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Accelerated path integral calculations for many-body systems

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Abstract. We present a generalization of a recently developed method for accelerated Monte Carlo calculation of path integrals of generic many particle systems. Using this method and the derived hierarchy of effective actions we calculate the energy spectra of a two particle model with quartic interaction for several values of coupling and demonstrate agreement with analytical results governing the increase in efficiency of the new method.

Keywords: Path integral, Effective action, Many-body systems

1. Introduction

Path integrals present a compact formalism for dealing with quantum theories [1, 2, 3]. In analytical approaches, path integrals allow for a generalization and extension of quantization methods to more complex physical systems, including systems with no classical counterparts [4]. Path integrals give an ideal mathematical framework for dealing with symmetries (e.g. gauge symmetry, symmetry breaking, anomalies), and for deriving nonperturbative results [5, 6]. Originally introduced in quantum mechanics and later most widely used in high energy theory, path integrals are today used in almost all areas of physics, ranging from the condensed matter, 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 and in modern finance [7], especially in option pricing applications [8, 9]. The downside of the formalism is that the mathematical properties of path integrals are not sufficiently well understood, and that an extremely small number of path integrals can be solved exactly [10]. An extensive overview of the path integral formalism and its various applications can be found in [11]. Although functional formalism has been used to derive many general approximation techniques (e.g. perturbation theory, semiclassical expansion, variational methods) along with a host of model-specific approximation techniques, many interesting models cannot be analyzed analytically in sufficient detail, with required precision, or in a given sector, and need to be treated numerically.

The definition of path integrals as a limit of multiple integrals over a discretized theory makes their numerical evaluation quite natural. The most applicable and efficient numerical method for such calculations is based on various Monte Carlo (MC) techniques [12]. Path Integral Monte Carlo (PIMC) simulations represent a general tool for numerical evaluation of properties of complex quantum and statistical systems. PIMC techniques dominate over other numerical

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methods for calculating integrals of high dimensionality. Reviews of some key PIMC variants (Metropolis, Green's function MC, Diffusion MC, Fourier PIMC) can be found in refs. [12, 13]. Notwithstanding the successes of these modern numerical integration methods, path integrals remain notoriously demanding of computing. This presents the main obstacle for tackling many important physical problems. The slow convergence of numerical methods is the direct result of our limited analytical knowledge of the properties of path integrals. Substantial new speedup can only follow from key new analytical input.

Considerable research effort has been devoted to the development of approaches that will enable faster numerical convergence to the continuum. Efficient implementation of PIMC algorithms, coupled with various physical system approximations, has resulted in important advances in the application of path integrals to real-world problems [14, 15, 13]. Another line of research has been the construction of discretized effective actions that speed up convergence of discretized physical quantities to the continuum limit. This has been done through the application of generalized Trotter formulas [16, 17, 18, 19], improvements in short-time propagation [20, 21, 22], and the application of various model-specific improvements to the action [23, 24]. A comparison of several of these approaches is given in ref. [25].

A recently developed method for analytical construction of improved discretized effective actions [26, 27, 28], based on the study of relationship between discretizations of different coarseness [29, 30], has led to substantial speedup of numerical path-integral calculations of several orders of magnitude for transition amplitudes, partition functions and expectation values. The discretized effective actions within this approach are labeled by a level number p, leading to $1/N^p$ convergence to the continuum limit, where N is the discretization coarseness. Up to now, the method has been limited to one-particle one-dimensional systems. The key new step that we present in this paper is the generalization of this formalism to generic non-relativistic many-particle systems in arbitrary dimensions.

The organization of the paper is as follows: Section 2 introduces the hierarchy of effective discretized actions and gives a brief overview of previously obtained results. The new and extended (many particles, higher dimensions) analytical approach to the construction of these effective actions is presented in Section 3. Section 4 presents numerical results that demonstrate the validity of the analytically derived speedup in convergence. The efficiency of the new approach is further demonstrated in Section 5 through the calculation of energy spectra of several models, which extend the results previously obtained in refs. [31, 32]. We conclude the paper with a brief summary of obtained results, indicating what we see to be the next steps in our line of research and its future applications. The Appendix gives the level $p = 5$ discretized effective action, leading to $1/N^5$ convergence to the continuum limit for path integral calculations of general quantum many-body systems in arbitrary number of dimensions. Higher level effective actions have been derived and are available on our web site [33].

2. Effective actions

We present a method for systematically increasing the efficiency of PIMC calculations of a general quantum theory. 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, with Hamiltonian of the form $\hat{H} = \hat{K} + \hat{V}$, where $\hat{K}$ is the usual kinetic energy operator, and $\hat{V}$ is the potential describing interparticle interactions and interactions with external fields. The above set of theories encompasses a large number of physically relevant models. However, as we shall see from the derivations, the method is in principle applicable to all quantum theories.

