Speeding up the Convergence of Path Integral Monte Carlo

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Overview

- Introduction to Path Integrals and Monte Carlo
  - General properties of path integrals
  - Formulation of the path integral formalism
  - Monte Carlo approach
  - Discretized effective actions
- Improving effective actions: Gaussian halving
  - Integral equation for the effective action
  - Euler's summation formula for path integrals
  - Expectation values ad estimators
  - Numerical results
- Improving effective actions: Recursive approach
  - Effective actions for many-body systems
  - Diagrammatic representation of effective actions
  - Recursive relations for estimators
  - Numerical results
- Concluding remarks

General properties of path integral formalism (1)

- Functional formalism in quantum theories allows:
  - easy treatment of symmetries (including gauge symmetries)
  - derivation of non-perturbative results (solitons, instantons)
  - establishing of connections between different theories, or different sectors of the same theory (bosonisation, duality)
  - quantization (including generalizations to systems with classical analogues)
- Rich cross-fertilization of ideas from high energy physics and condensed matter / statistical mechanics
- Applications to all fields of physics, chemistry, material science, even quantitative finance and economics

General properties of path integral formalism (2)

- In path integral formalism it is very easy to derive:
  - semiclassical expansion
  - perturbative expansion
  - various variational methods
- However, mathematical properties of path integrals are far from being completely understood
- Many important models and theories, or their interesting sectors, still require numerical treatment
  - Path Integral Monte Carlo (PIMC) is one of the most applicable methods
  - Very popular $\mathrm{M(RT)}^2$ (Metropolis) algorithm ensures optimal efficiency which, unfortunately, may be insufficient for some applications
  - The lack of the knowledge on path integrals directly translates into the inefficiency of our numerical algorithms

General properties of path integral formalism (3)

- Basic ideas on path integral formalism can be found in: P. A. M. Dirac, Physikalische Zeitschrift der Sowietunion **3**, 64 (1933) - Lagrangian formulation of quantum mechanics
- Richard Feynman developed the formalism we use today [R. P. Feynman, Rev. Mod. Phys. **20**, 367 (1948)]
- Contrary to the classical physics, where (usually) there is only one trajectory of the system for a given set of initial (boundary) conditions, in path integral formalism of the quantum theory we have to take into account all possible evolutions
- Each of possible trajectories contributes to the transition amplitude through the additive factor $\exp(\frac{i}{\hbar}S)$, where $S = \int L dt$ is the action corresponding to the given trajectory

Formulation of the path integral formalism (1)

- Path integrals originally introduced in quantum mechanics, where the amplitude for transition from some initial state $|\alpha\rangle$ to some final state $|\beta\rangle$ during a time interval T can be written as
$$A(\alpha, \beta; T) = \langle \beta | e^{\frac{i}{\hbar}\hat{H}T} | \alpha \rangle$$
- The same approach can be used in statistical physics, where partition function Z can be written in a similar fashion
- Path integrals in statistical physics / condensed matter are usually called imaginary-time path integrals, since they can be formally obtained from quantum-mechanical expressions through the formal replacement
$$\frac{i}{\hbar}T \to -\beta_t = \frac{1}{k_B T_t}$$
where T_t is the (thermodynamic) temperature of the system

Formulation of the path integral formalism (2)

- For technical reasons, usually we use imaginary time even in quantum mechanical problems ($\frac{i}{\hbar}T \to -\frac{1}{\hbar}T$)
- The standard derivation of the formalism starts from the identity

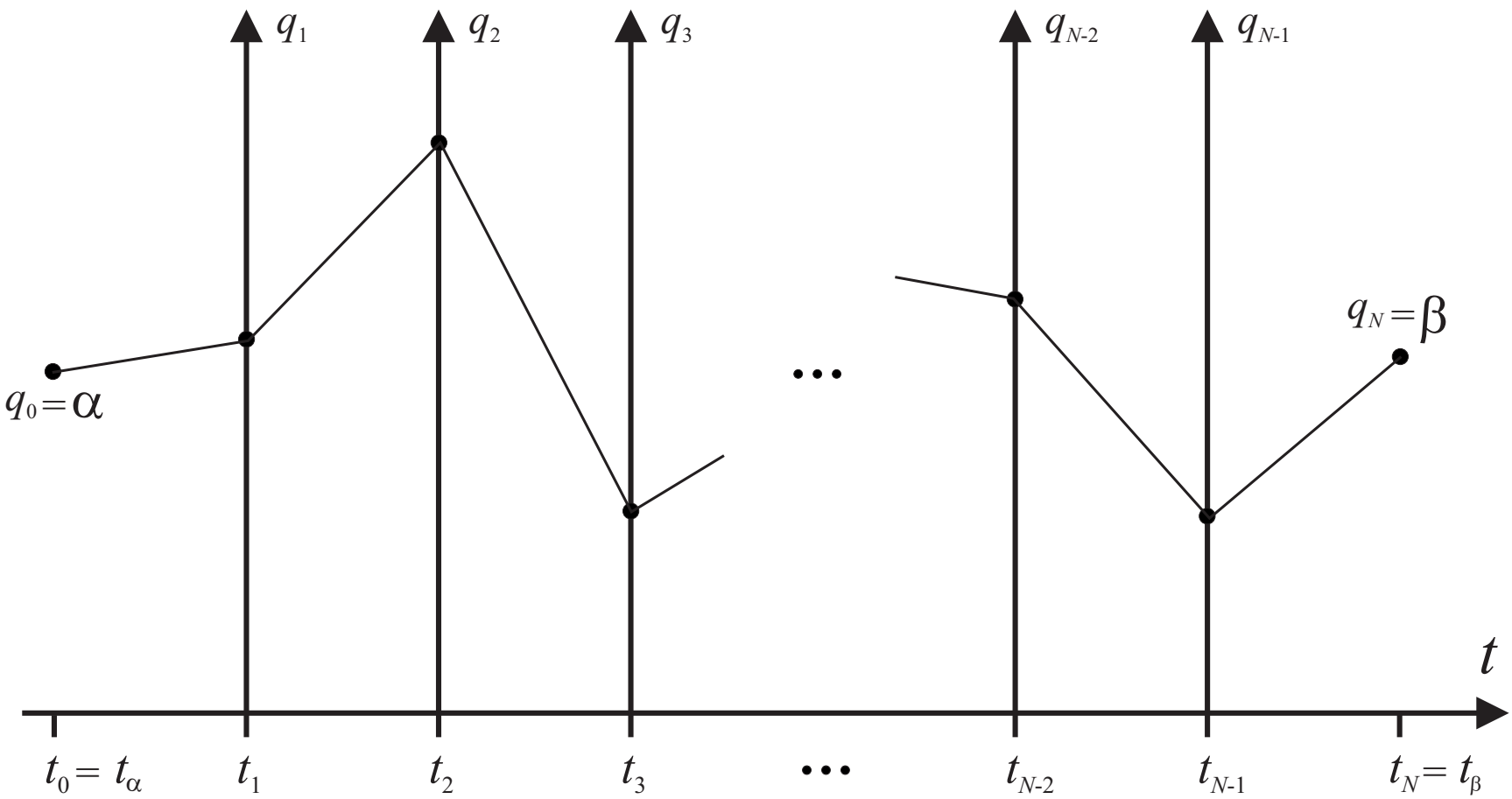
$$A(\alpha,\beta;T) = \int dq_1 \cdots dq_{N-1} A(\alpha,q_1;\epsilon)\cdots A(q_{N-1},\beta;\epsilon)\,,$$

which is obtained by dividing the evolution into N steps of the lenght $\epsilon = T/N$, and by insertion of $N-1$ resolutions of the identity operator between short-time evolution operators. This expression is exact.

- Next step is approximate calculation of short-time amplitudes up to the first order in ϵ, and we get ($\hbar = 1$)

$$A_N(\alpha,\beta;T) = \frac{1}{(2\pi\epsilon)^{N/2}} \int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

Illustration of the discretization of trajectories



Formulation of the path integral formalism (3)

- Continual amplitude $A(\alpha, \beta; T)$ is obtained in the limit $N \to \infty$ of the discretized amplitude $A_N(\alpha, \beta; T)$,

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

- Discretized amplitude A_N is expressed as a multiple integral of the function e^{-S_N}, where S_N is called discretized action
- For a theory defined by the Lagrangian $L = \frac{1}{2}\dot{q}^2 + V(q)$, (naive) discretized action is given by

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

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

Basics of Monte Carlo (1)

- Monte Carlo (MC) can be defined as a method for solving mathematical problems by using (pseudo-)random numbers
- If implemented properly, MC is guaranteed to converge to the exact value being calculated
- MC allows estimation of errors for calculated quantities, with clear statistical interpretation
- Calculation of integrals is the most common mathematical problem solved using MC method

Basics of Monte Carlo (2)

- MC calculates integrals using the following identity

$$I = \int_\alpha^\beta f(x)\,dx = \int_\alpha^\beta \frac{f(x)}{p(x)} p(x)\,dx = \left\langle \frac{f}{p} \right\rangle_p ,$$

where p is any given probability distribution function (PDF), satisfying

$$p \geq 0\,, \quad \int_\alpha^\beta p(x)\,dx = 1$$

- In the MC approach, integral I is calculated by estimating the above average value over some statistical sample

$$I = \left\langle \frac{f}{p} \right\rangle_p \approx I_{N_{MC}} = \frac{1}{N_{MC}} \sum_{i=1}^{N_{MC}} \frac{f(x_i)}{p(x_i)}$$

Basics of Monte Carlo (3)

- Numbers $\{x_i \,|\, i = 1, \ldots N_{MC}\}$ have to be generated from a chosen PDF $p(x)$
- Now the error of MC estimate for I can be defined as a standard deviation for the above average

$$\Delta I_{N_{MC}} = \sqrt{\frac{1}{N_{MC}} \left[\left\langle \left(\frac{f}{p} \right)^2 \right\rangle_p - \left\langle \frac{f}{p} \right\rangle_p^2 \right]}$$

- Central limit theorem guarantees that, for an ensemble of samples, each of the same size N_{MC}, the obtained estimates $I_{N_{MC}}$ would be distributed according to the Gaussian distribution, centered at I, with the standard deviation given by $\Delta I_{N_{MC}}$
- Statistical interpretation of errors now easy (σ-intervals)

Basics of Monte Carlo (4)

- MC error can be always reduced by increasing the size of the sample N_{MC}, since it scales as $1/\sqrt{N_{MC}}$
- In other methods (trapezoid rule, Simpson's formula, Bode's formula etc.), typically $\Delta I \sim \Delta x^k$, where Δx is the size of the integration step
- In d dimensions, time of calculation for such algorithms is $T_{CPU} \sim (1/\Delta x)^d \sim \Delta I^{-d/k}$, or, in other words,

$$\Delta I \sim T_{CPU}^{-k/d}$$

- In MC approach we have $T_{CPU} \sim N_{MC}$, so

$$\Delta I_{MC} \sim T_{CPU}^{-1/2}$$

- Now it is obvious why for high dimensional integrals MC dominates over all other methods, since k/d becomes much smaller than $1/2$ as d increases, whatever the value of k

Basics of Monte Carlo (5)

