

ACCELERATED PATH-INTEGRAL CALCULATIONS VIA EFFECTIVE ACTIONS

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We give an overview of a recently developed method which systematically improves the convergence of generic path integrals for transition amplitudes, partition functions, expectation values, and energy spectra. This was achieved by analytically constructing a hierarchy of discretized effective actions indexed by a natural number p and converging to the continuum limit as $1/N^p$. We analyze and compare the ensuing increase in efficiency of several orders of magnitude, and perform series of Monte Carlo simulations to verify the results.

Keywords: Effective action; Many-body system; Monte Carlo simulation.

1. Introduction

Path integral formalism offers a general framework for treatment of quantum theories.¹ Functional integrals provide easy way for generalization and extension of quantization methods to more complex physical systems, including systems with no classical counterparts. Originally introduced in quantum mechanics and later most widely used in high energy theory and condensed matter, path integrals can today be found in almost all areas of physics, ranging from atomic, molecular and nuclear physics, to the physics of polymers, biophysics, and chemistry. Moreover, path integrals are starting to play important roles in several areas of mathematics, even in modern finance. An up to date overview of the path integral formalism and its various applications can be found in Kleinert's book.²

The definition of path integrals as a limit of multiple integrals over a discretized theory makes their numerical evaluation quite natural. However, path integrals remain notoriously demanding of computing. Considerable research effort has been devoted to the development of approaches that enable faster numerical convergence to the continuum. Efficient imple-

mentation of path integral Monte Carlo algorithms, coupled with various model-related approximations, has enabled the application of path integrals to real-world problems.³ For a long time the state of the art result was $1/N^4$ convergence of discretized partition functions.^{4,5} This was achieved using a generalized form⁶ of the Trotter formula. However, it is only the integral over all the diagonal amplitudes (i.e. cyclicity of the trace) that has the $O(1/N^4)$ behavior, so such approach cannot be applied to the calculation of general amplitudes or associated (non-thermal) expectation values.

A recently developed method for analytical construction of improved discretized effective actions,⁷⁻⁹ based on the study of relationship between discretizations of different coarseness,^{10,11} has led to substantial speedup of numerical path-integral calculations of several orders of magnitude. Until now, the method has been limited to one-particle one-dimensional systems. Here we present the generalization of this formalism to generic non-relativistic many-particle quantum systems in arbitrary dimensions.

2. Improved Discretized Effective Actions

The presented method is applicable to all quantum theories. For simplicity, we illustrate the details of the derivation on the case of a non-relativistic quantum system consisting of M distinguishable particles in d spatial dimensions, interacting through the potential V . The imaginary time amplitude $A(a, b; T)$ for a transition from initial state $|a\rangle$ to final state $|b\rangle$ in time T is given as the $N \rightarrow \infty$ limit of the discretized amplitude

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

In this expression, N is the discretization coarseness (number of time slices), while S_N is the naively discretized action,

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

Here the time step is $\varepsilon = T/N$, while discretized velocities are defined as $\delta_{n,i} = q_{n+1,i} - q_{n,i}$, and mid-point coordinates $\bar{q}_n = (q_n + q_{n+1})/2$. The index n goes over N time steps, and index i goes over M particles.

The above definition of the path integral requires the transition from continuum to discretized theory, i.e. the introduction of coarseness N . Such expressions converge to the continuum very slowly, typically as $O(1/N)$.

