Effective Actions Approach for Improving Numerical Calculation of Path Integrals

A. Balaž, A. Bogojević, I. Vidanović, A. Belić

Scientific Computing Laboratory
Institute of Physics Belgrade
Pregrevica 118, 11080 Belgrade, Serbia
http://scl.phy.bg.ac.yu/
e-mail: antun@phy.bg.ac.yu

Overview

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Introduction (1)

- Path (functional) integrals in quantum theories allow
  - Easy treatment of symmetries (including gauge symmetries)
  - Derivation of non-perturbative results (solitons, instantons)
  - Showing connections between different theories, or different sectors of the same theory (bosonisation, duality)
  - Quantization (including generalizations to systems with no classical counterparts)
- Rich cross-fertilization of ideas from high energy and condensed matter / statistical mechanics
- Applications in all areas of physics, chemistry, material science, even finance and economics

Introduction (2)

- Path integral formalism can be used for deriving
  - Semiclassical expansion
  - Perturbative expansion
  - Variational methods
- However, mathematical properties of path integrals are far from being sufficiently well understood
- Many important models (or their interesting sectors) require numerical treatment
  - Path Integral Monte Carlo (PIMC) is the most applicable method
  - Widely used M(RT)^2 (Metropolis) algorithm provides optimal efficiency which is, still, unsatisfactory in many cases
  - Our lack of knowledge on path integrals translates into inefficiency of our numerical algorithms

Introduction (3)

- Basic notion of path integral formalism can be found in a paper by Dirac [P. A. M. Dirac, *Physikalische Zeitschrift der Sowietunion* **3**, 64 (1933)] - Lagrangian formulation of quantum mechanics
- Fully developed by Feynman [R. P. Feynman, *Rev. Mod. Phys.* **20**, 367 (1948)]
- Contrary to classical physics, where there is only one trajectory for a given set of boundary conditions, in path integral formalism all possible evolutions must be taken into account
- Each possible trajectory contributes to the transition amplitude by a factor $\exp\{\frac{i}{\hbar}S\}$, where $S = \int L dt$ is the action that corresponds to the given trajectory

Path integrals in quantum mechanics (1)

- Path integrals are originally introduced in quantum mechanics, where new expression is obtained for amplitude for a transition from initial state $|a\rangle$ to final state $|b\rangle$ in time T,
$$A(a,b;T) = \langle b|e^{\frac{i}{\hbar}\hat{H}T}|a\rangle$$
- The same approach can be taken in statistical physics, and partition function can be expressed in a very similar form
- Path integrals in statistical physics are said to be imaginary-time path integrals,
$$\frac{i}{\hbar}T \to -\beta = \frac{1}{k_B T_t}$$
where T_t is the temperature
- It is very common to work in imaginary-time, even when considering quantum mechanics ($\frac{i}{\hbar}T \to -\frac{1}{\hbar}T$)

Path integrals in quantum mechanics (2)

- The usual derivation starts with the following identity:

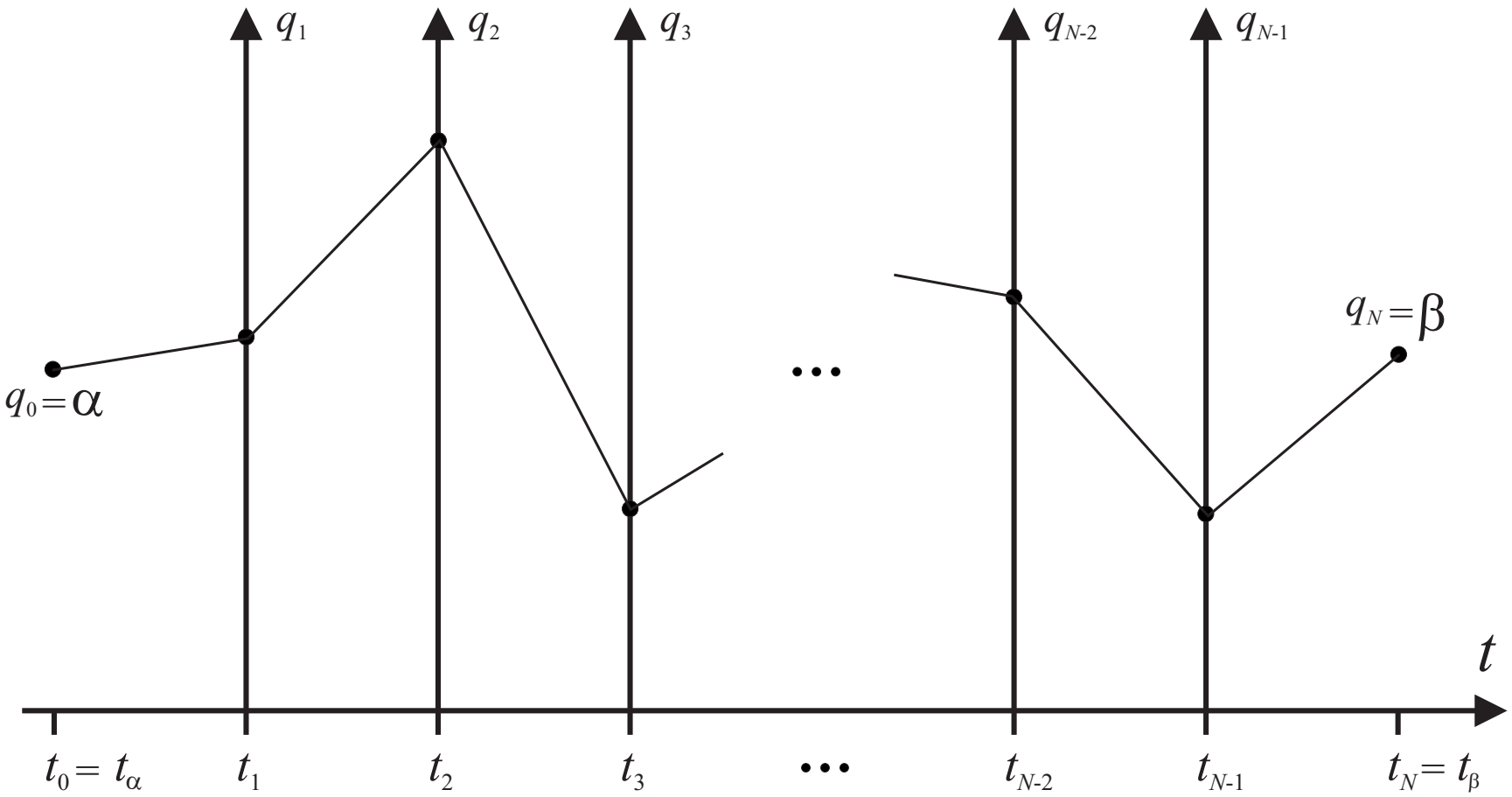
$$A(a,b;T) = \int dq_1 \cdots dq_{N-1} A(a,q_1;\varepsilon) \cdots A(q_{N-1},b;\varepsilon)\,.$$

