Extension of the SPEEDUP Path Integral Monte Carlo Code*

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Formulation of the path integral formalism [1/3]

- Many-body model in non-relativistic quantum theory

$$\hat{H} = \sum_{i=1}^{M} \frac{\hat{\mathbf{p}}_i^2}{2m_i} + \hat{V}(\hat{\mathbf{q}}_1, \ldots, \hat{\mathbf{q}}_M)$$

- Solution is usually expressed in terms of eigenvalues and eigenfunctions
- Complete analytic solution can be also expressed in terms of general transition amplitudes

$$A(\mathbf{a}, \mathbf{b}; T) = \langle \mathbf{b} | e^{-iT\hat{H}/\hbar} | \mathbf{a} \rangle$$

$|\mathbf{a}\rangle$ - initial state, $|\mathbf{b}\rangle$ - final state, T - time of propagation

- For technical reasons, we switch to imaginary (Euclidean) time in numerical calculations

Formulation of the path integral formalism [2/3]

- The standard derivation starts from the identity (we use 1D system, for simplicity)

$$A(a,b;T) = \int dq_1 \cdots dq_{N-1}\, A(a,q_1;\varepsilon)A(q_1,q_2;\varepsilon)\cdots A(q_{N-1},b;\varepsilon)$$

  dividing the evolution into N steps of the length $\varepsilon = T/N$.
- Approximation: calculation of short-time amplitudes up to the first order in ε ($\hbar = 1$)

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

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

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

Formulation of the path integral formalism [3/3]

- Discretized amplitude $A_N(a, b; T)$ 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 $L = \frac{1}{2}\dot{q}^2 + V(q)$, the usual naive discretized action is given by

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

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

Numerical calculation of path integral [1/2]

- Path integral formalism is ideally suited for numerical approach, with physical quantities defined as expectation values with respect to the exponential of the action, discretized in the form of a multiple-integral expression, with the normalization (partition function):

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

- Monte Carlo (MC) is the method of choice for calculation of such integrals
- 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 calculation of path integral [2/2]

- 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 limit as slow as $1/N$
- Using special techniques and properties 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)

Discretized effective actions [1/2]

- 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
- They must vanish in the $N \to \infty$ limit, and should not change continuum values of amplitudes
- Fortunately, such additional terms in discretized actions can be chosen in a smart way so as to speed up the convergence of path integrals

Discretized effective actions [2/2]

- 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 $1/N^4$

Recursive approach [1/3]

- Recursive method for deriving the discretized effective actions is based on solving the underlying Schrödinger equation for the amplitude
- This approach is by far the most efficient, both for one-body and many-body systems in arbitrary number of dimensions
- Recursive approach gives transition amplitudes in terms of the ideal discretized action

$$A(a,b;T) = \frac{1}{\sqrt{2\pi T}}\, e^{-S^*(a,b;T)}$$

- This expression is correct not only for short times of propagation, but also for arbitrary large T

Recursive approach [2/3]

- Ideal effective potential is introduced by

$$S^*(a,b;T) = T\left[\frac{1}{2}\left(\frac{b-a}{T}\right)^2 + W\right]$$

  where W is the (ideal) effective potential
- The effective potential allows systematic and hierarchic double expansion in the form

$$W(x,\bar{x};\varepsilon) = \sum_{m=0}^{\infty}\sum_{k=0}^{m} c_{m,k}(x)\,\varepsilon^{m-k}\bar{x}^{2k}$$

- If we restrict the above sum over m to $p-1$, the effective potential $W_p(x,\bar{x};\varepsilon)$ gives expansion of the effective action S_p^* to order ε^p, and hence the level designation p for both the effective action and the corresponding potential W_p

Recursive approach [3/3]

- In Path Integral Monte Carlo simulations for calculation of long time amplitudes, the use of level p effective action leads to significantly improved convergence of discretized amplitudes
- Discretized amplitudes calculated with the level p effective action converge as fast as ε^p to the continuum values, i.e. as $1/N^p$, where N is the number of time steps used in the discretization.

