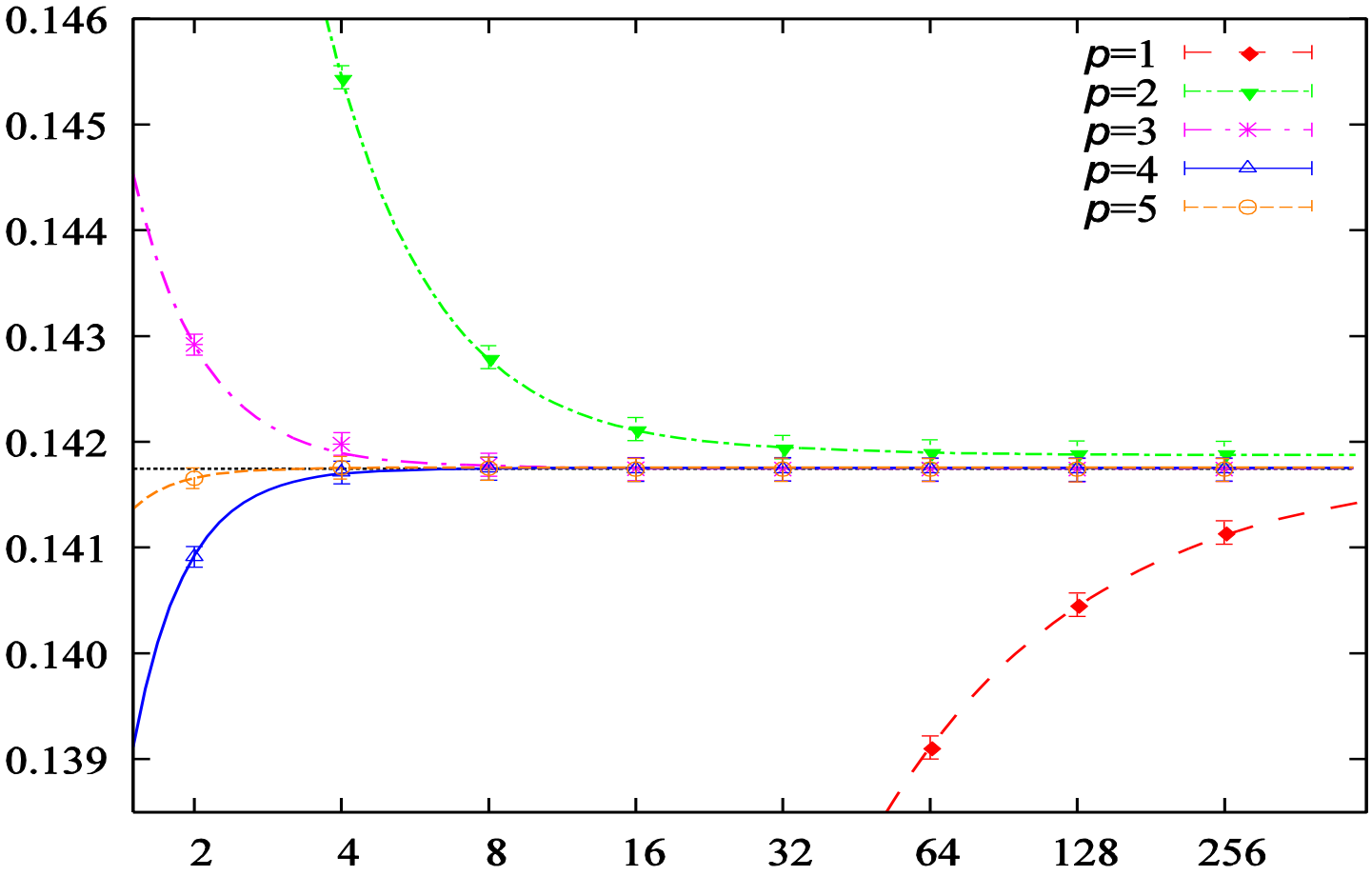
$$F(\beta) = -\frac{1}{\beta}\ln Z(\beta)$$

- Partition function is calculated via transition amplitudes:

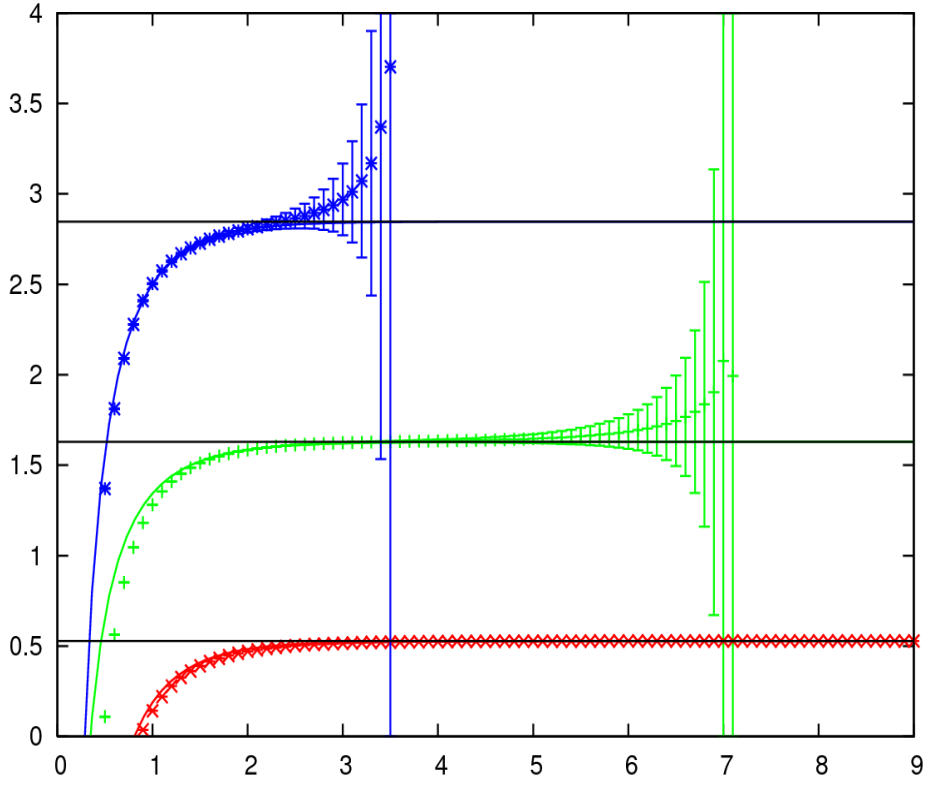
$$Z(\beta) = \int_{-\infty}^{\infty} A(q_i, q_i; \beta)\ dq_i$$

Numerical results -

free energy versus propagation steps



Numerical results - calculating energy spectra



- Dependance of the free energy F on propagation time T for the anharmonic oscillator with quartic coupling $g=1$. The horizontal lines correspond to the energy levels E_n determined from the fits

- Numerical simulations were performed with $p=9$ level improved actions, $N=256$, and $N_{MC}=10^7$

Numerical results - calculating energy spectra

- First few energy levels can be extracted by calculating free energies at set of temperatures

No acceleration

g	E_0	E_1	E_2	E_3
0	0.49992 (2)	1.504 (6)	2.45 (7)	3.5 (7)
0.1	0.50298 (2)	1.522 (7)	2.45 (7)	3.4 (7)
1	0.52756 (2)	1.642 (5)	2.68 (6)	
10	0.67333 (4)	2.26 (1)		
100	1.1618 (1)	4.12 (3)		

Acceleration level 5

g	E_0	E_1	E_2	E_3
0	0.50028 (4)	1.51 (1)	2.5 (1)	3.2 (5)
0.1	0.50354 (7)	1.498 (9)	2.6 (1)	4.1 (4)
1	0.52825 (4)	1.616 (7)	2.8 (1)	
10	0.67402 (5)	2.22 (1)	4.1 (4)	
100	1.1614 (4)	4.16 (8)		
1000	2.3613 (7)			