  It is obtained by dividing time evolution into N time steps of the length $\varepsilon = T/N$, and by inserting $N-1$ decompositions of the identity between short time evolution operators. The above expression is exact.

- The next step is approximative calculation of short-time amplitudes up to the first order in ε, and one obtains ($\hbar = 1$)

$$A_N(a,b;T) = \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{N}{2}} \int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

Illustration of the discretization of trajectories



Path integrals in quantum mechanics (3)

- The continuum amplitude $A(a,b;T)$ is recovered as $N \to \infty$ limit of the discretized amplitude $A_N(a,b;T)$,

$$A(a,b;T) = \lim_{N\to\infty} A_N(a,b;T)$$

- The discretized amplitude A_N is expressed as a multiple integral of e^{-S_N}, where S_N is the discretized action
- For a theory of the form

$$S = \int_0^T dt \left(\frac{1}{2}\,\dot{q}^2 + V(q)\right) ,$$

the (naive) discretized action is given as

$$S_N = \sum_{n=0}^{N-1} \left(\frac{\delta_n^2}{2\varepsilon} + \varepsilon V(\bar{q}_n)\right) ,$$

where $\delta_n = q_{n+1} - q_n$ and $\bar{q}_n = \frac{1}{2}(q_{n+1} + q_n)$.

Numerical calculation of path integrals (1)

- The path integral formalism is ready-made for numerical computations
- Physical quantities are given in terms of discretized expressions in the form of multiple integrals like

