Parallelization of Path Integral Monte Carlo Calculation of Transition Amplitudes

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Introduction

- 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

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

- Discretization 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 $1/N$.

Formulation of the path integral formalism (1)

- Amplitudes for transition from an initial state $|\alpha\rangle$ to a final state $|\beta\rangle$ in time T can be written as

$$A(\alpha, \beta; T) = \langle \beta | e^{-\frac{i}{\hbar}\hat{H}T} | \alpha \rangle$$

- For technical reasons, usually we use imaginary time
- The standard derivation starts from the identity

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

dividing the evolution into N steps of the length $\epsilon = T/N$. This expression is exact.

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

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

Formulation of the path integral formalism (2)

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

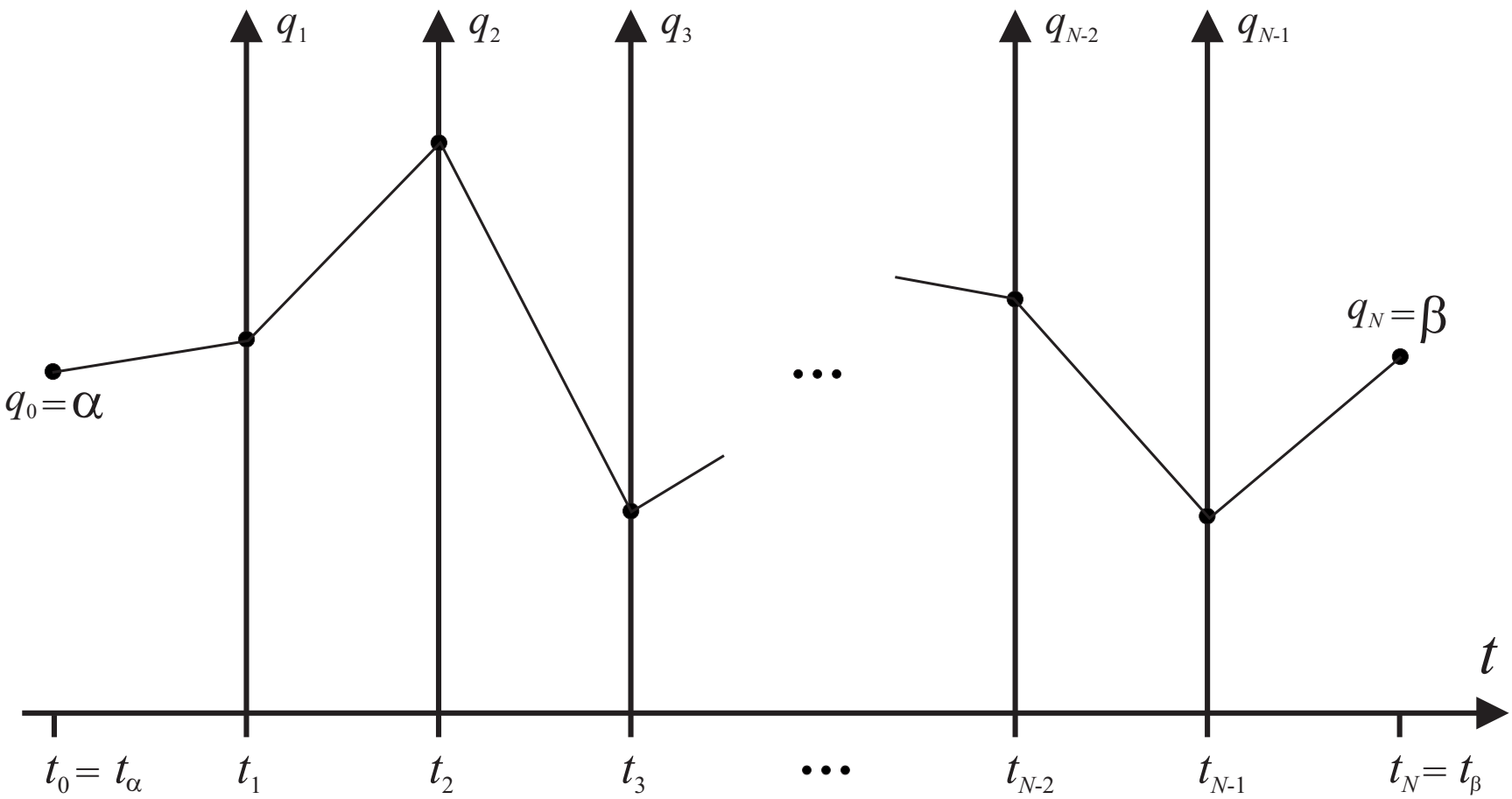
$$A(\alpha, \beta; T) = \lim_{N \to \infty} A_N(\alpha, \beta; T)$$