Numerical results – energy expectation values

J. Grujic, A. Bogojevic, A. Balaz, *Phys. Lett. A 360, 217 (2006)*

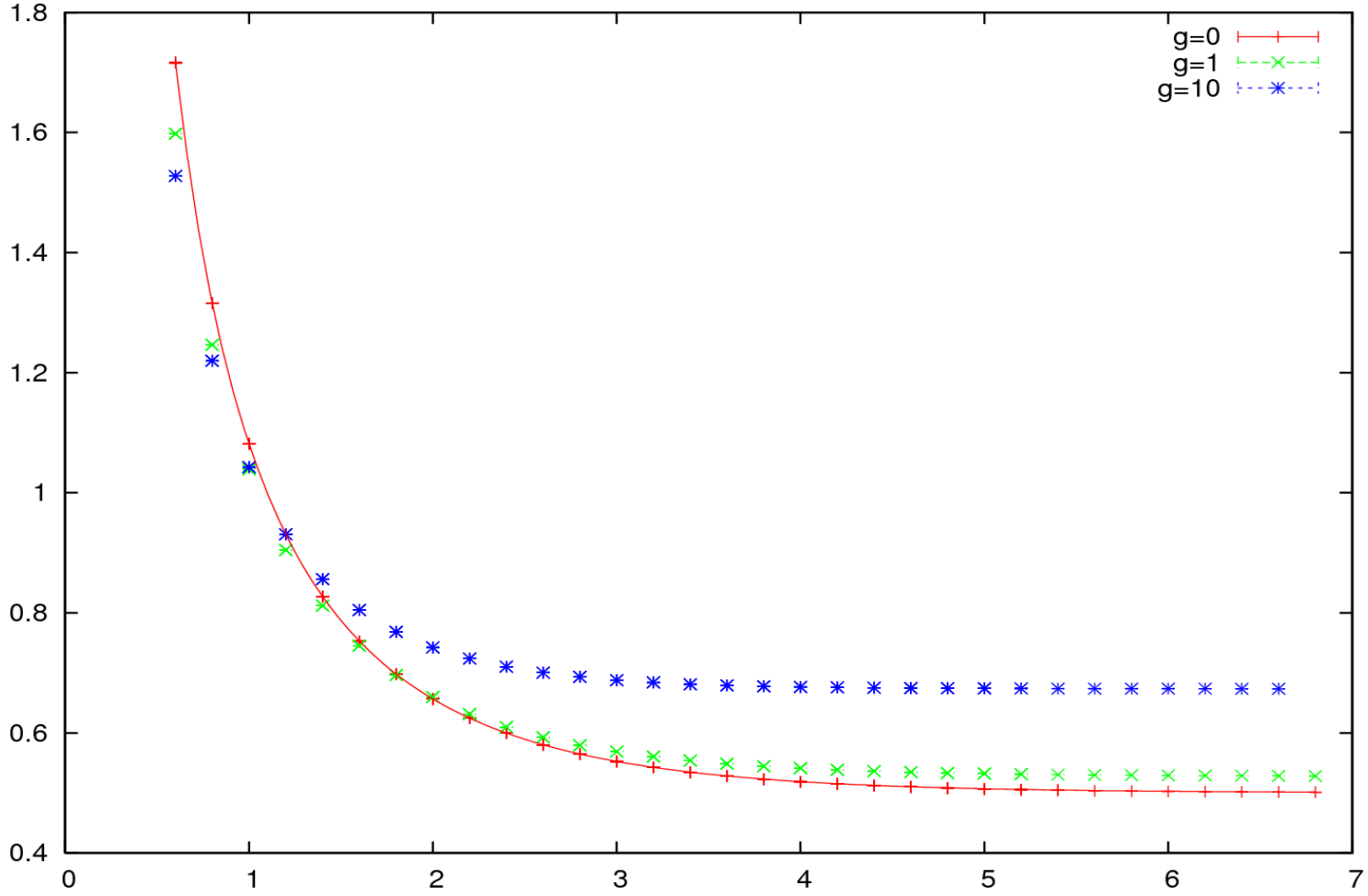
- Estimating mean values of observable

$$\sim O(a)e^{-S(a)}$$

- Effective estimators $O^{(p)}$ were needed for efficient calculation

- Effective virial and kinetic estimators of energy were calculated, so that $E^{(p)}_N - E^{(p)}_\infty \sim 1/N^p$

Numerical results – energy expectation values



Some later expeditions into convergence at warp speed

- A. Bogojevic, I. Vidanovic, A. Balaz, and A. Belic:
  "Fast Convergence of Path Integrals for **Many-Body Systems**"
  Phys. Lett. A **372**, 3341 (2008).
- A. Balaz, A. Bogojevic, I. Vidanovic, and A. Pelster:
  "**Recursive Schroedinger Equation Approach** to Faster Converging Path Integrals", Phys. Rev. E 79, 036701 (2009).
  Phys. Rev. E 80, 066706 (2009).
- A. Balaz, I. Vidanovic, A. Bogojevic, and A. Pelster:
  "Ultra-fast Converging Path-integral Approach **for Rotating Ideal Bose-Einstein Condensates**",
  Phys. Lett. A 374, 1539 (2010).
- A. Balaz, I. Vidanovic, A. Bogojevic, A. Belic, and A. Pelster:
  "Fast Converging Path Integrals for **Time-Dependent Potentials**: I. **Recursive Calculation** of Short-Time Expansion of the Propagator"
  J. Stat. Mech.-Theory Exp. , P03004 (2011).
- A. Balaz, I. Vidanovic, A. Bogojevic, A. Belic, and A. Pelster:
  "Fast Converging Path Integrals for **Time-Dependent Potentials**: II. Generalization to **Many-Body Systems and Real-Time Formalism**"
  J. Stat. Mech.-Theory Exp. , P03005 (2011).

SPEEDUP Code for Calculation of Transition Amplitudes Via the Effective Action Approach

A. Balaz, I. Vidanovic, D. Stojiljkovic, D. Vudragovic, A. Belic, and A. Bogojevic, Commun. Comput. Phys. **11**, 739 (2012).

- Components:
- Mathematica package
  - symbolic derivation
  - effective actions
- C package
  - Monte Carlo calculations
  - transition amplitudes
  - expectation values

SPEEDUP CAPABILITIES

- SUPPORTS:
  - GENERIC ONE-DIMENSIONAL SYSTEMS
  - MULTI-DIMENSIONAL POTENTIALS
  - MANY-BODY SYSTEMS
  - EFFECTIVE ACTIONS UP TO $p = 18$ CAN BE GENERATED AUTOMATICALLY.

Conclusions

- Standard path integrals converge as ~$1/N$.
- Effective actions improve convergence to ~$1/N^p$.
- Energy spectra can be extracted efficiently.
- Expectation values benefit from the same acceleration.
- SPEEDUP transformed the method into a practical computational tool.

Thank you for your attention!

A short story

- I met Antun in 1998 in Petnica Science Center.
- In 2000. he mentored my high school graduation theses on general theory of relativity.
- Ways to contribute to science:
  - Doing research ★
  - Advocating for science and influencing policymakers ★ (securing funds and equipment)
  - Education and mentorship! ★ ★ ★

Questions?