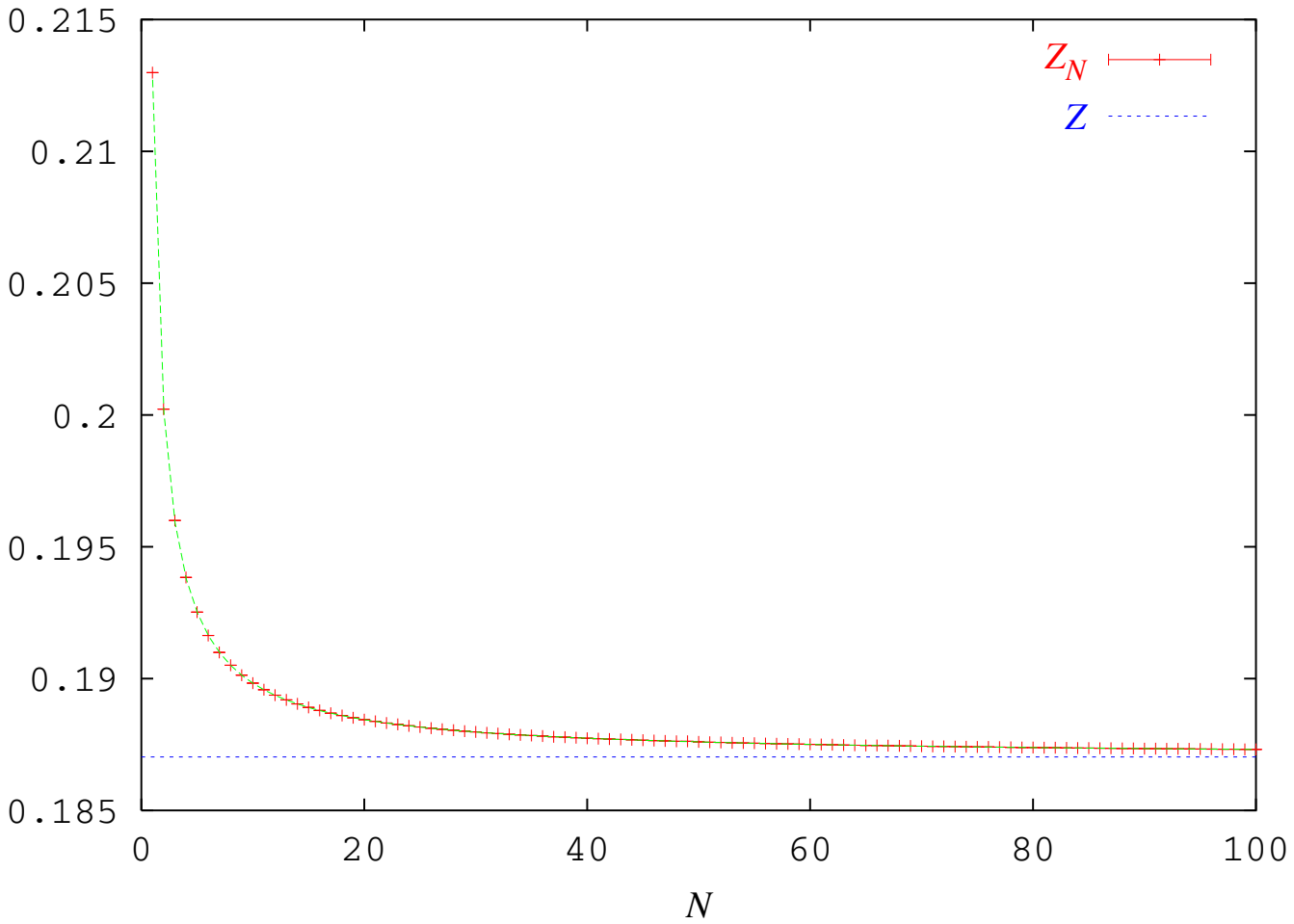
$$\int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

- Monte Carlo integration method is tailored for integrals of high dimensionality - it dominates over all other methods
- However, while multiple integrals can be calculated accurately and efficiently with MC method, $N \to \infty$ limit remains to be done
- This is the weak point of the above constructive definition of path integrals

Numerical calculation of path integrals (2)

- The discretization used for the definition of path integrals is not unique; in fact, the choice of discretization is *extremely* important
- The naively discretized action in the mid-point prescription leads to amplitudes that converge to the continuum as $1/N$
- Using some special tricks one can achieve better convergence (e.g. left prescription leads to $1/N^2$ convergence when partition functions, i.e. traces, are calculated)
- However, this cannot be done in a systematic way, nor is applicable in all cases (left prescription cannot be used for systems with ordering ambiguities)

Typical convergence of naively discretized path integrals to the continuum as $1/N$



Effective discretized actions (1)

- Discretized actions can be classified according to the speed of convergence of corresponding path integrals
- Different discretized actions can be introduced, containing various terms additional to the naive discretized action
- These additional terms must vanish in $N \to \infty$ limit, and must not change the continuum amplitudes; e.g.

$$\sum_{n=0}^{N-1} \varepsilon^3 V'(\bar{q}_n) \to \varepsilon^2 \int_0^T dt\, V'(q(t)) \to 0$$

- Additional terms can be added to discretized action in such a way as to improve the convergence of discretized path integrals

Effective discretized actions (2)

- Such improved discretized actions have been previously constructed using a variety of approaches, including:
  - Generalized Trotter-Suzuki formulas
  - Improvements in short-time propagation
  - Expansions in number of derivatives
- This has improved the convergence of generic path integral partition functions from $1/N$ to $1/N^4$
- The Li-Broughton effective potential

$$V^{LB} = V + \frac{1}{24}\varepsilon^2 V'^2 .$$

  in the left prescription gives the $1/N^4$ convergence $Z_N^{LB} = Z + O(1/N^4)$
- Derivation from the generalized Trotter formula uses the cyclic property of the trace - the $1/N^4$ convergence only holds for the partition function

Effective discretized actions (3)

- Substantial improvement has recently been made through the study of the relationship between discretizations of different coarseness and deriving the unique integral equation governing the flow to the continuum
- This investigations allowed us to systematically derive effective discretized actions which give give improved $1/N^p$ convergence of discretized path integrals
- Here we present equivalent approach, based on the calculation of ε-expanded short-time amplitudes
- The presented approach is easily generalizable to many-particle systems in arbitrary dimensions, which is an important advantage compared to earlier method

Ideal discretization (1)

- An ideal discretized action S^* would imply $A_N = A$ for all amplitudes and all discretizations N
- For massless free particles the naive and ideal discretized actions are the same
- The general completeness relation

$$A(a,b;T) = \int dq_1 \cdots dq_{N-1}\, A(a,q_1;\varepsilon) \cdots A(q_{N-1},b;\varepsilon)\,,$$

determines the ideal discretized action S_n^* for propagating for time ε to be

$$A(q_n,q_{n+1};\varepsilon) = (2\pi\varepsilon)^{-\frac{1}{2}}\ e^{-S_n^*}$$

- The ideal discretized action S^* is simply the sum of expressions S_n^*

Ideal discretization (2)