- Main challenges
  - optimal choice of PDF $p(x)$
  - efficient generation of random numbers from a chosen PDF
- It can be shown that the optimal PDF is actually just the normalized function f; BUT the normalization is exactly what we want to calculate, so this does not help
- However, this means that PDF should look as much as possible like the function f; usually we decompose the system into exactly solvable part and small perturbation, so exactly solvable part is ideal choice for p
- M(RT)^2 (Metropolis) algorithm is a general solution to the second challenge
  - problem of correlations must be carefully dealt with
  - efficiency must be tuned

Numerical approach to the calculation of path integrals (1)

- Path integral formalism is ideally suited for numerical approach, with physical quantities defined by discretized expressions as multiple integrals of the form

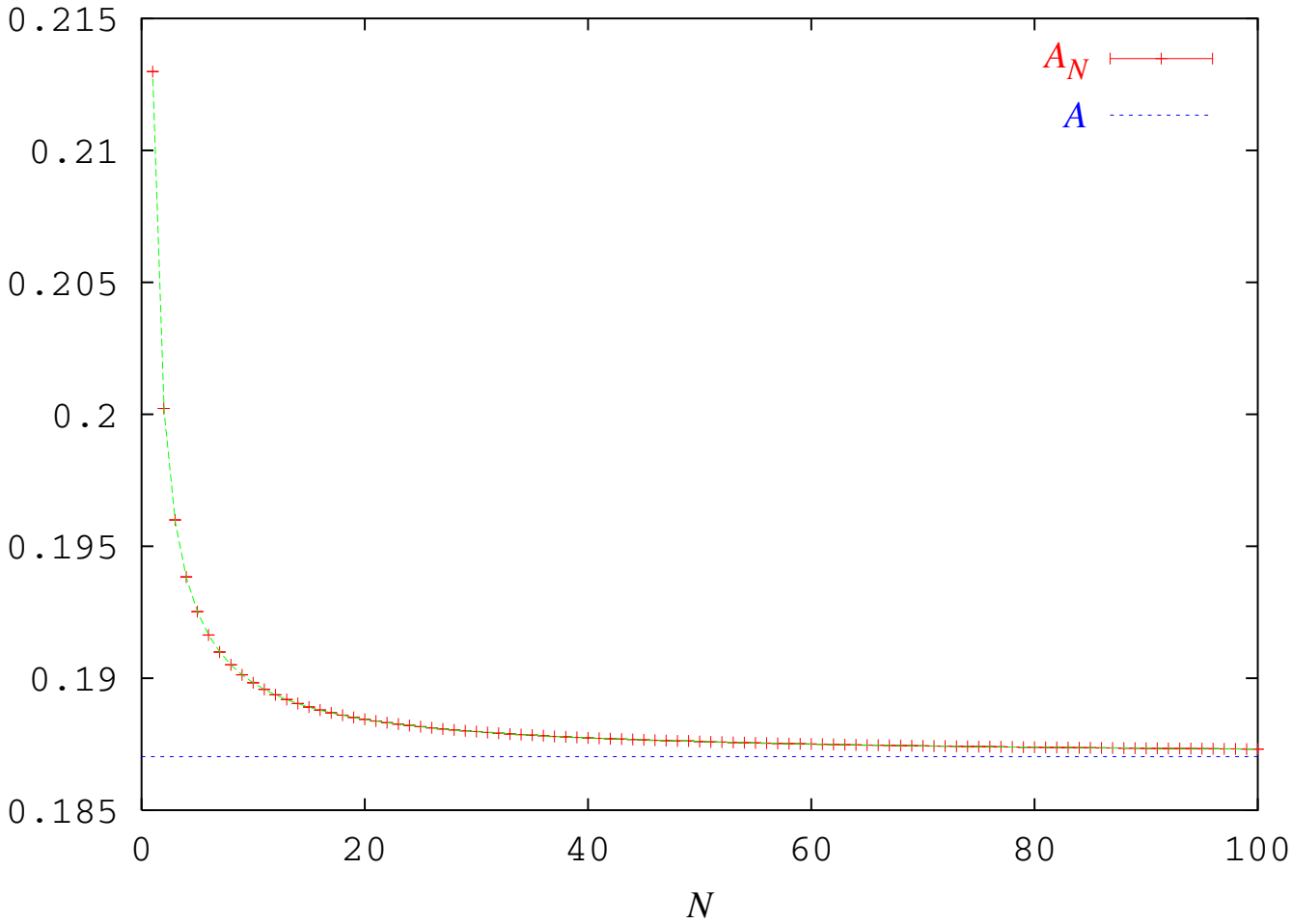
$$\int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

- Monte Carlo (MC) is the method of choice for calculation of such intergals
- However, although multiple integrals can be calculated very accurately and efficiently by MC, there still remains the difficult $N \to \infty$ limit
- This is what makes the outlined constructive definition of path integrals difficult to use in practical applications

Numerical approach to the calculation of path integrals (2)

- Discretization used in the definition of path integrals is not unique; in fact, the choice of the discretization is of *essential* importance
- Naive discretized action (in the mid-point prescription) gives discretized amplitudes converging to the continuum as slow as $1/N$
- Using special tricks we can get better convergence (e.g. left prescription gives $1/N^2$ convergence when partition function is calculated)
- However, this cannot be done in a systematic way, nor it can be used in all cases (e.g. left prescription cannot be used for systems with ordering ambiguities)

Typical $1/N$ convergence of naively discretized path integrals



Discretized effective actions (1)

- Discretized actions can be classified according to the speed of convergence of discretized path integrals to continuum values
- It is possible to introduce different discretized actions which contain some additional terms compared to the naive discretized action
- These additional terms must vanish in the $N \to \infty$ limit, and should not change continuum values of amplitudes, e.g.

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

- Additional terms in discretized actions are chosen so that they speed up the convergence of path integrals

Discretized effective actions (2)

- Improved discretized actions have been earlier constructed through several approaches, including
  - generalizations of the Trotter-Suzuki formula
  - improvements in the short-time propagation
  - expansion of the propagator by the number of derivatives
- This improved the convergence of general path integrals for partition functions from $1/N$ to $1/N^4$
- Li-Broughton effective potential

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

  in the left prescription gives $1/N^4$ convergence
- Derivation of the above expression from the generalized Trotter formula makes use of the cyclic property of the trace, hence $1/N^4$ convergence is obtained for partition functions only

Improving effective actions: Gaussian halving

- We present here an approach enabling a substantial speedup in the convergence of path integrals through studying the connection between different discretizations of the same theory
- Using this approach we have derived the integral equation connecting discretized effective actions of different coarseness and allows their systematic derivation. This leads to improved $1/N^p$ convergence of path integrals for sone-particle systems in $d = 1$
- The equivalent approaches enabling generalization of obtained results to many-body systems were also developed.

Ideal discretization (1)

- Ideal discretized action S^* is defined as the action giving exact continual amplitudes $A_N = A$ for any discretization N
- For massless free particle, naive discretized action is ideal
- From the completeness relation

$$A(\alpha, \beta; T) = \int dq_1 \cdots dq_{N-1}\, A(\alpha, q_1; \epsilon) \cdots A(q_{N-1}, \beta; \epsilon)\,,$$

it follows that the ideal discretized action S_n^* for the propagation time ϵ is given by

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

- Ideal discretized action S^* is the sum of terms S_n^*

Ideal discretization (2)

- In general case, the ideal discretized action can be written as

$$S_n^* = \frac{\delta_n^2}{2\epsilon} + \epsilon W_n \,,$$

where W is the effective potential which contains $V(\bar{q}_n)$ and corrections

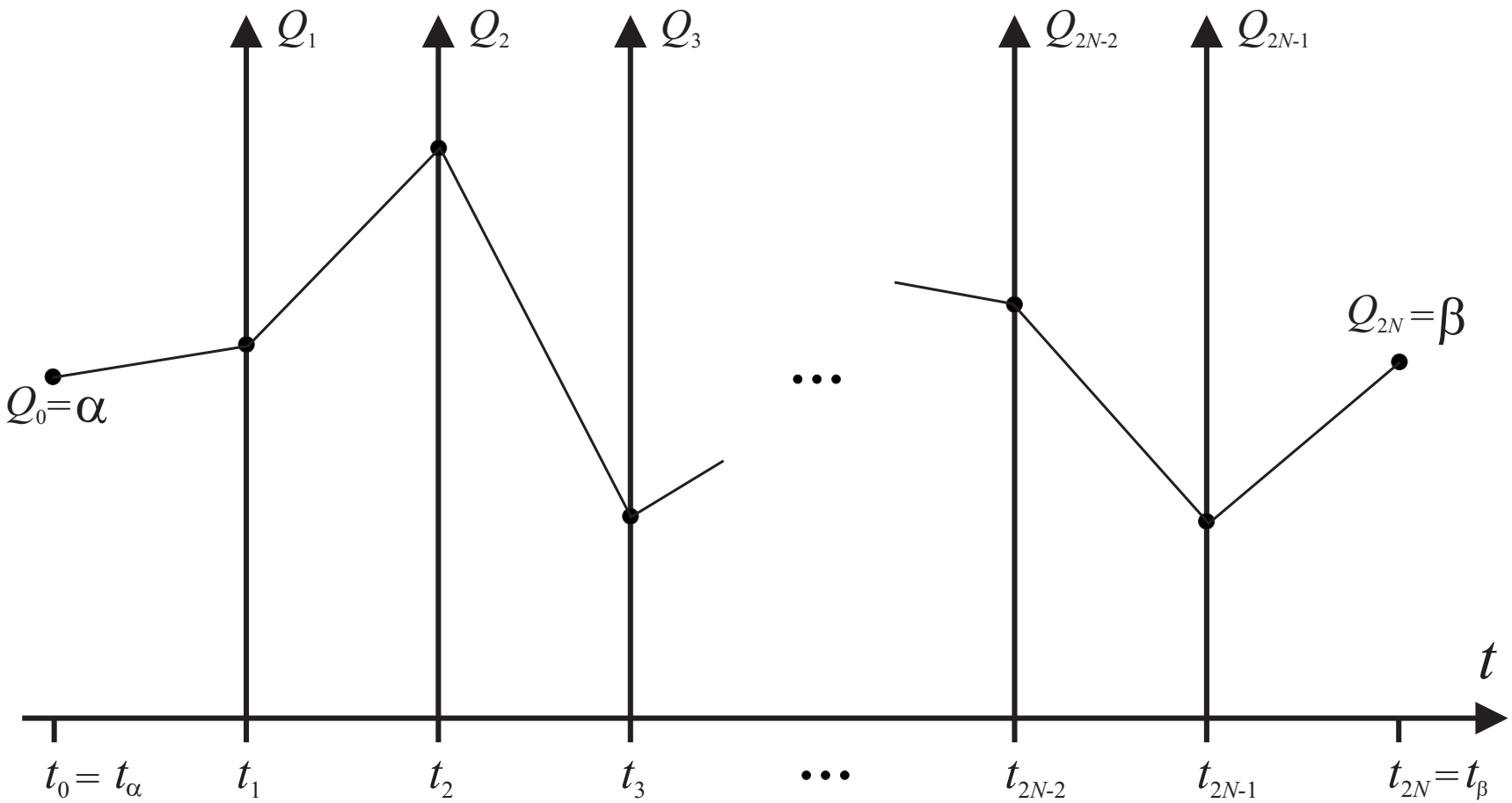
- From the definition of the ideal discretized action it follows