Overview

- Discretization of the propagation time with level p effective action leads to discretized amplitudes in the form

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

where $S_N^{(p)}$ stands for the discretized level p effective action

$$S_N^{(p)} = \sum_{k=0}^{N-1} \left[\frac{2\bar{x}_k^2}{\varepsilon} + \varepsilon \, W_p(x_k, \bar{x}_k; \varepsilon) \right]$$

abbreviations:

$$q_0 = a, \; q_N = b, \; x_k = (q_{k+1} + q_k)/2, \; \bar{x}_k = (q_{k+1} - q_k)/2$$

Bisection method [1/2]

- Discretized trajectory $q(t) = \{q_0, q_1, \ldots q_N\}$ is constructed using the bisection method
  - Procedure starts from bisection level $n = 0$ - initial and final position of the particle
  - At bisection level $n = 1$ the propagation is divided into two time-steps - coordinate q of the particle at the moment $T/2$
  - The coordinate q is generated from the Gaussian probability density function centered at $(a + b)/2$ and with the width $\sigma_1 = \sqrt{T/2}$
  - The procedure continues iteratively
  - At each bisection level n, new coordinates are generated in the middle of each time step from Gaussians centered at mid-point of coordinates generated at level $n - 1$, with the width $\sigma_n = \sqrt{T/2^n}$

Bisection method [2/2]

- Numbers η from the Gaussian centered at zero are generated by Box-Müller method

$$\eta = \sqrt{-2\sigma_n^2 \ln \xi_1}\, \cos 2\pi\xi_2$$

  ξ_1 and ξ_2 are generated from the uniform distribution on the interval $U = [0, 1]$ (SPRNG library)
- If the target bisection level is s, then at bisection level $n \leq s$

$$q\Big[(1+2i)\cdot 2^{s-n}\Big] = \eta_i + \frac{1}{2}\left(q\Big[i\cdot 2^{s-n+1}\Big] + q\Big[(i+1)\cdot 2^{s-n+1}\Big]\right)$$

  where i runs from 0 to $2^{n-1} - 1$

Monte Carlo approach [1/2]

- Monte Carlo method uses pseudo-random numbers for calculation of the integrals
- For d-dimensional integral on a unit cube U^d, with ξ_i sequence of pseudo-random d-dimensional points in U^d, MC estimate of the integral of the function $f(\mathbf{x})$ is given by the average of the function f evaluated at the MC sample of points ξ_i
- According to the central limit theorem, such estimate converges to the exact value of the integral when the number of MC samples N_{MC} goes to infinity

Monte Carlo approach [2/2]

- Furthermore, central limit theorem states that the statistical distribution of numerical results obtained using large number of independent MC samples is a Gaussian, centered at the exact value of the integral, with the variance $\sigma^2(f)/N_{MC}$, where $\sigma^2(f)$ is given by the analytic formula

$$\sigma^2(f) = \int_{U^d} f^2(\mathbf{x})d\mathbf{x} - \left(\int_{U^d} f(\mathbf{x})d\mathbf{x} \right)^2$$

  and can be estimated as well from a single MC run
- This gives clear statistical interpretation of errors when MC method is used: the distribution of deviations is a Gaussian with the expected standard deviation:

$$\sqrt{\sigma^2(f)/N_{MC}}$$

- Convergence rate is proportional to $N_{MC}^{-1/2}$

Quasi-MC approach [1/3]

- There are many known quasi-random sequences: Halton, **Sobol**, Faure
- Sobol's sequence is used for implementation of the SPEEDUP quasi-MC algorithm
- In order to verify the quasi-MC algorithm, we have considered calculation of the Gaussian-type integrals