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

Illustration of the discretization of trajectories



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

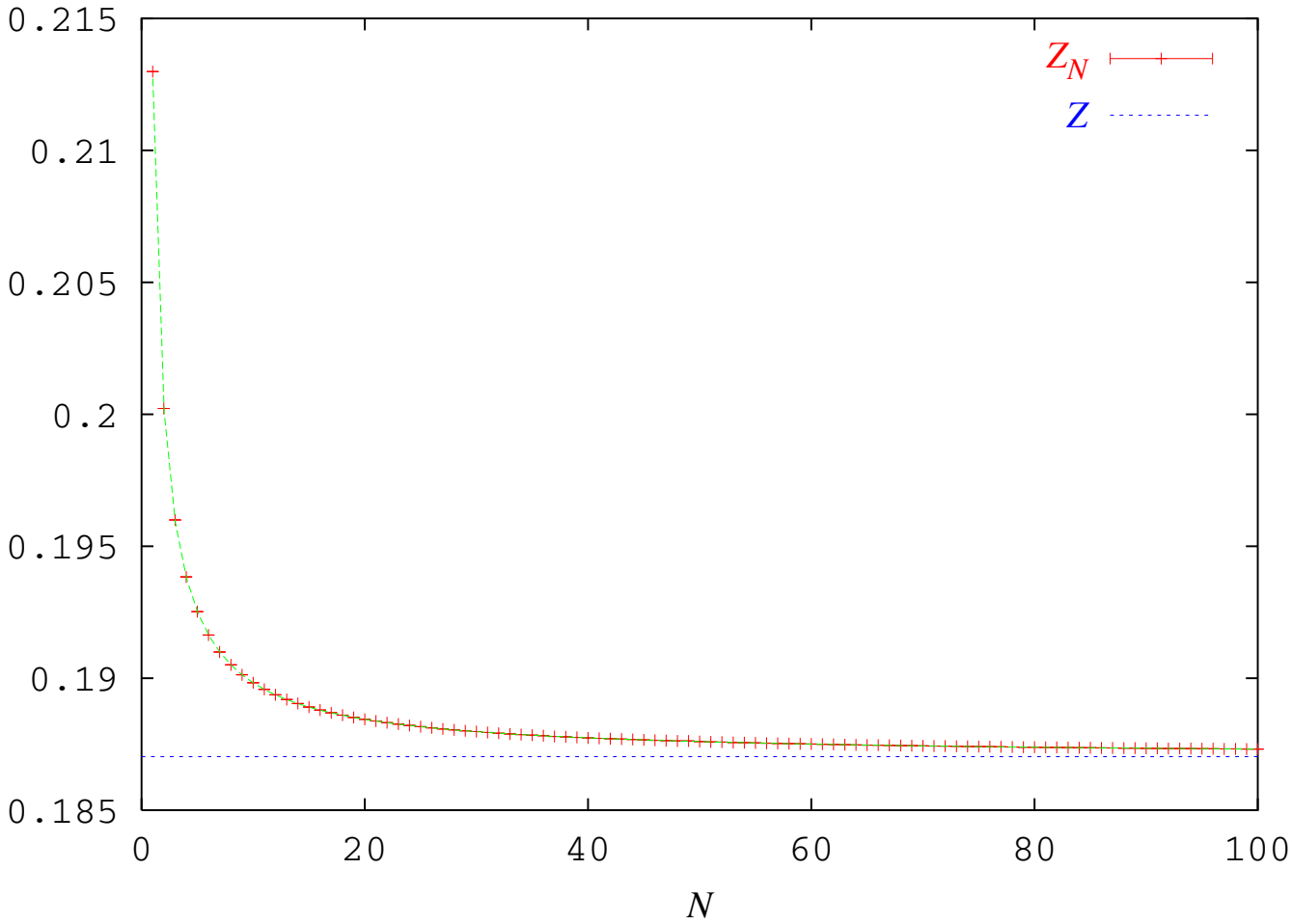
$$\int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