$$W_n = W(\delta_n, \bar{q}_n; \epsilon)$$

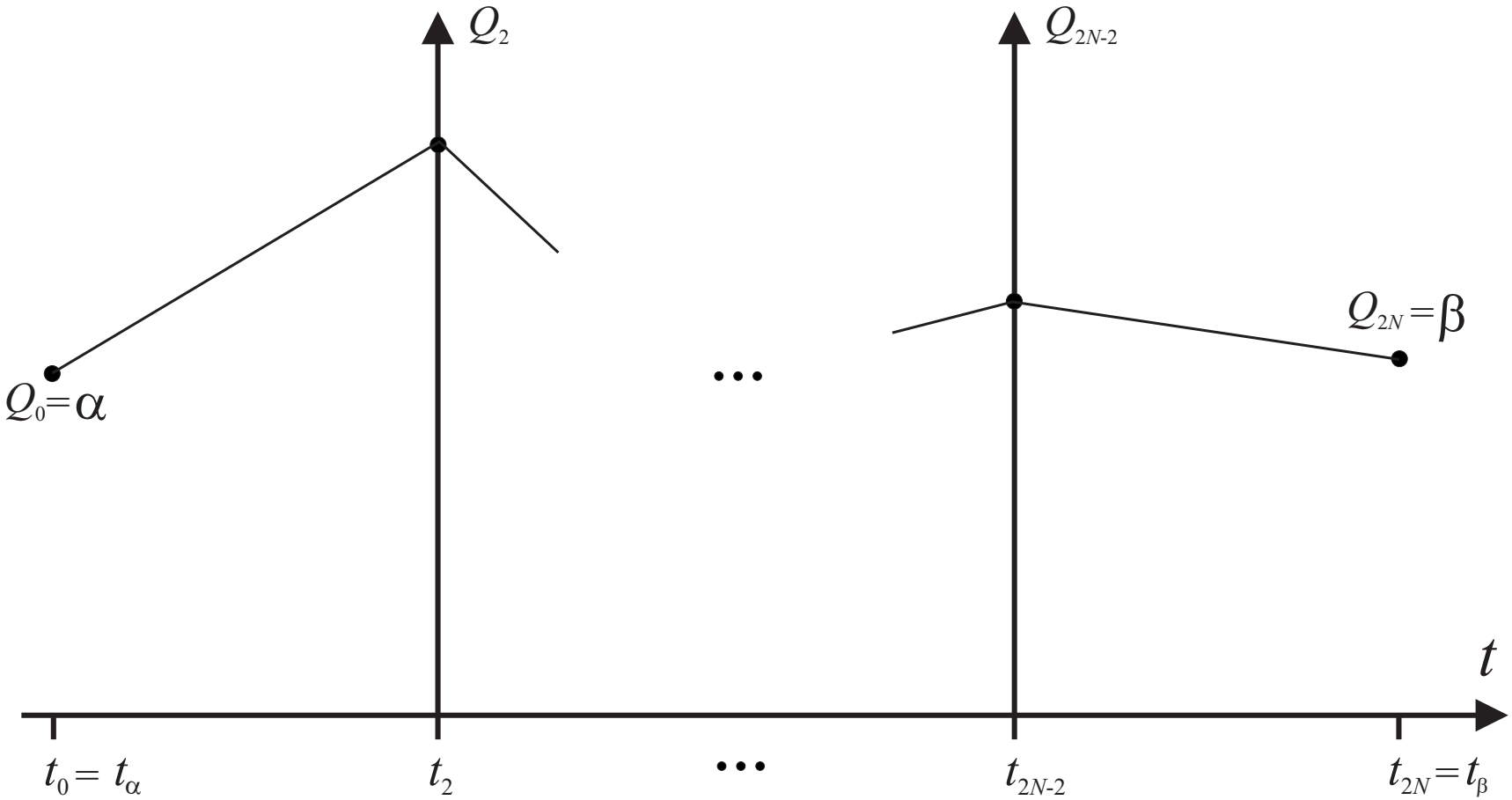
- From the reality of imaginary-time amplitudes, i.e. from the hermiticity of real-time amplitudes we obtain

$$W(\delta_n, \bar{q}_n; \epsilon) = W(-\delta_n, \bar{q}_n; \epsilon)$$

Relation between different discretizations (1)



Relation between different discretizations (2)



Relation between different discretizations (3)

- If we integrate out all odd-numbered coordinates, for a given discretized $2N$-action we get the effective N-action

$$e^{-\widetilde{S}_N} = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{N}{2}} \int dx_1 \cdots dx_N \; e^{-S_{2N}}$$

- However, if we use the ideal discretized action, then we get

$$e^{-S^*_N} = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{N}{2}} \int dx_1 \cdots dx_N \; e^{-S^*_{2N}}$$

Integral equation for the effective action

- From previous relation we obtain integral equation for the effective potential in the form

$$e^{-\epsilon_N W(\delta_n,\bar{q}_n;\epsilon_N)} = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dy\, e^{-\frac{2}{\epsilon_N}y^2} \times G\left(\bar{q}_n + y; q_n, q_{n+1}, \frac{\epsilon_N}{2}\right),$$

where function G is defined as

$$-\frac{2}{\epsilon_N} \ln G(x; q_n, q_{n+1}, \epsilon_N) = W\left(q_{n+1} - x, \frac{q_{n+1}+x}{2}; \epsilon_N\right) + W\left(x - q_n, \frac{x+q_n}{2}; \epsilon_N\right)$$

Euler's summation formula (1)

- For ordinary integrals Euler's summation formula reads

$$I[f] = \int_0^T f(t)dt = \sum_{n=1}^{N} f(t_n)\epsilon_N - \frac{\epsilon_N}{2}\sum_{n=1}^{N} f'(t_n)\epsilon_N + \frac{\epsilon_N^2}{6}\sum_{n=1}^{N} f''(t_n)\epsilon_N + \dots$$

- It allows the integral $I[f]$ to be written as a series in time step ϵ_N,

$$I[f] = I_N[f^{(p)}] + O(\epsilon_N^p)\,,$$

where $f^{(p)}$ is the corresponding initial part of the ideal discretized function f^*.

- Using the obtained integral equation for W, we will derive Euler's summation formula for path integrals

Euler's summation formula (2)

- When we expand function G in a series in the first argument around $\bar{q}_n$, we get the following equation for W

$$W(\delta_n, \bar{q}_n; \epsilon_N) = -\frac{1}{\epsilon_N} \ln \left[\sum_{k=0}^{\infty} \frac{G^{(2k)}\left(\bar{q}_n; q_n, q_{n+1}, \frac{\epsilon_N}{2}\right)}{(2k)!!} \left(\frac{\epsilon_N}{4}\right)^k \right]$$

- Further application of asymptotic expansion makes use of the expansion of the ideal effective potential in a series

$$W(\delta_n, \bar{q}_n; \epsilon_N) = \sum_{k=0}^{\infty} \delta_n^{2k} \, g_k(\bar{q}_n; \epsilon_N)$$

- From the equation for W we get a system of differential equations for functions g_k

Euler's summation formula (3)

- If we expand functions g_k into series in the time step ϵ

$$g_k(\bar{q}_n;\epsilon_N) = \sum_{m=0}^{p-k-1} \epsilon_N^m \, g_{km}(\bar{q}_n) \qquad (k = 0, \ldots, p-1)$$

  we obtain a system of equations that is easily decoupled and can be solved in functions g_k
- Note that in the above expression the sum is limited according to the consistency condition which follows from the diffusion relation $\delta^2 \propto \epsilon$
- Boundary condition for the above system is $g_{00} = V$, obtained from limits $\delta_n^2 \to 0$ and $\epsilon_N \to 0$, in which W reduces to

$$W(0, \bar{q}_n; 0) = V(\bar{q}_n)$$

Euler's summation formula (4)

- To level $p = 3$ we get

$$g_0(\bar{q}_n;\epsilon_N) = V(\bar{q}_n) + \epsilon_N \frac{V''(\bar{q}_n)}{12} + \epsilon_N^2 \left[-\frac{V'(\bar{q}_n)^2}{24} + \frac{V^{(4)}(\bar{q}_n)}{240} \right]$$

$$g_1(\bar{q}_n;\epsilon_N) = \frac{V''(\bar{q}_n)}{24} + \epsilon_N \frac{V^{(4)}(\bar{q}_n)}{480}$$

$$g_2(\bar{q}_n;\epsilon_N) = \frac{V^{(4)}(\bar{q}_n)}{1920}$$

- Ideal effective action on the convergence level p is given as

$$S_N^{(p)} = \sum_{n=0}^{N-1} \left[\frac{\delta_n^2}{2\epsilon_N} + \epsilon_N \sum_{k=0}^{p-1} \delta_n^{2k}\, g_k(\bar{q}_n;\epsilon_N) \right]$$

- This ensures the improved convergence
$A_N^{(p)}(\alpha,\beta;T) = A(\alpha,\beta;T) + O(\epsilon_N^p)$

Expectation values and estimators

- To obtain expectation values of physical quantities in the path integral formalism, we calculate average values of estimators - functions of discretized coordinates q_n representing physical quantities. The average is taken over $\exp(-S_N)$.
- Naive expressions for estimators must be also improved, consistently to improvements made to the discretized action
- For instance, on the level $p = 2$ virial estimator for the energy is given by