- We will calculate the ideal discretized action by expanding it in power series in ε, i.e. by systematically calculating

$$A(q_n, q_{n+1}; \varepsilon) = (2\pi\varepsilon)^{-\frac{1}{2}} \left(e^{-S_n^{(p)}(q_n, q_{n+1}; \varepsilon)} + O(\varepsilon^{p+1}) \right)$$

  up to the desired order ε^p.
- First step is to shift integration variable $q = \xi + x$ about a fixed referent trajectory ξ (same boundary conditions)

$$A(q_n, q_{n+1}; \varepsilon) = e^{-S_n[\xi]} \int_{x(-\varepsilon/2)=0}^{x(\varepsilon/2)=0} [dx] \; e^{-\int_{-\varepsilon/2}^{\varepsilon/2} ds \left(\frac{1}{2}\dot{x}^2 + U(x;\xi) \right)}$$

- Time is also shifted from $t \in [n\varepsilon, (n+1)\varepsilon]$ to $s \in [-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}]$, and

$$S_n[\xi] = \int_{-\varepsilon/2}^{\varepsilon/2} ds \left(\frac{1}{2}\dot{\xi}^2 + V(\xi) \right) , \; U(x;\xi) = V(\xi+x) - V(\xi) - x\ddot{\xi}$$

Ideal discretization (3)

- The amplitude may now be written as

$$A(q_n, q_{n+1}; \varepsilon) = \frac{e^{-S_n[\xi]}}{(2\pi\varepsilon)^{\frac{1}{2}}} \left\langle e^{-\int_{-\varepsilon/2}^{\varepsilon/2} ds\, U(x;\xi)} \right\rangle ,$$

  where $\langle ... \rangle$ denotes the expectation value with respect to the free massless particle action
- The above expression holds for any choice of referent trajectory ξ
- Since we are using expansion in small time step ε, to retain all terms of the desired order it is necessary to take into account that the short time propagation of the considered class of theories satisfies the diffusion relation $\delta_n^2 \propto \varepsilon$
- So, keeping all terms proportional to $\varepsilon^k \delta_n^{2l}$ with $k + l \leq p$ will be sufficient for obtaining the desired precision

Ideal discretization (4)

- The sought-after free particle expectation value can calculated using the series expansion

$$\left\langle e^{-\int ds\, U(x;\xi)} \right\rangle = 1 - \int ds \left\langle U(x;\xi) \right\rangle + \frac{1}{2} \int\int dsds' \left\langle U(x;\xi) U(x';\xi') \right\rangle + \ldots$$

- By expanding $U(x;\xi)$ around the tajectory ξ, we get

$$U(x;\xi) = x(V'(\xi) - \ddot{\xi}) + \frac{1}{2} x^2 V''(\xi) + \ldots$$

- Expectation values $\langle x(s) \ldots x(s') \rangle$ can be calculated in the usual way, by introducing a generating functional for the free-particle theory whose propagator is:

$$\Delta(s,s') = \frac{1}{\varepsilon} \theta(s-s') \left(\frac{\varepsilon}{2} - s \right) \left(\frac{\varepsilon}{2} + s' \right) + s \leftrightarrow s'$$

Ideal discretization (5)

- Using Wick's theorem, one easily finds $\langle x(s) \rangle = 0$, $\langle x(s)x(s') \rangle = \Delta(s, s')$, etc.
- Note that the calculation of the generating functional (and also of the expectation values) is the same, irrespective of the choice of ξ
- In all cases the action and the boundary conditions for the field x are the same, and so the propagator is always given by the above formula
- However, different choices of ξ are related to different approximation techniques:
  - the choice of classical trajectory for ξ corresponds to the semiclassical expansion
  - the choice of a linear referent trajectory for ξ leads to short-time expansion

Ideal discretization (6)

- In order to perform the remaining integrations over s, due to the explicit dependence of the referent trajectory on s, we first expand the potential and all its derivatives in the expression for U around some reference point
- We choose $\bar{q}_n$ as that reference point, corresponding to the mid-point prescription
- Once one chooses the referent trajectory $\xi(s)$, all expectation values that need to be calculated are given in terms of quadratures
- By choosing linear referent trajectories $\xi(s) = \bar{q}_n + \frac{\delta_n}{\varepsilon} s$ and calculating up to terms of order ε^2 (level $p = 2$), we obtain for the action

$$S_n[\xi] = \varepsilon \left(\frac{1}{2} \frac{\delta_n^2}{\varepsilon^2} + V(\bar{q}_n) + \frac{\delta_n^2}{24} V''(\bar{q}_n) \right) + O(\varepsilon^3)$$

Ideal discretization (7)

- For the remaining free particle expectation value up to the level $p = 2$ we get

$$\left\langle e^{-\int ds\, U(x;\xi)} \right\rangle = 1 - \frac{\varepsilon^2}{12} V''(\bar{q}_n) + O(\varepsilon^3) = e^{-\frac{\varepsilon^2}{12} V''(\bar{q}_n)} + O(\varepsilon^3)$$