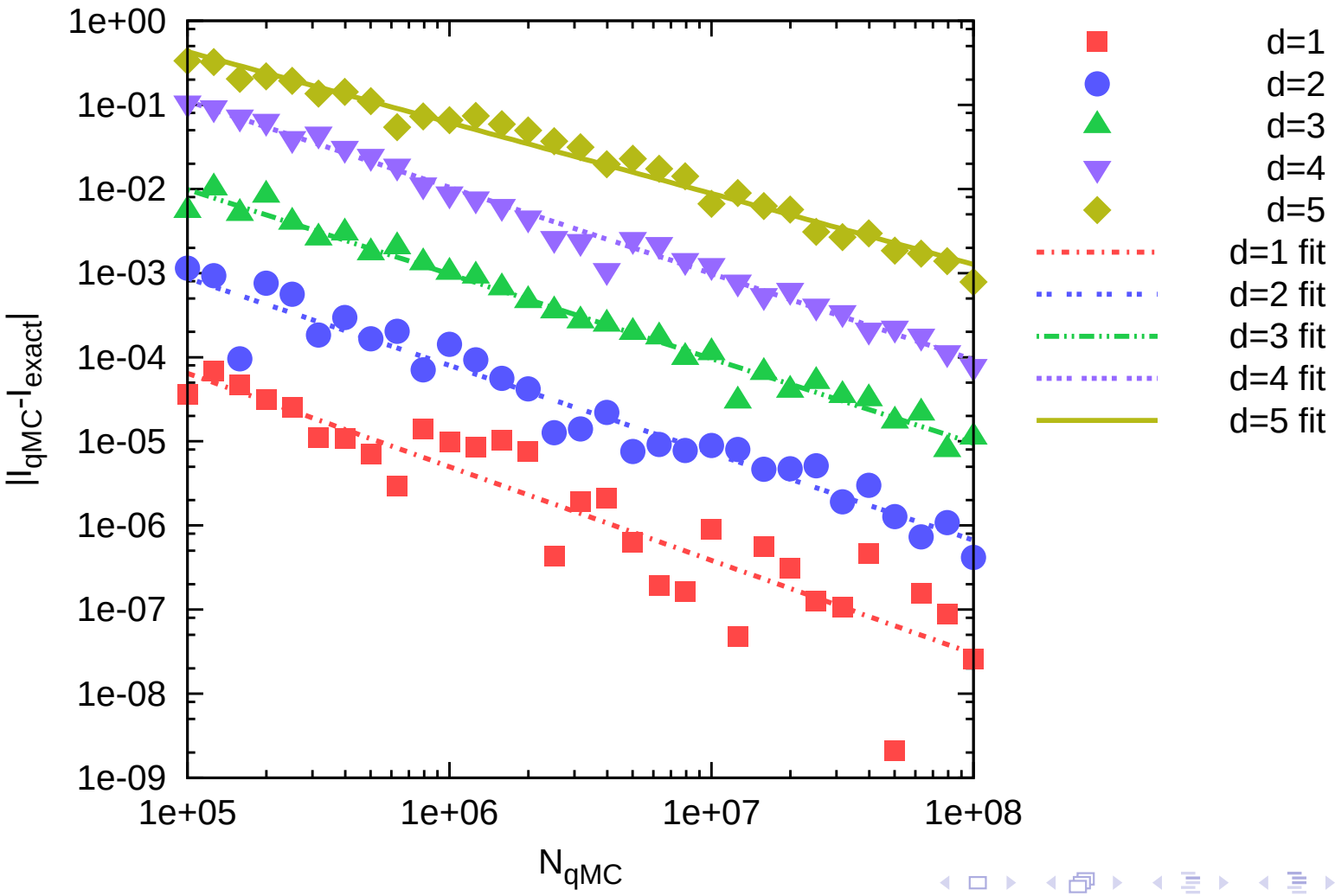
$$I = \int_{U^d} \exp\Big(-\sum_{i=1}^{d} x_i^2\Big) d\mathbf{x}$$

- We have performed numerical calculations using large numbers of independent quasi-MC samples for different values of dimensionality d