One of the key features of definition (1) is that the discretization is not unique. In fact, the choice of discretization strongly affects convergence of

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discretized amplitudes to the continuum. In a recent paper¹⁰ we have shown that for a general theory there exists an ideal discretization (equivalently, an ideal discretized action S^*), giving the exact (continuum limit) result for *any* discretization coarseness N

$$A_N^*(a, b; T) = A(a, b; T).$$

This is easily seen if we recall that the defining relation for path integrals as the continuum limit of discretized amplitudes follows from the completeness relation

$$A(a, b; T) = \int dq_1 \cdots dq_{N-1} A(a, q_1; \varepsilon) \cdots A(q_{N-1}, b; \varepsilon), \quad (3)$$

through the substitution of short-time amplitudes $A(q_n, q_{n+1}; \varepsilon)$ calculated to first order in time step ε . A faster converging result may be obtained by evaluating the amplitudes under the integral in Eq. (3) to higher orders in ε . From the above relation we directly see that the ideal discretized action S^* leads to exact propagation, and is given in terms of the exact amplitude,

$$A(q_n, q_{n+1}; \varepsilon) = (2\pi\varepsilon)^{-\frac{Md}{2}} e^{-S_n^*}. \quad (4)$$

The ideal discretized action S^* is simply the sum of expressions S_n^* . We will use Eq. (4) to calculate the ideal discretized action as a power series in ε , which starts from the naive action (2) as the zeroth order term. The details of this expansion have been inspired by an analogous derivation given in Kleinert's book.² The outlined approach makes possible the systematic improvement of numerical convergence of path integral calculations, and the construction of a hierarchy of discretized actions $S_N^{(p)}$, denoted by level number p , giving improved convergence

$$A_N^{(p)}(a, b; T) = A(a, b; T) + O(1/N^p). \quad (5)$$

In order to calculate the short-time amplitude to the desired order in ε , we shift integration variable $q = \xi + x$ about a fixed referent trajectory ξ , and the time to $s \in [-\varepsilon/2, \varepsilon/2]$, so that the short-time amplitude becomes

$$A(q_n, q_{n+1}; \varepsilon) = e^{-S_n[\xi]} \int_{x(-\varepsilon/2)=0}^{x(\varepsilon/2)=0} [dx] e^{-\int_{-\varepsilon/2}^{\varepsilon/2} ds \left(\frac{1}{2} \dot{x}^2 + U(x; \xi) \right)}. \quad (6)$$

The referent trajectory ξ satisfies the same boundary conditions as q , which implies that x vanishes at the boundaries. The action $S_n[\xi]$ is defined as

$$S_n[\xi] = \int_{-\varepsilon/2}^{\varepsilon/2} ds \left(\frac{1}{2} \dot{\xi}^2 + V(\xi) \right), \quad (7)$$

and $U(x; \xi) = V(\xi + x) - V(\xi) - x\ddot{\xi}$. The amplitude may now be written as

$$A(q_n, q_{n+1}; \varepsilon) = \frac{e^{-S_n[\xi]}}{(2\pi\varepsilon)^{\frac{Md}{2}}} \left\langle e^{-\int_{-\varepsilon/2}^{\varepsilon/2} ds U(x; \xi)} \right\rangle, \quad (8)$$

where $\langle \dots \rangle$ denotes expectation values with respect to free massless theory. The above expression holds for any choice of referent trajectory ξ .

Expansion in powers of U gives

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

where $x' = x(s')$, $\xi' = \xi(s')$, and $U(x; \xi)$ is further expanded around the referent trajectory ξ . The expectation values of products $\langle x_i(s) \dots x_j(s') \rangle$ is calculated through the use of the massless free theory generating functional. Note that the generating functional (and as a result the expectation values) do not depend on the choice of ξ . However, different choices of ξ are related to different approximation techniques: the choice of classical trajectory for ξ corresponds to the semiclassical expansion, while the choice of a linear referent trajectory is the simplest way to obtain short-time expansion.

In order to perform the remaining integrations over s in Eq. (8), due to the explicit dependence of the referent trajectory on s , we first expand the potential U and all its derivatives around some reference point. For example, in the mid-point prescription, we choose \bar{q}_n as that reference point. Once one chooses the trajectory $\xi(s)$, all expectation values in Eq. (8) are given in terms of quadratures. In this way we obtain a double expansion for S^* in ε and in $\delta n, i^2$. In order to retain only the terms that contribute up to a certain order in ε , we further use the fact that the short time propagation of the considered class of theories satisfies, to leading order, the diffusion relation $\delta_{n,i}^2 \propto \varepsilon$.