- Now we easily obtain the level $p = 2$ discretized effective action

$$S_N^{(p=2)} = \sum_{n=0}^{N-1} \varepsilon \left(\frac{1}{2} \left(\frac{\delta_n}{\varepsilon} \right)^2 + V(\bar{q}_n) + \frac{\varepsilon}{12} V''(\bar{q}_n) + \frac{\delta_n^2}{24} V''(\bar{q}_n) \right)$$

- One can easily derive higher level effective actions
- Generalization to many-particle systems in arbitrary dimensions is straightforward and has been done

Numerical results (1)

- We have conducted a series of PIMC simulations of transition amplitudes for a two-dimensional system of two particles interacting through potential

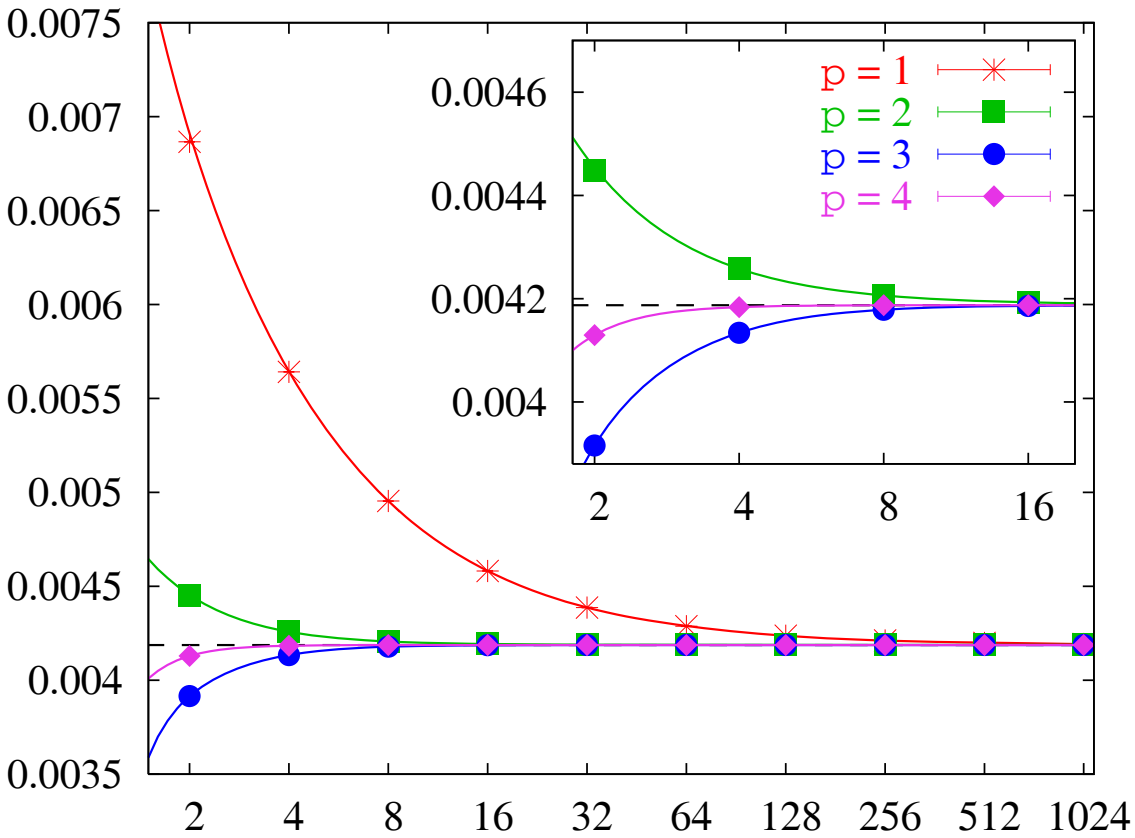
$$V(\vec{r}_1, \vec{r}_2) = \frac{1}{2}(\vec{r}_1 - \vec{r}_2)^2 + \frac{g_1}{24}(\vec{r}_1 - \vec{r}_2)^4 + \frac{g_2}{2}(\vec{r}_1 + \vec{r}_2)^2$$

- Numerical simulations, based on our SPEEDUP PIMC code, have been performed for different values of couplings g_1 and g_2 and for variety of initial and final states
- The continuum amplitudes $A^{(p)}$ have been estimated by fitting polynomials in $1/N$ to the discretized values $A_N^{(p)}$