Quasi-MC approach [2/3]

- Obtained distribution of numerical estimates for the value of the integral was always found to be a Gaussian, whose parameters can be found by fitting
- Obtained distributions were centered on the exact values of integrals within the errors estimated by the fitted widths of Gaussians
- Deviations were proportional to N_{qMC}^{-1}, which is a significant improvement over the standard MC convergence speed

Quasi-MC approach [3/3]



SPEEDUP code modification

- Quasi-random numbers instead of pseudo-random ones
- Implementation of Sobol's sequence that allows generation of quasi-random numbers in a large number of dimensions
- Box-Müller method to obtain the trajectories according to the bisection algorithm

Distribution [1/3]

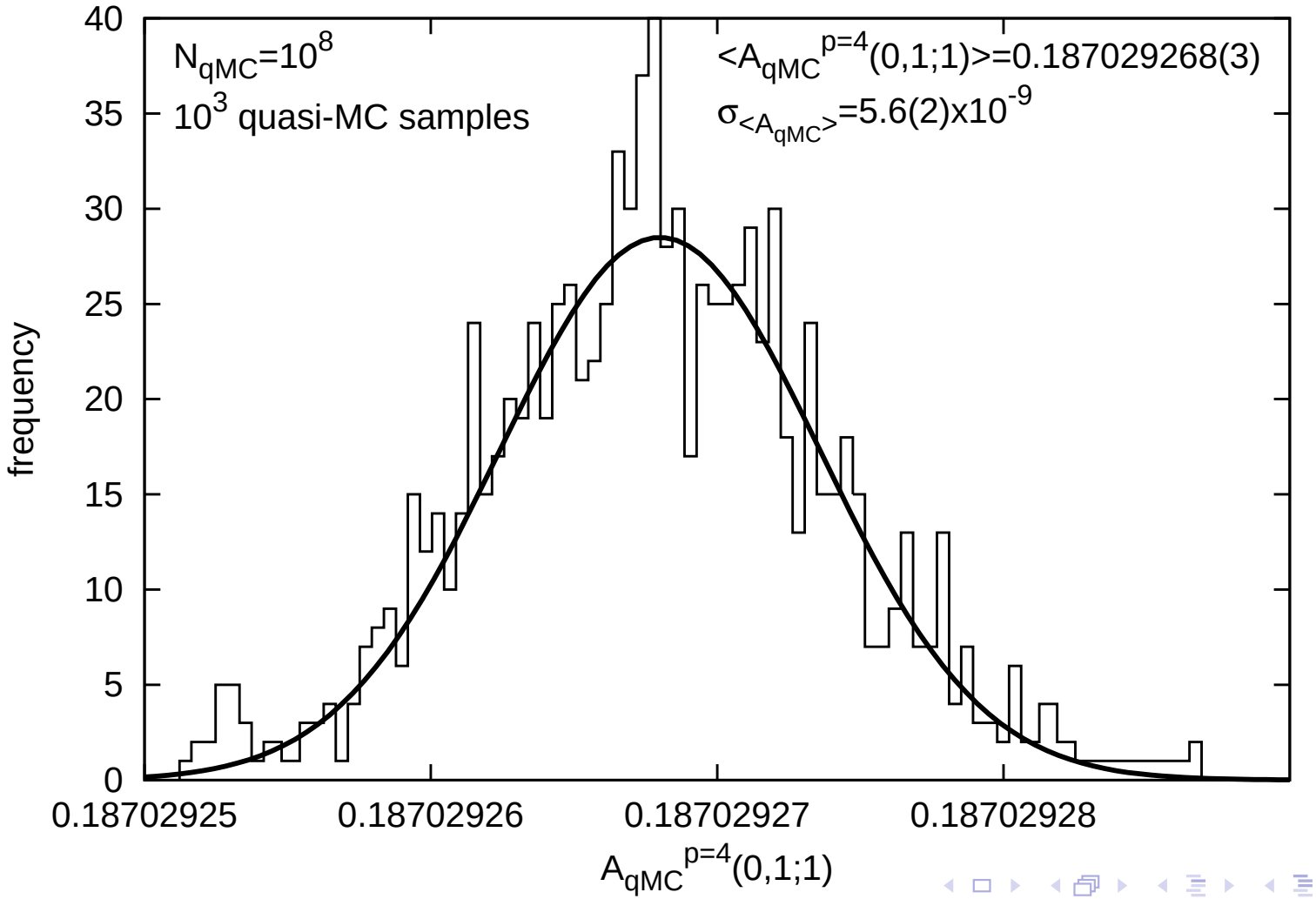
- Statistical distribution of the obtained results on a large ensemble of samples
- Quasi-MC SPEEDUP algorithm is tested for the example of calculation of the transition amplitudes $A(0,1;1)$ for the anharmonic potential