The explicit analytical expressions for the many-particle discretized effective action have been so far derived for $p \leq 12$. The derived expressions become algebraically more complex, and such calculations require the use of some of the available packages for symbolic calculus. Note that, in principle, there are no obstacles in going to as high values of p as desired. The derived higher level effective actions can be found on our web site.¹² We stress that it would also be quite interesting to attack the problem of solving Eq. (4) through the use of other approximation schemes, particularly those that are non-perturbative in ε , e.g. the Feynman-Kleinert variational approach.¹³⁻¹⁵

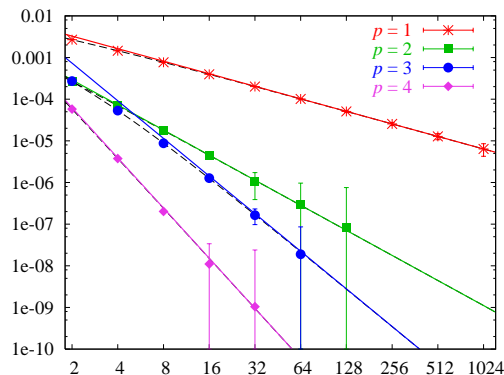


Fig. 1. Deviations of amplitudes from the continuum limit vs. N for two-particle system (9) in two dimensions. Solid lines give the leading $1/N^p$ behavior, while dashed lines correspond to the fitted polynomial functions.

3. Numerical Results

In order to verify the analytically derived speedup in convergence of discretized path integrals, we have performed a series of path integral Monte Carlo simulations of transition amplitudes for a two-dimensional system of two particles interacting through the potential

$$V(\vec{r}_1, \vec{r}_2) = \frac{1}{2}(\vec{r}_1 - \vec{r}_2)^2 + \frac{g_1}{24}(\vec{r}_1 - \vec{r}_2)^4 + \frac{g_2}{2}(\vec{r}_1 + \vec{r}_2)^2. \quad (9)$$

All numerical simulations were done using the latest version of our SPEEDUP¹² program that has been extended so as to include multi-particle multi-dimensional systems. The simulations have been performed for different values of couplings g_1 and g_2 and for a variety of initial and final states. The associated continuum limit amplitudes $A^{(p)}$ have been estimated by fitting polynomials in $1/N$ to the discretized values $A_N^{(p)}$, according to the analytically derived relation (5). For all values of p the fitted continuum values $A^{(p)}$ agree within the error bars. Figure 1 gives the plot of the deviations of discretized amplitudes from the continuum limit for two-particle system (9) in two dimensions, with $g_1 = 10$, $g_2 = 0$, $T = 1$, and initial and final states $a = (0, 0; 0.2, 0.5)$, $b = (1, 1; 0.3, 0.6)$. The number of MC samples was from 10^6 for $p = 1$ to 10^{10} for $p = 4$. The increase of level p leads to an ever faster approach to the continuum. The obtained $1/N^p$ dependence gives explicit verification of the analytically derived increase in convergence. As a result of the newly presented method, the usual simu-

lations proceed much faster than by using standard calculation schemes. Note that even the $p = 4$ curve corresponds to a precision of four decimal places in the case of an extremely coarse discretization such as $N = 2$.

4. Conclusions

We have presented a derivation of discretized effective actions leading to substantial, systematic speedup of numerical calculation of path integrals of a generic many-particle non-relativistic theory. The derived speedup holds for all path integrals - for transition amplitudes, partition functions, expectation values, energy levels. The newly calculated discretized effective actions agree with previous approaches. The obtained analytical results have been numerically verified through simulations of path integrals for an anharmonic oscillator with quartic coupling for two particles in two spatial dimensions. The two principle advantages of the new method are: simpler derivation and straightforward generalization to more complex systems.

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