$$A_N^{(p)} = A^{(p)} + \frac{B^{(p)}}{N^p} + \frac{C^{(p)}}{N^{p+1}} + \ldots$$

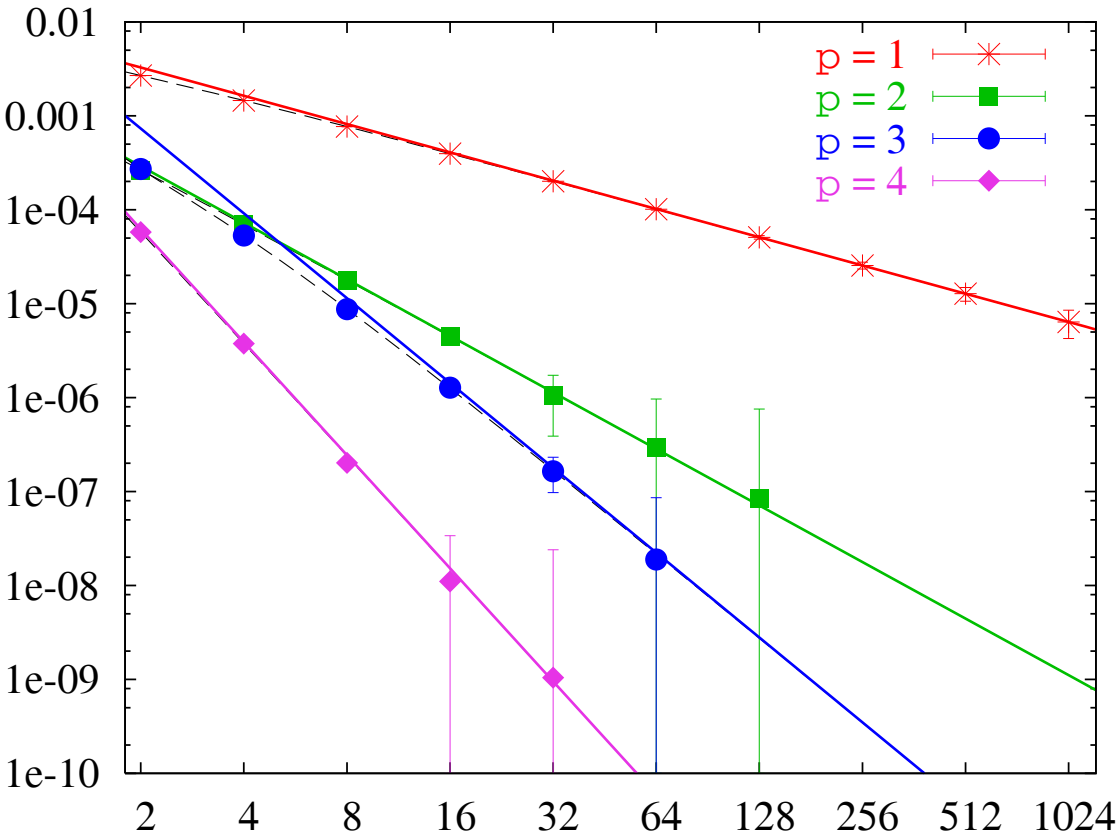
- For all values of p the fitted continuum values $A^{(p)}$ agree within the error bars

PIMC: Convergence to the continuum



Amplitude for the oscillator with large quartic anharmonicity $g_1 = 10$, $g_2 = 0$, $T = 1$, $N_{MC} = 10^6$, initial and final states $a = (0, 0; 0.2, 0.5)$, $b = (1, 1; 0.3, 0.6)$.

PIMC: Deviations from the continuum



Deviations from the continuum of amplitudes for the oscillator with large quartic anharmonicity $g_1 = 10$, $g_2 = 0$, $T = 1$, $N_{MC} = 10^6$ $(p = 1)$, 10^7 $(p = 2)$, 10^9 $(p = 3)$, 10^{10} $(p = 4)$, initial and final states $a = (0, 0; 0.2, 0.5)$, $b = (1, 1; 0.3, 0.6)$.

Numerical results (2)

- One can also evaluate energy spectra of the model by calculating its partition function in the path integral formalism, and recalling $Z(T) = \sum_{n=0}^{\infty} d_n e^{-TE_n}$
- The free energy of the system, $F(T) = -\frac{1}{T} \ln Z(T)$, tends to the ground state energy E_0 in the large T limit.
- Auxiliary functions

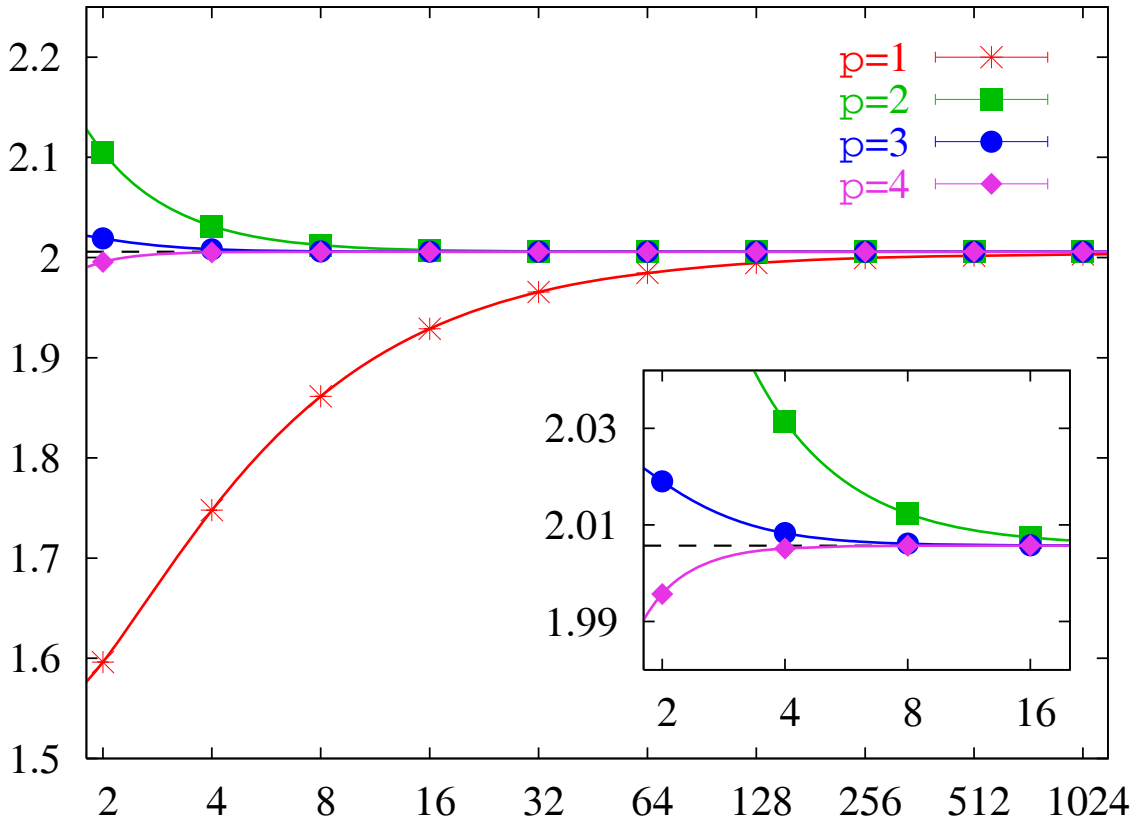
$$F^{(n)}(T) = -\frac{1}{T} \ln \frac{Z(T) - \sum_{i=0}^{n-1} d_i \; e^{-TE_i}}{d_n}$$