$$V(x) = \frac{1}{2} m\omega^2 x^2 + \frac{1}{24} g\, x^4$$

for the values of parameters $m = 1$, $g = 1$, with the level $p = 4$ effective action, and using the target bisection level $s = 8$ (255-dimensional integrals)

- Distribution the ensemble of 10^3 independently calculated transition amplitudes, each obtained from the sample of $N_{qMC} = 10^8$ trajectories

Distribution [2/3]



Distribution [3/3]

- In order to assess if the obtained estimate for the amplitude (mean value of the fitted Gaussian) is correct, we have used comparison with the MC SPEEDUP code with exceedingly large number of samples ($N_{MC} = 10^{12}$)
- With such a sample we achieved the comparable precision for the amplitude

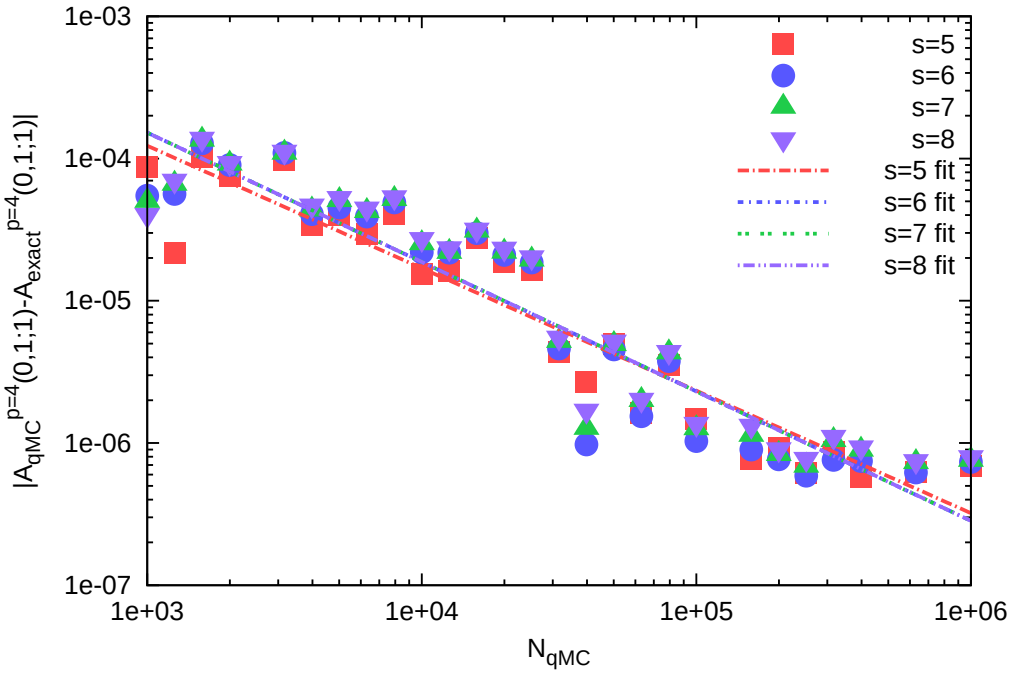
$$A_{exact}^{p=4} = 0.18702926(3)$$

which is used as our estimate for the exact value in further calculations of deviations of numerical results obtained from the quasi-Monte Carlo SPEEDUP code.