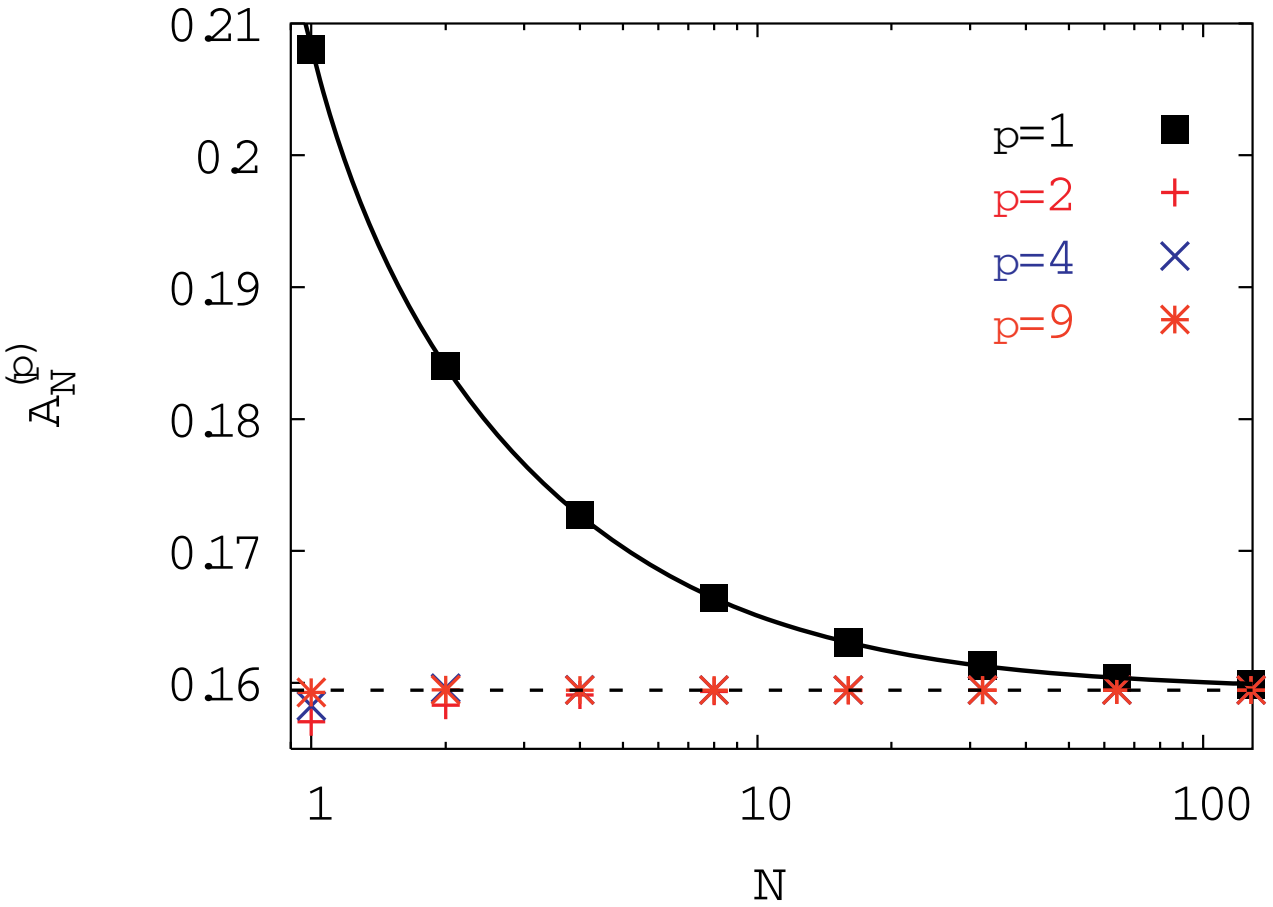
$$E_V^{(p=2)} = \frac{1}{N} \sum_{n=0}^{N-1} \left[V_n + \frac{\bar{q}_n}{2} V_n' + \frac{\epsilon_N}{6} V_n'' + \frac{\delta_n^2}{12} V_n'' + \frac{\bar{q}_n \epsilon_N}{24} V_n''' + \frac{\bar{q}_n \delta_n^2}{48} V_n''' \right]$$

Numerical results (1)

- To verify the derived speedup in the convergence of path integrals, we perform a series of PIMC simulations for the amplitudes of anharmonic oscillator $V_1(q) = \frac{1}{2}q^2 + \frac{\lambda}{4!}q^4$ and modified Pöschl-Teller potential $V_2(q) = -\frac{1}{2}\,\frac{a^2 b(b-1)}{\cosh^2 aq}$
- Numerical simulations were done using our SPEEDUP PIMC code for various values of parameters λ, a, b, as well as for various boundary conditions
- Continuum amplitudes $A^{(p)}$ are estimated by fitting of discretized values of amplitudes $A_N^{(p)}$ to polynomials in $1/N$

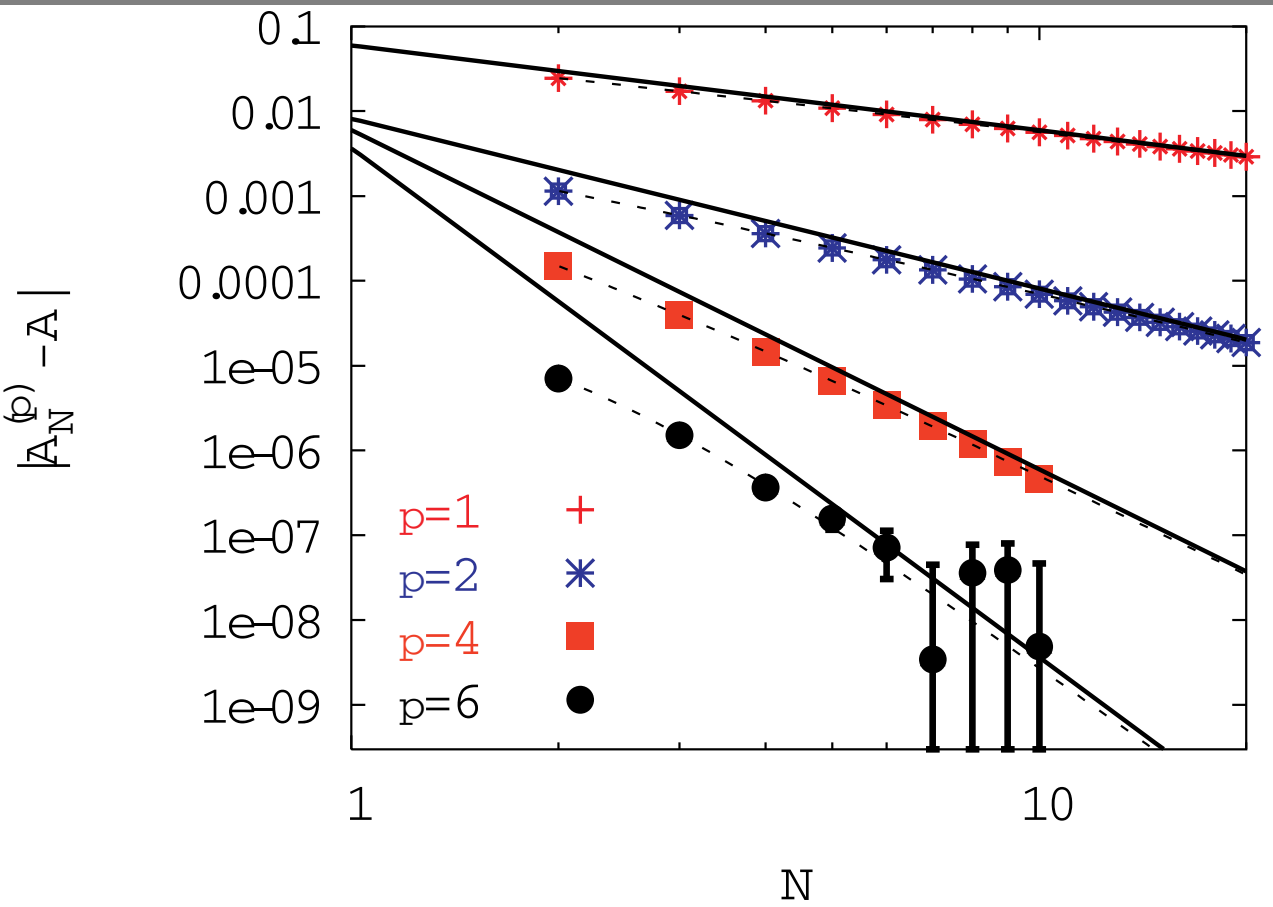
$$A_N^{(p)} = A^{(p)} + \frac{B^{(p)}}{N^p} + \frac{C^{(p)}}{N^{p+1}} + \dots$$

PIMC: Convergence to the continuum



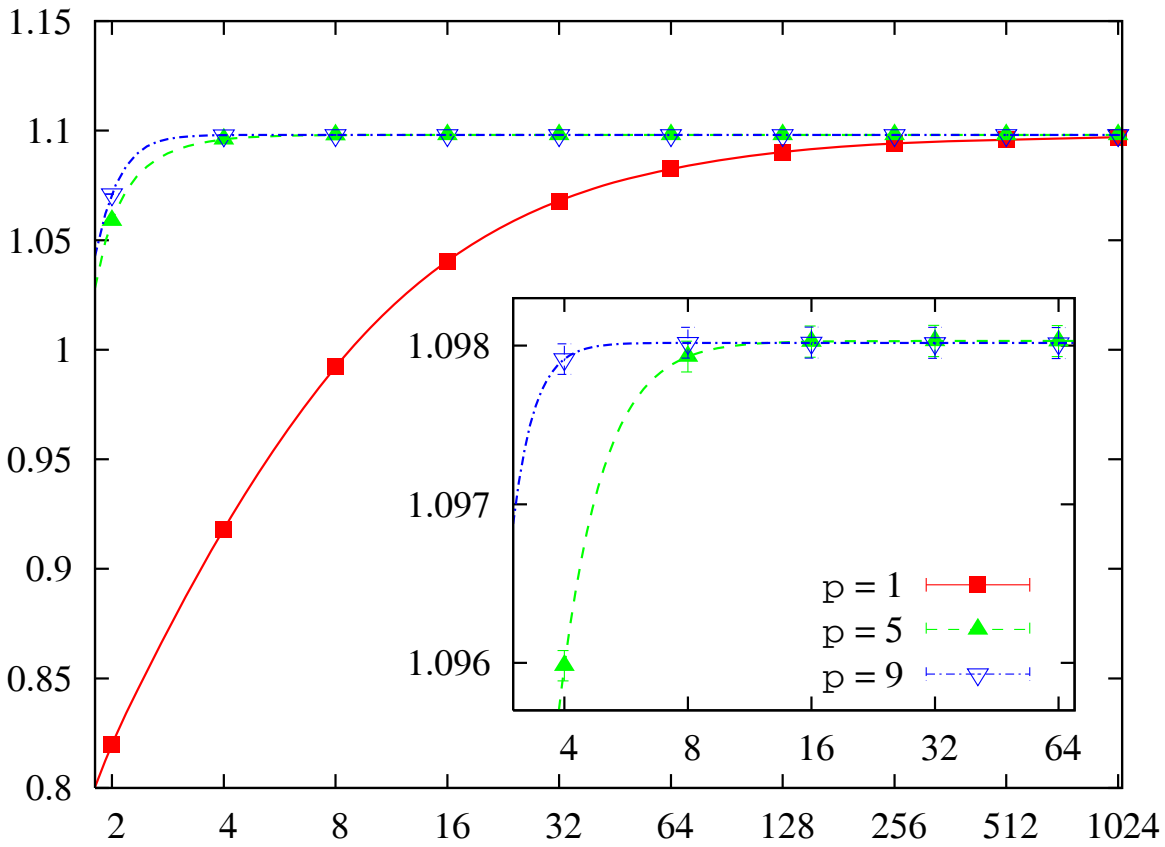
Amplitude for the oscillator V_1 with large anharmonicity $\lambda = 10$, $T = 1$, $N_{MC} = 9.2 \cdot 10^7$ for $\alpha = 0$, $\beta = 1$.