can be fitted for large T to

$$f^{(n)}(T) = E_n - \frac{1}{T} \ln(1 + ae^{-Tb})$$

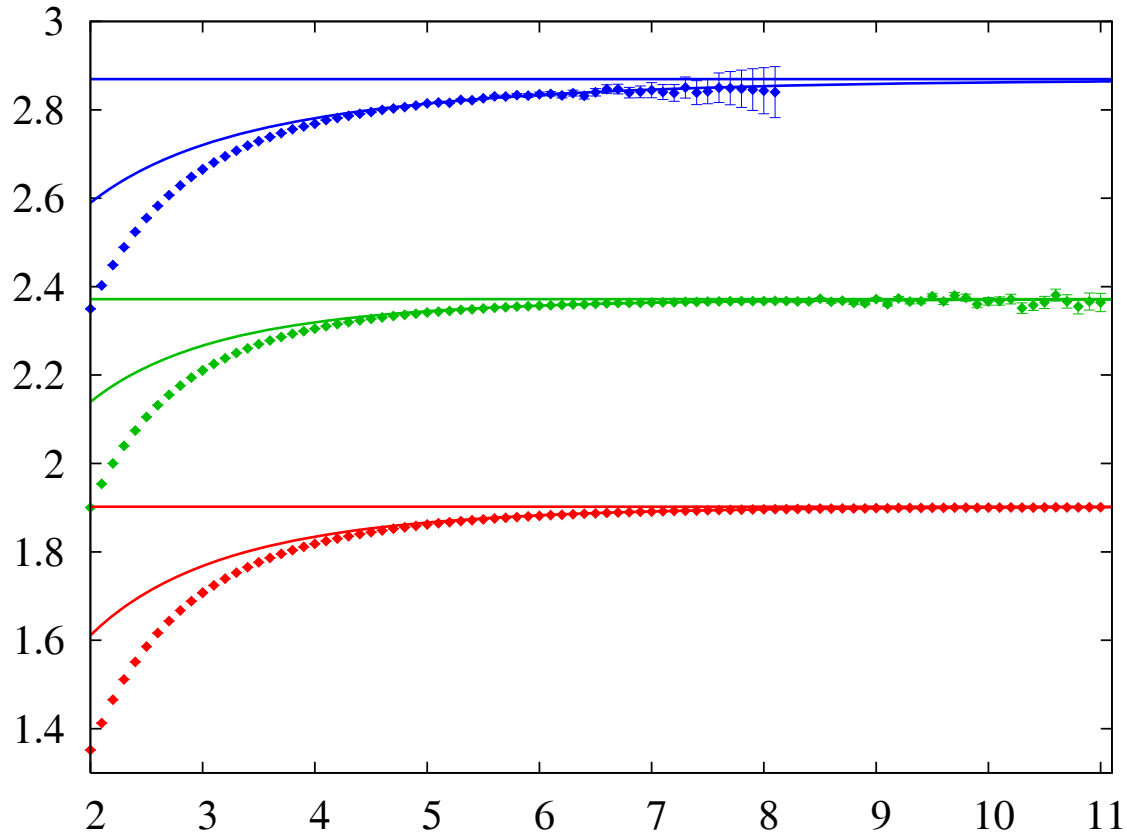
and tend to the corresponding energy levels E_n

PIMC: Convergence of the free energy



Convergence of discretized free energy to the continuum as functions of N for the system of two particles in two dimensions in a quartic potential with $g_1 = 1$, $g_2 = 1$, $T = 1$, $N_{MC} = 10^7$.

PIMC: Energy spectra calculation



Dependence of the free-energy and auxiliary functions $f^{(1)}$ and $f^{(2)}$ on T for the system in the quartic potential with $g_1 = 1/10$, $g_2 = 1/9$, $N_{MC} = 10^9$. We used $p = 5$ effective action and $N = 64$.