Deviation [1/2]

- Standard deviation of quasi-MC results cannot be estimated using the MC approach
- One approach would be to always study the distribution and estimate the standard deviation from an ensemble of samples
- This takes a considerable amount of time, which is not justified if there are other means to reliably estimate the deviation
- We have studied dependence of the deviation from the exact value of the amplitude as a function of the size of the sample N_{qMC}

Deviation [2/2]

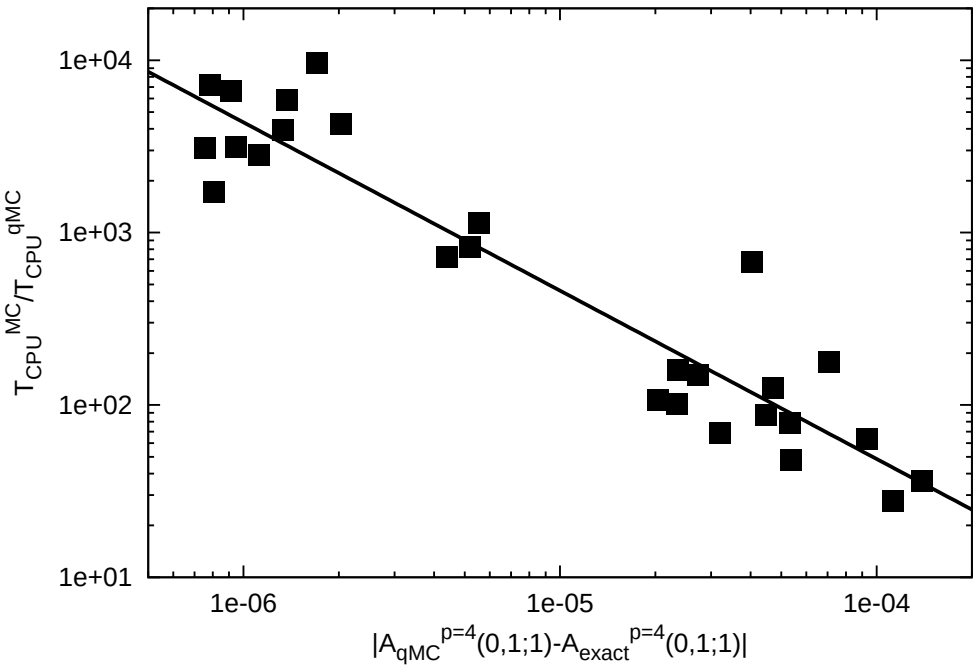


- Exact value of the amplitude is obtained by the MC algorithm
- We found approximate scaling of deviations to be N_{qMC}^{-1} for all values of the target bisection level

Speedup [1/2]

- N_{qMC}^{-1} scaling leads to the improved performance of quasi-MC algorithm compared to the standard MC method
- Generation of pseudo-random and quasi-random numbers is of similar complexity
- Therefore, the fact that one needs much smaller size of quasi-MC sample in order to obtain the same accuracy as with the MC algorithm leads to a significant speedup

Speedup [2/2]



- Even for a moderate value of the required precision Δ, one obtains improvement of many orders of magnitude, approximately proportional to $1/\Delta$

Conclusions

- We have implemented quasi-MC extension of the SPEEDUP code for calculation of quantum mechanical transition amplitudes using the effective action approach
- Quasi-MC SPEEDUP algorithm uses Sobol's set of quasi-random numbers
- Distribution of numerical results obtained using the quasi-MC algorithm is Gaussian
- $1/N_{qMC}$ scaling of deviations leads to a significant speedup of the quasi-MC algorithm compared to the standard MC approach for the same accuracy of results