PIMC: Deviations from the continuum



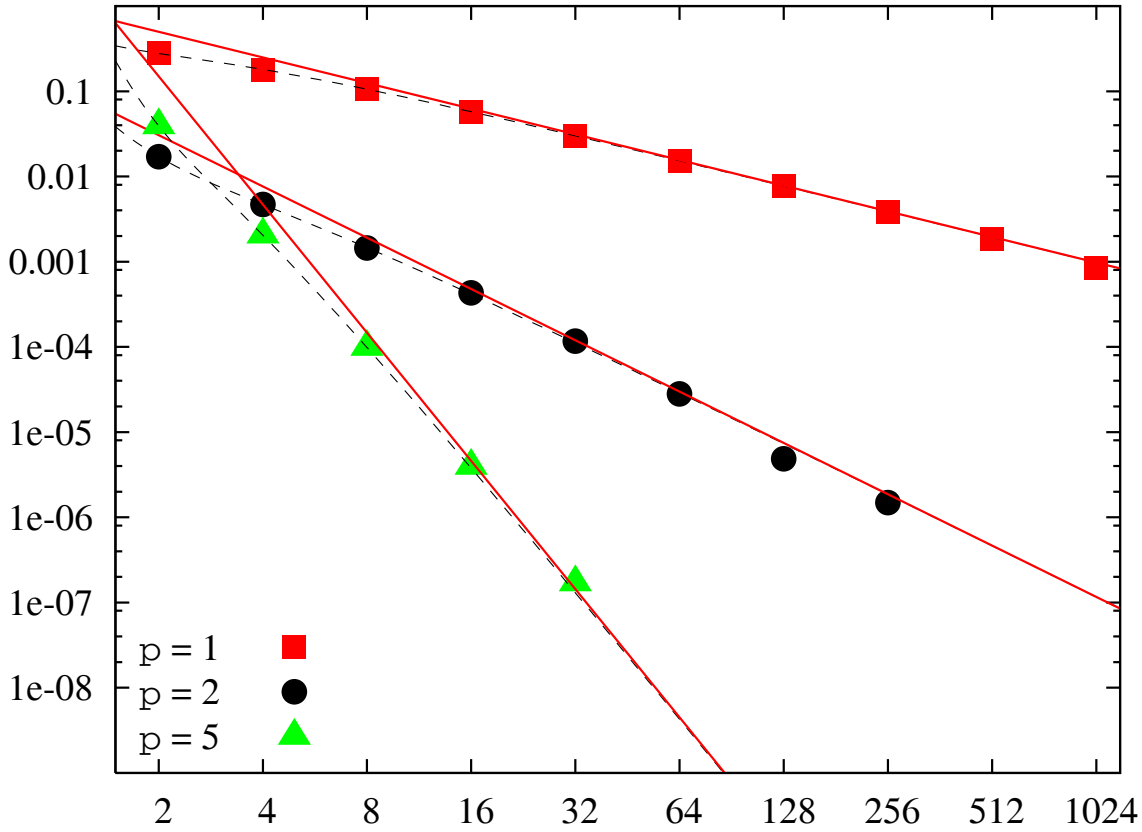
Deviations from the continuum amplitudes for the oscillator V_1 with large anharmonicity $\lambda = 10$, $T = 1$, $N_{MC} = 9.2 \cdot 10^9$ $(p = 1, 2)$, $9.2 \cdot 10^{10}$ $(p = 4)$, $3.68 \cdot 10^{11}$ $(p = 6)$ for $\alpha = 0$, $\beta = 1$.

PIMC: Convergence of expectation values



Convergence of discretized thermal expectation values to continuum as a function of N for V_1 with $\lambda = 24$, $T = 1$, $N_{MC} = 10^9$.

PIMC: Deviations from the continuum



Deviations of discretized thermal expectation values from the continuum as a function of N for V_1 with $\lambda = 24$, $T = 1$, $N_{MC} = 10^9$.

Numerical results (2)

- From the partition function it is possible to find energy spectra of the system if we use $Z(T) = \sum_{n=0}^{\infty} d_n e^{-TE_n}$
- Free energy of the system, $F(T) = -\frac{1}{T} \ln Z(T)$, tends to the ground-state energy E_0 for large propagation time T
- If we intoduce auxiliary functions

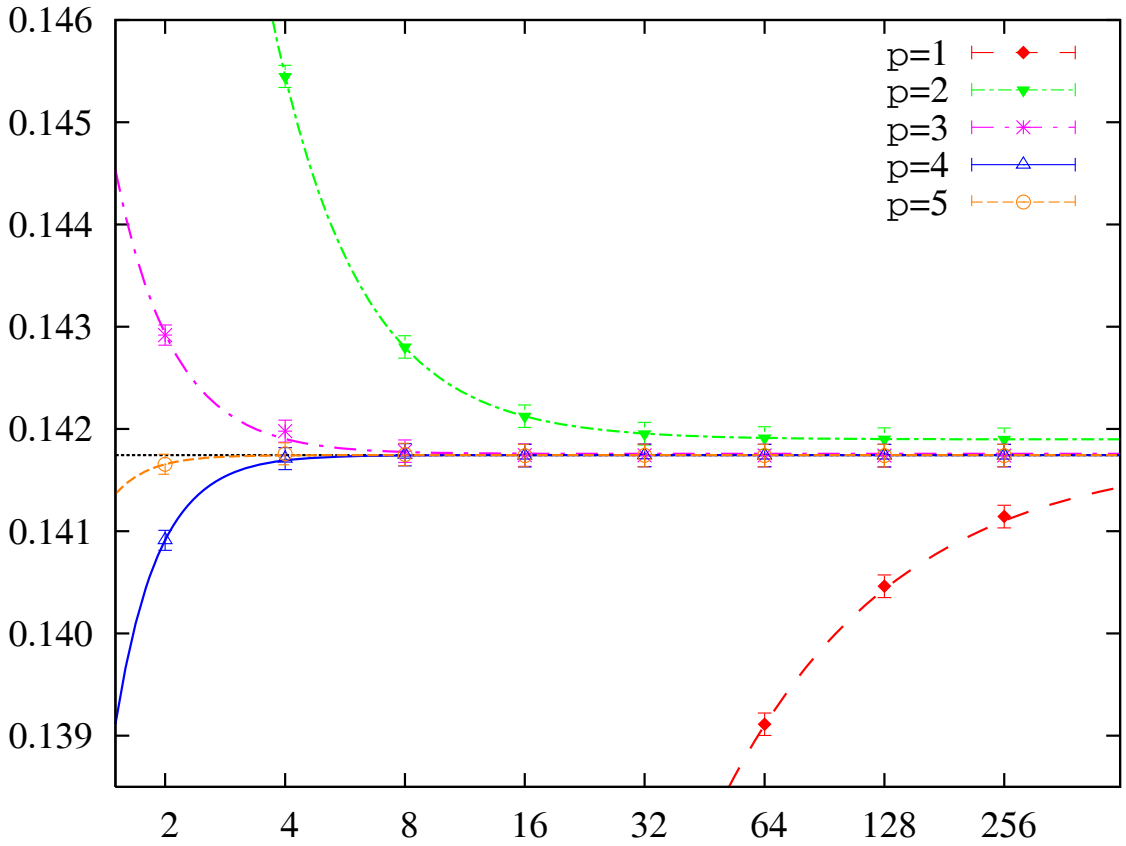
$$F^{(n)}(T) = -\frac{1}{T} \ln \frac{Z(T) - \sum_{i=0}^{n-1} d_i \; e^{-TE_i}}{d_n}$$

they can be fitted for large propagation time to

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

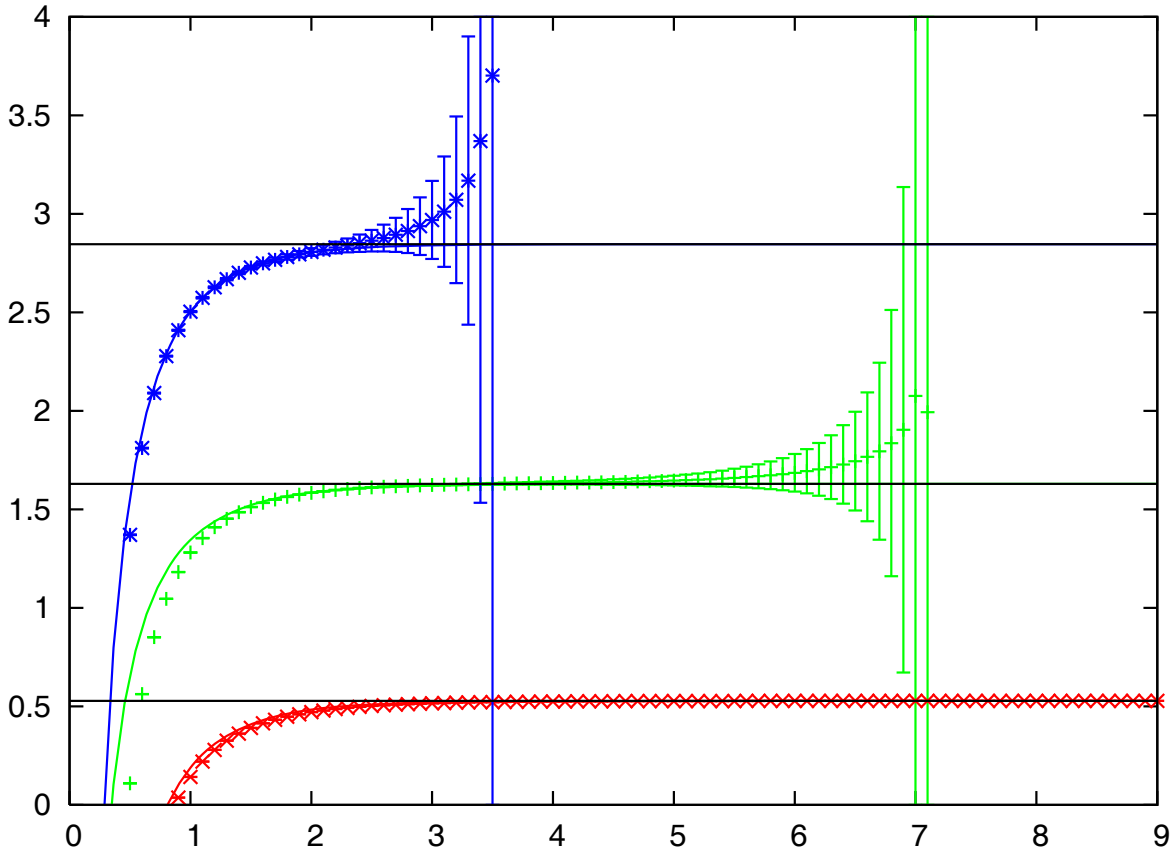
and they tend to corresponding energy levels E_n

PIMC: Convergence of the free energy



Convergence of the discretized free energy to continuum as a function of N for V_1 with $\lambda = 1$, $T = 1$, $N_{MC} = 10^7$.

PIMC: Calculation of energy spectra



Time dependence of the free energy and auxiliary functions $f^{(1)}$ and $f^{(2)}$ for V_1 with $\lambda = 1$, $N_{MC} = 10^7$ when $p = 9$ effective action and $N = 256$ is used.

PIMC: Lower energy levels of the anharmonic oscillator

λ	E_0	E_1	E_2	E_3
0	0.49993(2)	1.502(2)	2.48(6)	3.6(5)
0.1	0.50301(2)	1.516(1)	2.54(5)	3.5(2)
1	0.52765(2)	1.6295(8)	2.85(2)	3.98(7)
10	0.67335(2)	2.230(1)	4.12(2)	
100	1.16247(4)	4.058(6)		
1000	2.3578(2)			

Lower energy levels of a quartic anharmonic oscillator V_1, calculated with $N_{MC} = 10^7$, $p = 9$ effective action and $N = 256$.