PIMC: Low-lying energy levels of anharmonic oscillator

g_1	E_0	E_0^{pert}	E_1	E_2	E_3
0.0	1.8857(1)	1.88562	2.3571(6)	2.83(1)	3.3(2)
0.1	1.9019(2)	1.90187	2.374(2)	2.82(1)	—
1.0	2.0228(2)	2.03384	2.497(3)	2.94(3)	—
10	2.6327(6)	—	3.098(4)	3.57(3)	—

Low lying energy levels of the system in the quartic potential ($g_2 = 1/9$), calculated using $N_{MC} = 10^9$, level $p = 5$ effective action and $N = 64$. The degeneracies of the calculated energy levels are found to be $d_0 = 1$, $d_1 = 2$, $d_2 = 3$, $d_3 = 6$.

Current research

- Derivation of higher level effective actions for many-particle systems in arbitrary dimensions
- Efficient *Mathematica* implementation of symbolic derivation of effective actions
- Derivation of improved estimators for calculation of expectation values (kinetic energy, potential energy, heat capacity etc.)
- Derivation of simplified effective actions for calculation of partition functions (generalizations of Li-Broughton action)
- Monte Carlo implementation and numerical verification of derived effective actions and estimators
- Derivation of recursive relations for effective actions

Future research directions

- Extensive application of the new method for more efficient PIMC calculations in non-relativistic many-particle dynamics, in particular calculation of properties of Bose-Einstein condensation for systems of:
  - Noninteracting bosons in anharmonic rotating trap
  - Weakly interacting bosons in anharmonic rotating trap
- Extracting large β information by using variational methods to calculate the ideal discretized action.
- Generalization of method to more complex quantum systems:
  - Bosonic QFT
  - Fermionic QFT
  - Gauge theories
  - Topologically non-trivial spaces

Conclusions (1)

- Asymptotically expanding the ideal discretized action in ε to order ε^p gives us the effective discretized action $S_N^{(p)}$ whose amplitudes converge as $1/N^p$.
- Explicit analytical expressions for $S_N^{(p)}$ have been obtained for a general non-relativistic theory of M particles in d dimensions for higher values of p.
- The presented scheme is general, i.e. applicable to all path integral calculations. Most other approaches focus solely on partition functions (e.g. use cyclicity of the trace).
- The newly derived effective actions agree with previous approaches wherever comparison is possible (e.g. $S_N^{(p=4)}$ equals the Li-Broughton effective action, modulo terms vanishing for periodic boundary conditions).

Conclusions (2)

- The boundary-dependent terms in $S_N^{(p)}$ lead to sought-after $1/N^p$ convergence even when calculating amplitudes.
- PIMC calculations of amplitudes, partition functions, expectation values and energies of various theories confirm analytically derived speedup.
- Important additional advantages:
  - Simpler derivations;
  - Straightforward generalization to more complex systems (e.g. to QFT);
  - Important heuristical insights, such as $S[q_{\rm cl}] = S_N^*\big|_{\hbar=0}$, where $S[q]$ is the continuum action and $q_{\rm cl}$ is the classical trajectory passing through points $q_0\, q_1, \ldots, q_N$;
  - Possibility of obtaining large β information by calculating S_N^* variationally rather than through an asymptotic expansion in ε.

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Effective p=4 discretized action

$$
\begin{aligned}
S_N^{(p=4)} &= \sum \left\{ \varepsilon \left(\frac{1}{2} \frac{\delta_i \delta_i}{\varepsilon^2} + V \right) \right. \\
&+ \frac{\varepsilon^2}{12} \partial^2_{k,k} V + \frac{\varepsilon \delta_i \delta_j}{24} \partial^2_{i,j} V \\
&- \frac{\varepsilon^3}{24} \partial_i V \partial_i V + \frac{\varepsilon^3}{240} \partial^4_{i,i,j,j} V + \frac{\varepsilon^2 \delta_i \delta_j}{480} \partial^4_{i,j,k,k} V + \frac{\varepsilon \delta_i \delta_j \delta_k \delta_l}{1920} \partial^4_{i,j,k,l} V \\
&+ \frac{\varepsilon^4}{6720} \partial^6_{i,i,j,j,k,k} V - \frac{\varepsilon^4}{120} \partial_i V \partial^3_{i,k,k} V - \frac{\varepsilon^4}{360} \partial^2_{i,j} V \partial^2_{i,j} V \\
&- \frac{\varepsilon^3 \delta_i \delta_j}{480} \partial_k V \partial^3_{k,i,j} V + \frac{\varepsilon^3 \delta_i \delta_j}{13440} \partial^6_{i,j,k,k,l,l} V - \frac{\varepsilon^3 \delta_i \delta_j}{1440} \partial^2_{i,k} V \partial^2_{k,j} V \\
&+ \left. \frac{\varepsilon^2 \delta_i \delta_j \delta_k \delta_l}{53760} \partial^6_{i,j,k,l,m,m} V + \frac{\varepsilon \delta_i \delta_j \delta_k \delta_l \delta_m \delta_n}{322560} \partial^6_{i,j,k,l,m,n} V \right\}
\end{aligned}
$$