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



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 makes use of the cyclic property of the trace - the improvement is valid for partition functions only

Ideal discretization (1)

- Ideal discretized action S^* is defined as the action giving exact continual amplitudes $A_N = A$ for any discretization
- For the free particle, the 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

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

- 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

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

Improving effective actions (1)

- We present an approach enabling a substantial speedup in the convergence of path integrals
- Previously we have set up an approach based on the integral equation connecting discretized effective actions of different coarseness
- It allows the systematic derivation of effective actions and leadis to improved $1/N^p$ convergence for one-particle systems in $d = 1$ - Gaussian halving
- For many-body systems in arbitrary dimensions we have developed two equivalent approaches

Improving effective actions (2)

- First is based on direct calculation of ϵ-expansion of short-time amplitudes, expressed as expectation values of the corresponding free theory
  - following the original idea from the book by H. Kleinert
- Here we present second approach, based on solving recursive relations for the discretized action, derived from Schrödinger's equation for amplitudes.
- This approach is by far the most efficient, both for many-body and one-body systems.
- The presented results are highly related to recently developed systematic approach by Chin and collaborators for the arbitrary-order splitting of the evolution operator

Equation for the ideal effective potential (1)

- 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 (2)

- 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)

- The effective potential is given as a power series

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

where systematics in ϵ-expansion is ensured by $\epsilon \propto x^2$, and

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

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

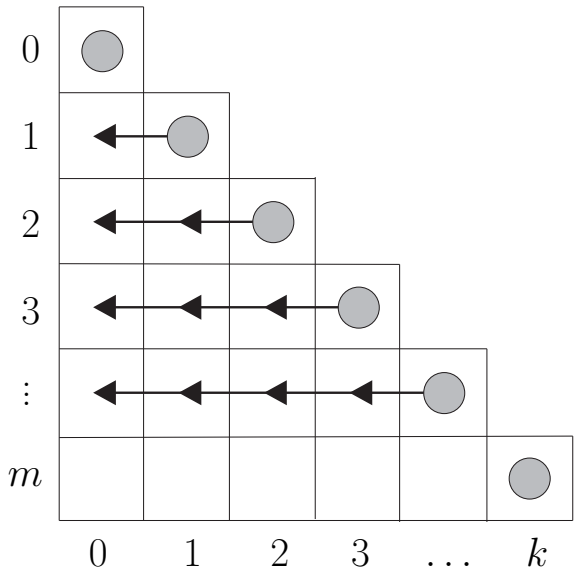
$$\begin{aligned}8\,(m+k+1)\,W_{m,k} = {} & \bar{\partial}^2 W_{m-1,k} + \partial^2 W_{m,k+1} - \\ & - \sum_{l=0}^{m-2}\sum_{r}(\bar{\partial}W_{l,r})\cdot(\bar{\partial}W_{m-l-2,k-r}) - \\ & - \sum_{l=1}^{m-2}\sum_{r}(\partial W_{l,r})\cdot(\partial W_{m-l-1,k-r+1})\end{aligned}$$

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 action for many-body systems (1)

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

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

Effective action for many-body systems (2)

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

Numerical results (1)