PIMC: Lower energy levels of the modified Pöschl-Teller potential

a	b	E_0	E_0^{exact}	E_1	E_1^{exact}
0.25	5.5	-0.6329(2)	-0.63281	-0.3819(7)	-0.38281
0.25	15.5	-6.5704(6)	-6.57031	-5.694(9)	-5.69531
0.5	5.5	-2.5313(3)	-2.53125	-1.530(3)	-1.53125
0.5	15.5	-26.281(1)	-26.2813	-22.80(3)	-22.7813

a	b	E_2	E_2^{exact}	E_3	E_3^{exact}
0.25	5.5	-0.18(2)	-0.19531	-0.09(3)	-0.07031
0.25	15.5	-4.92(2)	-4.88281	-3.8(4)	-4.13281
0.5	5.5	-0.80(2)	-0.78125	-0.31(6)	-0.28125
0.5	15.5	-19.6(5)	-19.5313	-16.9(9)	-16.5313

Lower energy levels of the modified Pöschl-Teller potential, calculated with $N = 256$, $p = 9$, $N_{MC} = 10^7$.

Improving effective actions: Recursive approach

- Gaussian halving is developed and applicable for single-particle one-dimensional systems only
- For many-body systems in arbitrary dimensions we have developed two equivalent approaches
- First is based on direct calculation of ϵ-expansion of short-time amplitudes, expressed as expectation values of the corresponding free theory
- Here we present second approach, based on solving recursive relations for the discretized action. These relations are derived from Schrödinger's equation for amplitudes.
- This approach is by far the most efficient, both for many-body and one-body systems.

Schrödinger's equation

- We start from Schrödinger's equation for the amplitude $A(q, q'; \epsilon)$ for a system of M non-relativistic particles in d spatial dimensions

$$\left[\frac{\partial}{\partial \epsilon} - \frac{1}{2}\sum_{i=1}^{M} \triangle_i + V(q)\right] A(q, q'; \epsilon) = 0$$

$$\left[\frac{\partial}{\partial \epsilon} - \frac{1}{2}\sum_{i=1}^{M} \triangle'_i + V(q')\right] A(q, q'; \epsilon) = 0$$

- Here $\triangle_i$ and $\triangle'_i$ are d-dimensional Laplacians over initial and final coordinates of the particle i, while q and q' are $d \times M$ dimensional vectors representing positions of all particles at the initial and final time.

Equation for the ideal effective potential

- If we express short-time amplitude $A(q, q'; \epsilon)$ by the ideal discretized effective potential W

$$A(q, q'; \epsilon) = \frac{1}{(2\pi\epsilon)^{dM/2}} \exp\left[-\frac{\delta^2}{2\epsilon} - \epsilon W\right]$$

we obtain equation for the effective potential in terms of $x = \delta/2$, $\bar{x} = (q + q')/2$, $V_\pm = V(\bar{x} \pm x)$

$$W + x \cdot \partial W + \epsilon \frac{\partial W}{\partial \epsilon} - \frac{1}{8}\epsilon \bar{\partial}^2 W - \frac{1}{8}\epsilon \partial^2 W + \frac{1}{8}\epsilon^2 (\bar{\partial} W)^2 + \\ + \frac{1}{8}\epsilon^2 (\partial W)^2 = \frac{V_+ + V_-}{2}$$

Recursive relations (1)

- As before, the effective potential is given as a series

$$W(x,\bar{x};\epsilon) = \sum_{m=0}^{\infty}\sum_{k=0}^{m} W_{m,k}(x,\bar{x})\,\epsilon^{m-k}$$

where

$$W_{m,k}(x,\bar{x}) = x_{i_1}x_{i_2}\cdots x_{i_{2k}}c_{m,k}^{i_1,\ldots,i_{2k}}(\bar{x})$$

- Coefficients $W_{m,k}$ are obtained from recursive relations

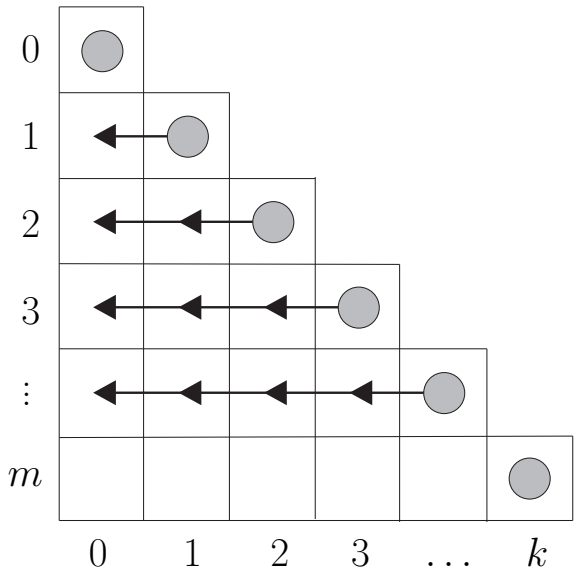
$$\begin{aligned}8\,(m+k+1)\,W_{m,k} = {} & \bar{\partial}^2 W_{m-1,k} + \partial^2 W_{m,k+1} - \\ & - \sum_{l=0}^{m-2}\sum_{r}(\bar{\partial}W_{l,r})\cdot(\bar{\partial}W_{m-l-2,k-r}) - \\ & - \sum_{l=1}^{m-2}\sum_{r}(\partial W_{l,r})\cdot(\partial W_{m-l-1,k-r+1})\end{aligned}$$

Recursive relations (2)

- Diagonal coefficients are easily obtained from recursive relations

$$W_{m,m} = \frac{1}{(2m+1)!}(x \cdot \bar{\partial})^{2m} V$$

- Off-diagonal coefficients are obtained by applying recursive relations in the following order



Effective actions for many-body systems

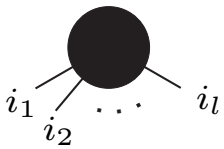
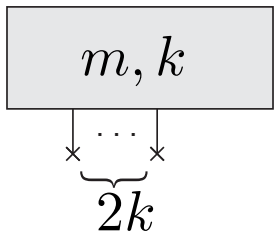
- To level $p = 3$, effective action is given by

$$
\begin{aligned}
W_{0,0} &= V \\
W_{1,1} &= \frac{1}{6}\,(x\cdot\bar{\partial})^2 V \\
W_{1,0} &= \frac{1}{12}\bar{\partial}^2 V \\
W_{2,2} &= \frac{1}{120}\,(x\cdot\bar{\partial})^4 V \\
W_{2,1} &= \frac{1}{120}(x\cdot\bar{\partial})^2\,\bar{\partial}^2 V \\
W_{2,0} &= \frac{1}{240}\,\bar{\partial}^4 V - \frac{1}{24}\,(\bar{\partial}V)\cdot(\bar{\partial}V)
\end{aligned}
$$

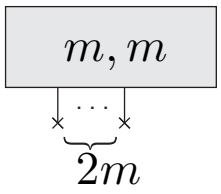
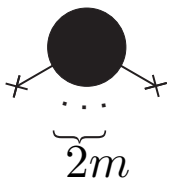
Diagrammatic form of effective actions (1)

- Derived recursive relations can be represented in a diagrammatic form if we introduce

$\delta_{ij} =$  , $x_i =$ 

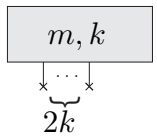
$\bar{\partial}_{i_1}\bar{\partial}_{i_2}\cdots\bar{\partial}_{i_l}V =$  , $W_{m,k} =$  .

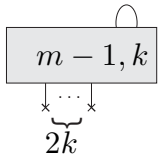
- Diagrammatic form of diagonal coefficients

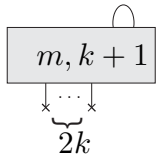
$W_{m,m} =$  $= \frac{1}{(2m+1)!}$  .

Diagrammatic form of effective actions (2)

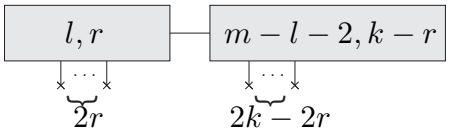
- Diagrammatic form of recursive relations

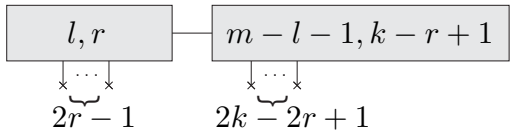
$8(m+k+1)$ 

$=$ 

$+(2k+2)(2k+1)$ 

$-$

$-\sum_{l=0}^{m-2}\sum_{r}$ 

$-\sum_{l=1}^{m-2}\sum_{r} 2r(2k-2r+2)$ 

.

- Solutions to level $p = 3$

$W_{0,0} =$  ,

$W_{1,1} = \frac{1}{6}$  $= \frac{1}{6}(1)^2$,

$W_{1,0} = \frac{1}{12}$  $= \frac{1}{12}(11)$,

$W_{2,2} = \frac{1}{120}$  $= \frac{1}{120}(1)^4$,

$W_{2,1} = \frac{1}{120}$  $= \frac{1}{120}(1)^2(11)$,

$W_{2,0} = \frac{1}{240}$  $-\frac{1}{24}$ 

$= \frac{1}{240}(11)^2 - \frac{1}{24}(12)$,

$W_{3,3} = \frac{1}{5040}$  $= \frac{1}{5040}(1)^6$,

$W_{3,2} = \frac{1}{3360}$  $= \frac{1}{3360}(1)^4(11)$,

Recursive relations for estimators

- For many-body estimators for expectation values we also derive recursive relations using the recursive relations for the effective action
- If we write action and virial estimator for the energy in the form

$$S_N^* = S_N^{(p=1)} + \sum_{p=2}^{\infty} \sum_{n=0}^{N-1} \sigma_n^{(p)} , \qquad E_V^* = E_V^{(p=1)} + \sum_{p=2}^{\infty} \sum_{n=0}^{N-1} e_{V,n}^{(p)}$$

then the corresponding recursive relation to level p reads

$$e_{V,n}^{(p)} = \frac{1}{T} \left(p + \frac{1}{2} \bar{q}_{n,i} \, \partial_i \right) \sigma_n^{(p)}$$

Numerical results (1)

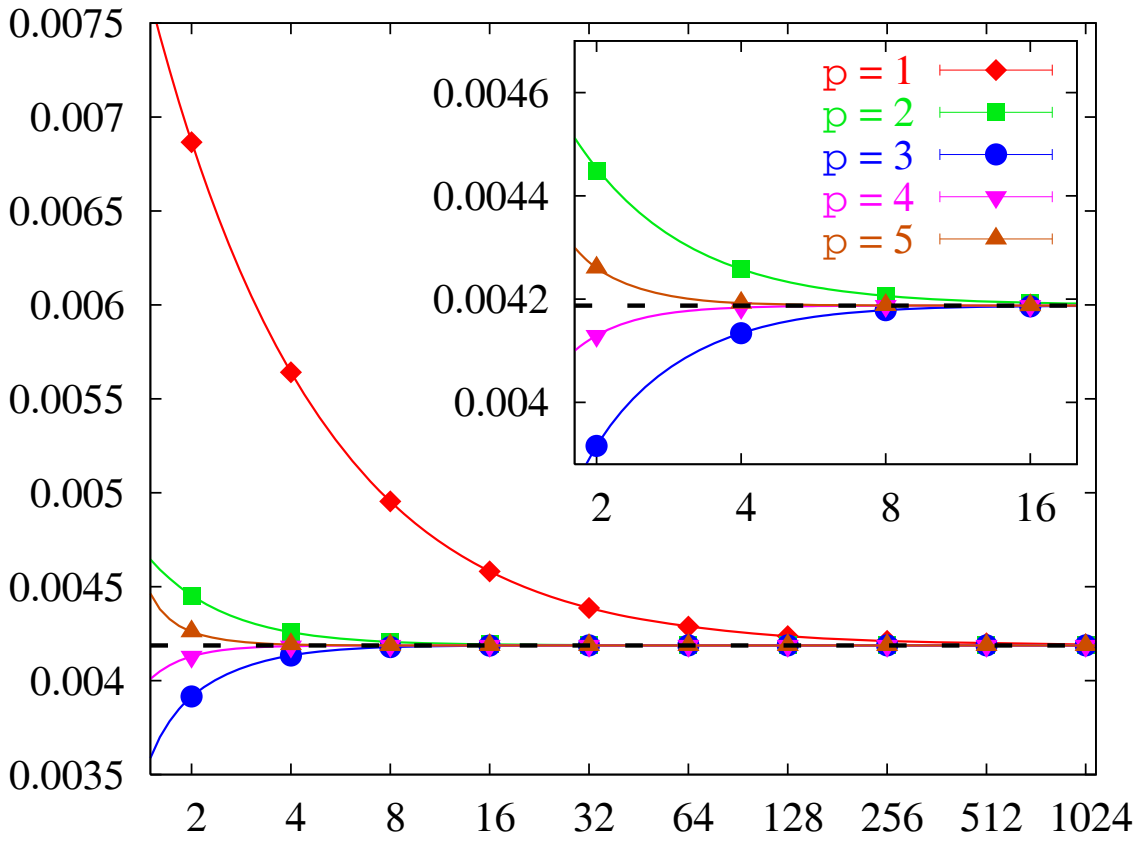
- To verify the derived speedup in the convergence of path integrals, we perform a series of PIMC simulations for amplitudes of a two-particle system in two dimensions in the potential

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

- Numerical simulations are done using our SPEEDUP PIMC code for various values of parameters g_1 and g_2, as well as for various boundary conditions
- Continuum amplitudes $A^{(p)}$ are estimated by fitting of discretized values of amplitudes $A_N^{(p)}$ to polynomials in $1/N$

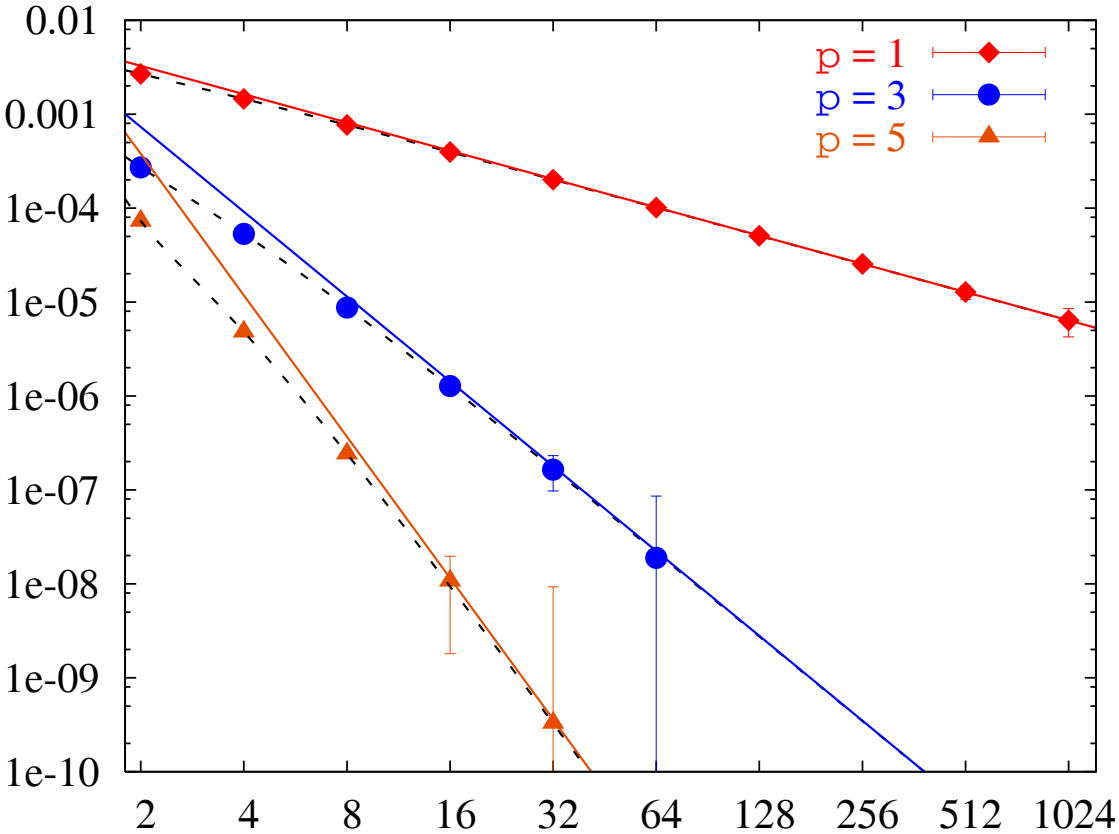
$$A_N^{(p)} = A^{(p)} + \frac{B^{(p)}}{N^p} + \frac{C^{(p)}}{N^{p+1}} + \dots$$

PIMC: Convergence to the continuum



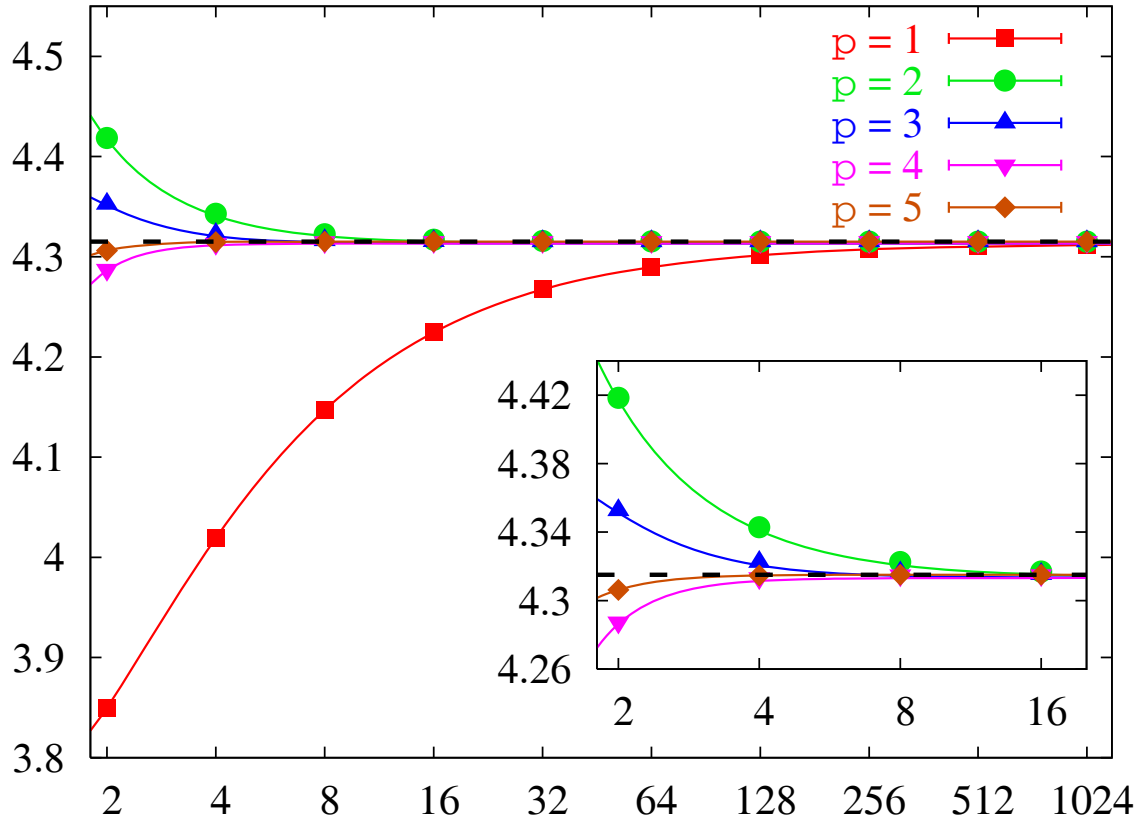
Amplitude for a quartic anharmonic oscillator with large anharmonicity $g_1 = 10$, $g_2 = 0$, $T = 1$, $N_{MC} = 10^6$ for $\alpha = (0, 0; 0.2, 0.5)$, $\beta = (1, 1; 0.3, 0.6)$.

PIMC: Deviations from the continuum



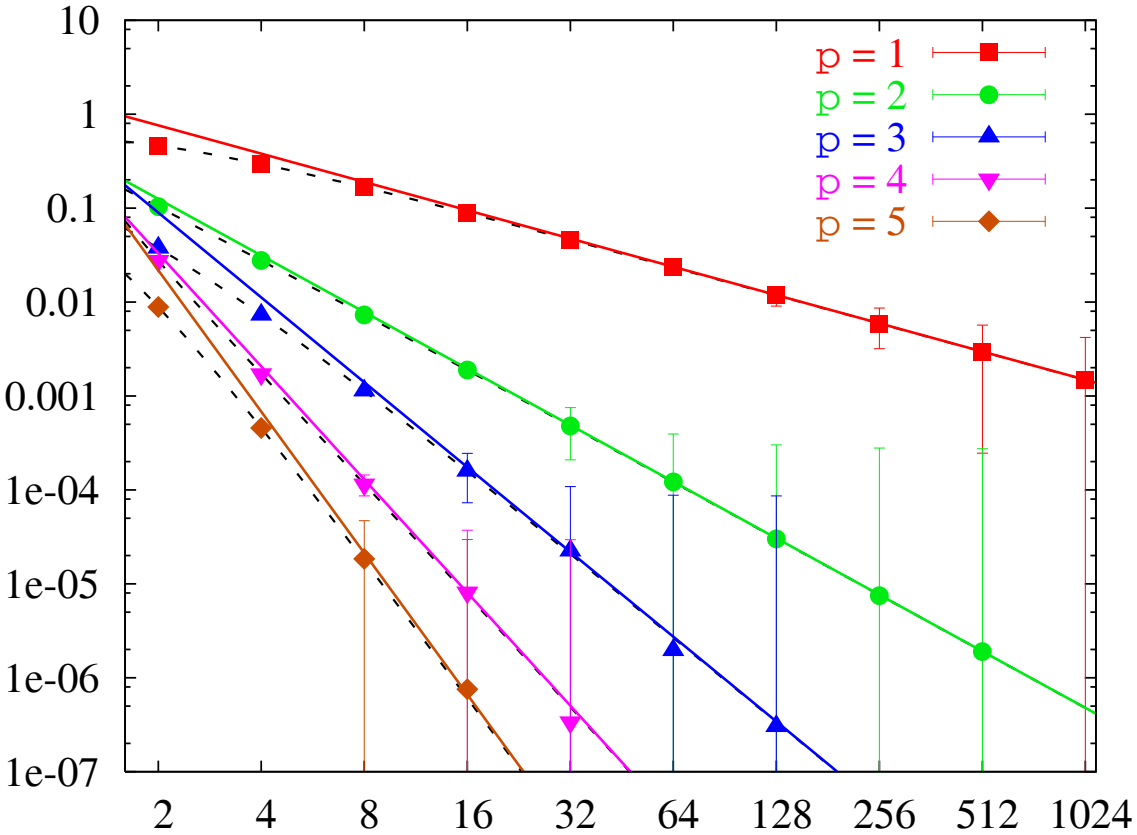
Deviations of amplitudes from the continuum for a quartic anharmonic oscillator with large anharmonicity $g_1 = 10$, $g_2 = 0$, $T = 1$, $N_{MC} = 10^6$ $(p = 1)$, 10^7 $(p = 2)$, 10^9 $(p = 3)$, 10^{10} $(p = 4)$, for $\alpha = (0, 0; 0.2, 0.5)$, $\beta = (1, 1; 0.3, 0.6)$.