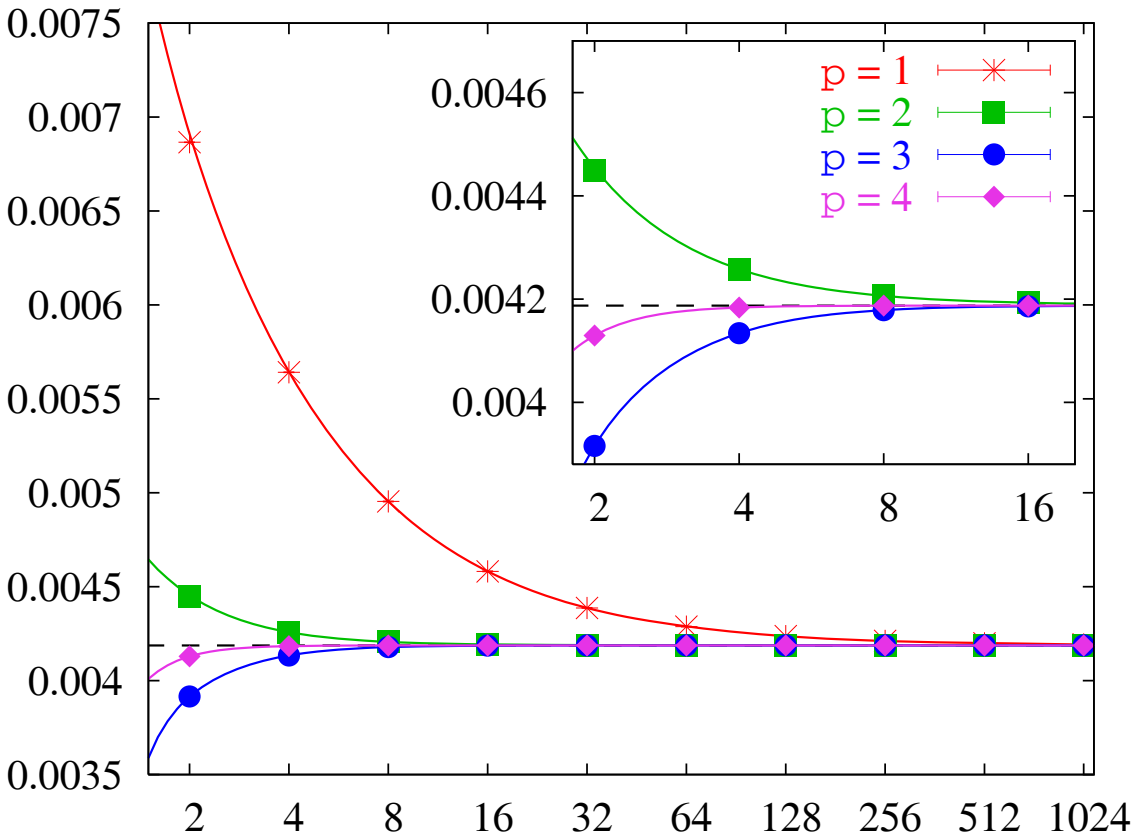
- We have conducted a series of PIMC calculations of transition amplitudes, e.g. 2P in 2D

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

  as well as for time-dependent potentials, http://arxiv.org/abs/0912.2743
- The continuum amplitudes $A^{(p)}$ have been estimated by fitting polynomials in $1/N$ to the discretized values $A_N^{(p)}$

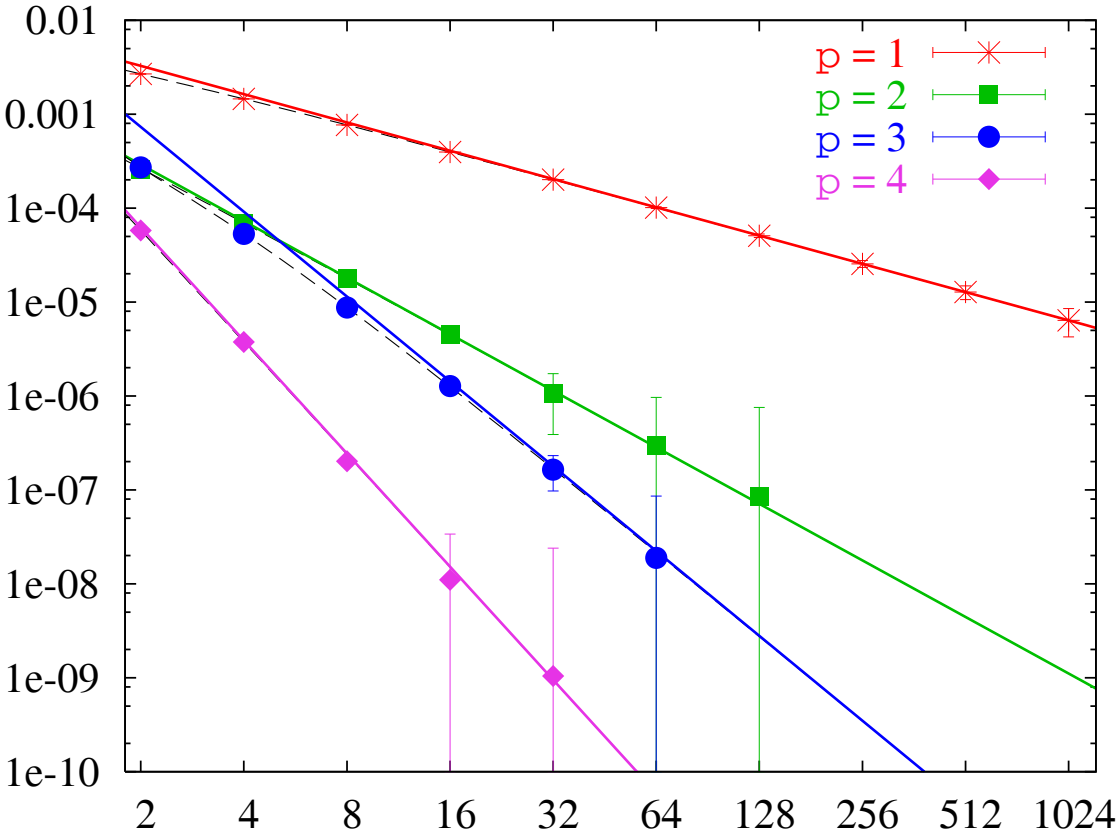
$$A_N^{(p)} = A^{(p)} + \frac{B^{(p)}}{N^p} + \frac{C^{(p)}}{N^{p+1}} + \dots$$

PIMC: Convergence to the continuum, 2P in 2D



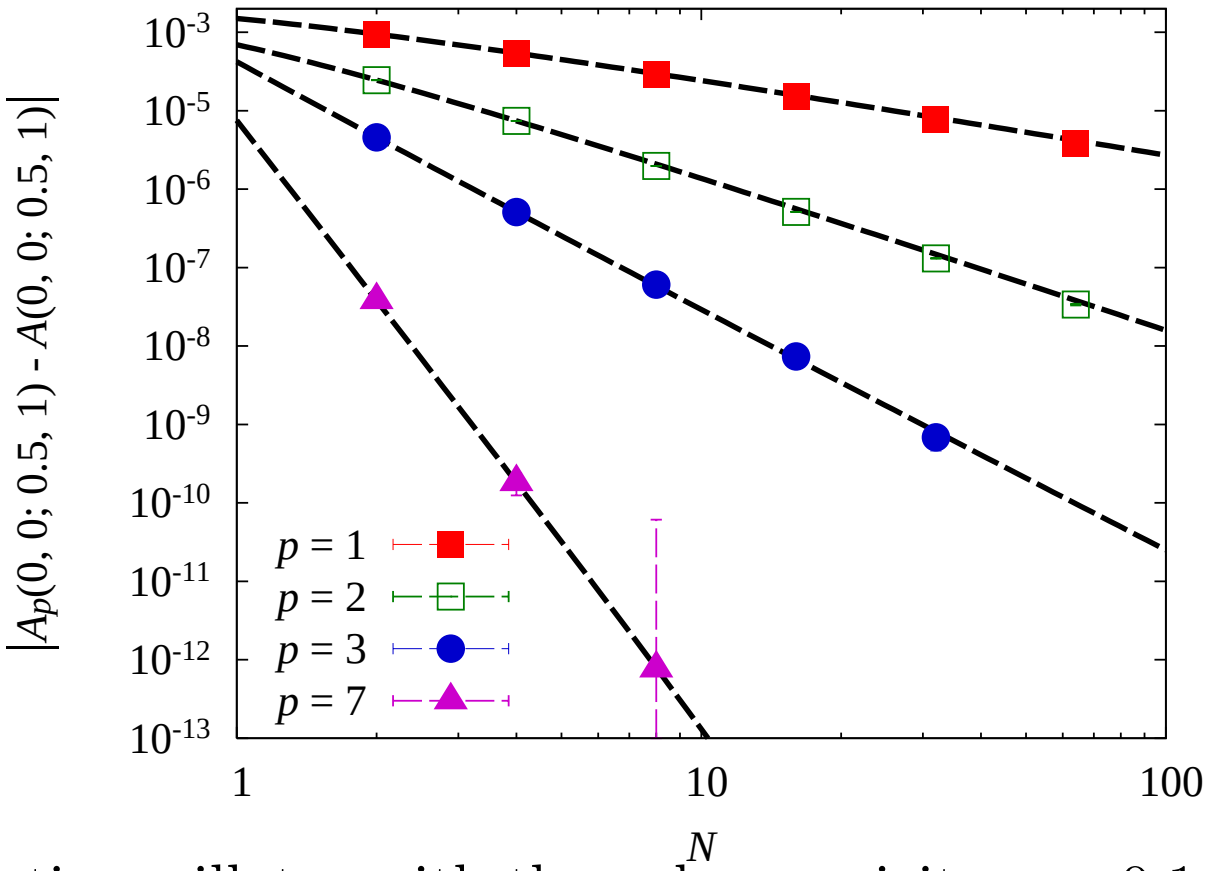
Amplitude for the oscillator with large quartic anharmonicity $g_1 = 10$, $g_2 = 0$, $T = 1$, $N_{MC} = 10^6$, initial and final states $a = (0, 0; 0.2, 0.5)$, $b = (1, 1; 0.3, 0.6)$.