PIMC: Convergence of expectation values



Convergence of discretized thermal expectation values of energy to continuum as a function of N for a system of two particles in two dimensions in a quartic potential with $g_1 = 1$, $g_2 = 1/9$, $T = 1$, $N_{MC} = 10^7$.

PIMC: Deviations from expectation values



Deviations from continuum expectation values of energy as a function of N for a system of two particles in two dimensions in a quartic potential with $g_1 = 1$, $g_2 = 1/9$, $T = 1$, $N_{MC} = 10^7 (p = 1)$, $10^9 (p = 2)$, $10^{10} (p = 3)$, $10^{11} (p = 4, 5)$.

Numerical results (2)

- From the partition function it is possible to find energy spectra of the system if we use $Z(T) = \sum_{n=0}^{\infty} d_n e^{-TE_n}$
- Free energy of the system, $F(T) = -\frac{1}{T} \ln Z(T)$, tends to the ground-state energy E_0 for large propagation time T
- If we intoduce auxiliary functions

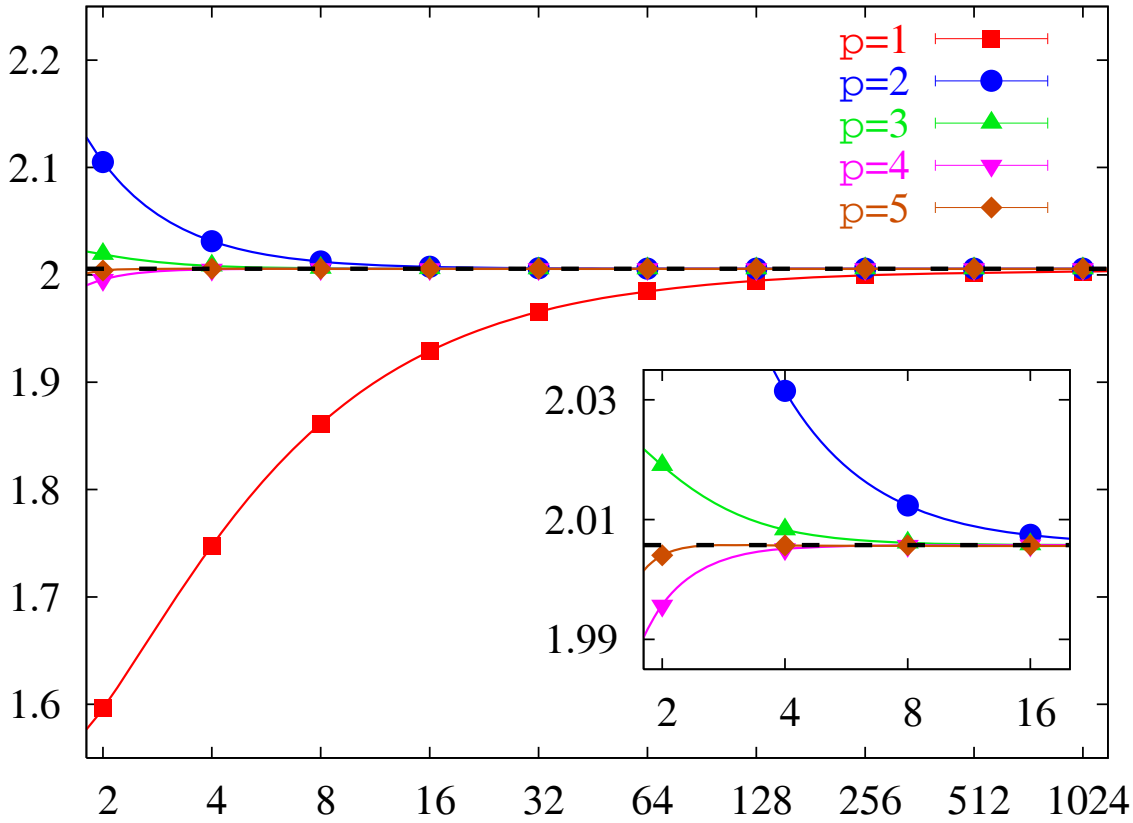
$$F^{(n)}(T) = -\frac{1}{T} \ln \frac{Z(T) - \sum_{i=0}^{n-1} d_i \; e^{-TE_i}}{d_n}$$

they can be fitted for large propagation time to

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

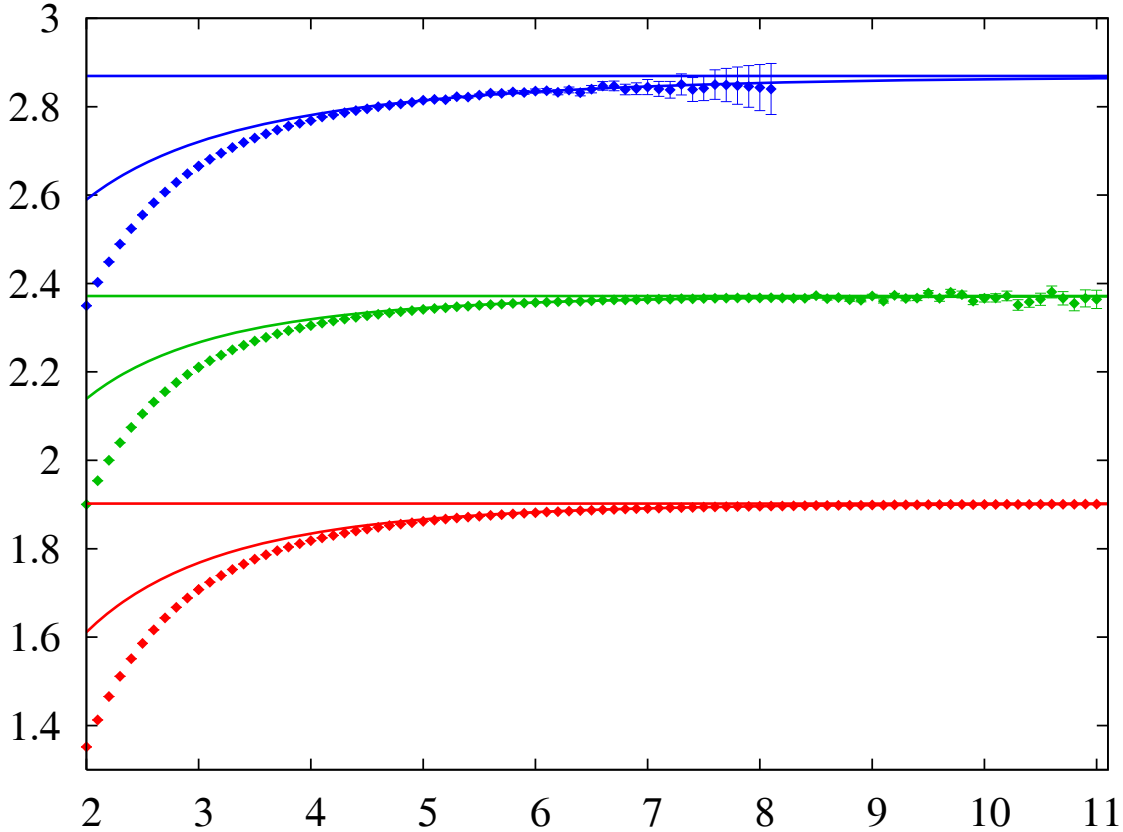
and they tend to corresponding energy levels E_n

PIMC: Convergence of the free energy



Convergence of the discretized free energy to continuum as a function of N for a 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: Calculation of energy spectra



Time dependence of the free energy and auxiliary functions $f^{(1)}$ and $f^{(2)}$ for a system of two particles in two dimensions in a quartic potential with $g_1 = 1/10$, $g_2 = 1/9$, $N_{MC} = 10^9$, using $p = 5$ effective action and $N = 64$.

PIMC: Lower energy levels of anharmonic oscillator (dM=4)

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)	—

Lower energy levels for a system of two particles in two dimensions in a quartic potential with $g_2 = 1/9$, calculated using $N_{MC} = 10^9$, $p = 5$ effective action and $N = 64$. Obtained degeneracies of calculated energy levels are $d_0 = 1$, $d_1 = 2$, $d_2 = 3$, $d_3 = 6$.

Conclusions (1)

- We introduced path integral formalism in quantum mechanics
- Monte Carlo method is presented, and its application to the calculation of path integrals (PIMC)
- We also presented a new method for numerical calculation of path integrals and expectation values for a general non-relativistic many-body quantum theory
- We derived discretized effective actions which allow deeper analytical understanding of the path integral formalism
  - Gaussian halving
  - ϵ-expansion of the short-time propagator
  - recursive approach
- In numerical approach, discretized effective actions of level p provide substantial speedup of Monte Carlo algorithm from $1/N$ to $1/N^p$

Conclusions (2)

- For single-particle one-dimensional theories we have derived discretized actions up to level $p = 35$, while for a general non-relativistic many-body theory up to level $p = 10$
- For special cases of potentials we have derived effective actions to higher levels ($p = 140$ for a quartic anharmonic oscillator in $d = 1$, $p = 67$ in $d = 2$, $p = 37$ for modified Pöschl-Teller potential)
- We have developed MC codes that implement the newly introduce approached and performed extensive numerical study through which the derived analytical results are verified
- We have derived *Mathematica* codes for automation of symbolic derivation of discretized effective actions for higher values of level p

Current and future applications

- Calculation of properties of Bose-Einstein condensates in fast-rotating magneto-optical traps
- Efficient calculation of ground state of various quantum systems, including the description of Bose-Einstein condensate by Gross-Pitaevskii (mean field) equation
- Quantum gases with disorder (Anderson localization)
- Improved estimators for expectations values (heat capacity, magnetization etc.)

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- Danica Stojiljković
- Jelena Grujić
- dr Axel Pelster

Effective discretized p=4 action

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