PIMC: Deviations from the continuum, 2P in 2D



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 $a = (0, 0; 0.2, 0.5)$, $b = (1, 1; 0.3, 0.6)$.

PIMC: Deviations from the continuum, time-dependent potential



Pure quartic oscillator with the anharmonicity $g = 0.1$, rescaled by the Grosche factor $\zeta(t) = \sqrt{t^2 + 1}$, $N_{MC} = 1.6 \cdot 10^{13}$

Parallelization

- The presented MC algorithm is inherently parallel, and its implementation is relatively easy in all frameworks
  - Message Passing Interface (MPI)
  - Threaded code (OpenMP)
  - Distributed computing (Grid)
- The essential ingredient is a good parallel generator of pseudo-random numbers
  - Large number of uncorrelated pseudo-random numbers
  - Large number of uncorrelated streams of pseudo-random numbers
  - Reproducibility
- We have used very well-known **SPRNG** generator

Parallelization strategy

- Initialization of the needed number of parallel processes/threads/Grid jobs
- Initialization of the needed number of parallel streams from SPRNG: each process/thread/job uses its own stream
- Accumulation of average values of all quantities (amplitudes, partition functions, expectation values)
  - No communication during the computation - ideal scalability of the code
- At the end, all accumulated quantities are collected by one designated process and further statistically processed
  - In the Grid context, this is done through a series of scripts after collecting output sandboxes, not within the Grid job

Pros and Cons

- MPI
  - Simple to program, implement, and use
  - Applicable only within one cluster
  - If one process fails, the whole simulation fails
- OpenMP
  - Simple to program, implement, and use
  - Applicable only within one SMP node
  - Could be combined with MPI in principle, although here this will not gain any performance
- Gridified version of the code
  - Simple to program, implement, and use
  - Applicable on many clusters
  - A needed number of *independent* jobs can be submitted, and failed jobs can be resubmitted, without affecting other jobs
  - If statistics is not sufficient, additional jobs can be easily submitted, with some reasonable planning in advance

Conclusions

- New method for numerical calculation of path integrals for a general non-relativistic many-body quantum theory
- Derived discretized effective actions allow deeper analytical understanding of the path integral formalism
- In the numerical approach, discretized effective actions of level p provide substantial speedup of Monte Carlo algorithm from $1/N$ to $1/N^p$
- Used Path Integral Monte Carlo algorithm can be easily parallelized in a number of available frameworks
- AEGIS, SEE-GRID-SCI and EGEE Grid infrastructures used for various applications of the SPEEDUP code
  - Numerical verification of the improved convergence
  - Exact diagonalization of the space-discretized matrix of the evolution operator (spectra)
  - Properties of fast-rotating Bose-Einstein condensates