In the path integral formalism, the imaginary time amplitude $A(a, b; T)$ for a transition from initial state[1] $|a\rangle$ to final state $|b\rangle$ in time T is given as the $N \to \infty$ limit of the discretized

[1] The set of positions of all particles in coordinate representation is described by an Md dimensional vector.

amplitude[2]

$$A_N(a,b;T) = \frac{1}{(2\pi\varepsilon)^{\frac{MNd}{2}}} \int \mathrm{d}q_1 \cdots \mathrm{d}q_{N-1}\ e^{-S_N}\,. \tag{1}$$

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

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

Vectors with one index (e.g. q_n) represent the set of positions of all particles after n time steps $\varepsilon = T/N$, while vectors with two indices (e.g. $q_{n,i}$) represent d-dimensional positions of particle i at time step $n\varepsilon$. We have also introduced discretized velocities $\delta_{n,i} = q_{n+1,i} - q_{n,i}$ and mid-point coordinates $\bar{q}_n = (q_n + q_{n+1})/2$. The $N \to \infty$ limit of the above discretized amplitude gives the continuum amplitude $A(a,b;T)$ in the mid-point prescription, symbolically written as

$$A(a,b;T) = \int_{q(0)=a}^{q(T)=b} [\mathrm{d}q]\ e^{-S[q(t)]}\,. \tag{3}$$

The above definition of path integral requires the transition from continuum to discretized theory, i.e. the introduction of coarseness N. Although well suited for numerical calculations, expressions given by equation (1) converge to the continuum very slowly, typically as $O(1/N)$, and it is quite natural to look for a discretization scheme leading to better convergence. It was shown in [29] that there is an ideal discretization (determined by the ideal discretized action S^*), giving for a general theory the exact (continuum limit) result for *any* discretization coarseness N

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

Note that for free particles S^* is in fact just the naively discretized action.

The defining relation for path integrals as the continuum limit of discretized amplitudes given by equation (1) follows from the completeness relation (decomposition of unity)

$$A(a,b;T) = \int \mathrm{d}q_1 \cdots \mathrm{d}q_{N-1}\ A(a,q_1;\varepsilon) \cdots A(q_{N-1},b;\varepsilon)\,, \tag{4}$$

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 to higher orders in ε. From the above completeness relation, it follows that the ideal discretized action S^* leads to exact propagation in time, and is given in terms of the exact amplitude, according to

$$A(q_n, q_{n+1};\varepsilon) = (2\pi\varepsilon)^{-\frac{Md}{2}}\ \ e^{-S^*_n}\,. \tag{5}$$

The ideal discretized action S^* is simply the sum of expressions S^*_n.

The knowledge of the ideal action S^* is equivalent to the knowledge of the exact expression for the amplitude A. At first, this would seem to indicate that nothing is to be gained by equation (5). This is, however, not the case. We will use equation (5) to input new analytical information into our numerical procedure by calculating amplitudes within some available analytical approximation scheme. For example, short time propagation can be calculated as a power series expansion in ε, which starts from the naive action (2). The details of this derivation have been inspired by [11] and are presented in Section 3. One can also attack the

[2] Throughout the paper, we use system of units in which $\hbar$ and masses of all particles are set to unity. If needed, those quantities can be easily recovered in all expressions using dimensional analysis.

problem of solving equation (5) using various other approximative schemes, especially in the case when short time approximation is not appropriate. The application of the Feynman and Kleinert variational approach [34, 35], further developed in [36, 37, 38, 39, 40], could prove very useful is such cases.

We can look at the problem of speeding up the numerical convergence of discretized path integral expressions from another point of view. Purely considering the discretization procedure, we can immediately conclude that (2) is not unique, and that the freedom we have in the discretization procedure can be effectively used to speed up numerical convergence of discretized path integral calculations.

The first type of freedom is associated with the prescription used. For the class of theories considered, i.e. theories without ordering ambiguities, we have the freedom to choose the points in which to evaluate the potential V. For example, we could choose the point $\alpha q_n + (1-\alpha) q_{n+1}$ for any $\alpha \in [0,1]$. As is well known, different choices correspond to different ordering prescriptions in the operator formalism. The choice of the middle point $\bar{q}_n$ ($\alpha = 1/2$) is the most common one. It corresponds to the symmetric or Weyl ordering of operators $\hat{p}$ and $\hat{q}$, and so always leads to a hermitian expression for the hamiltonian $\hat{H}$. Two other prescriptions are also often used. The left ordering prescription evaluates the potential at q_n ($\alpha = 1$), the left boundary of the interval $[q_n, q_{n+1}]$ (in the operator formalism this corresponds to taking the $\hat{p}$'s to the left of the $\hat{q}$'s in all the products that appear in the hamiltonian). Similarly, one defines the right ordering prescription ($\alpha = 0$). Although they lead to somewhat simpler looking expressions, the left and right prescriptions do not in general give hermitian hamiltonians. However, for the considered class of theories, all prescriptions lead to the same continuum amplitude – the discretized amplitudes do differ, but they tend to the same continuum limit. However, as we shall see at the end of this section, the choice of prescription does somewhat affect the speed of convergence.

The second, and more important freedom related to our choice of discretized action has to do with the introduction of additional terms that explicitly vanish in the continuum limit. In contrast to the first type of freedom in the discretization procedure which is present only if there are no ordering ambiguities, this second type of freedom exist for all theories. This freedom is much wider than the first one, allowing for a 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

$$A_N^{(p)}(a,b;T) = A(a,b;T) + O(1/N^p). \tag{6}$$

We designate such improved discretized actions as effective actions. For example, the term

$$\sum_{n=0}^{N-1} \sum_{i=1}^{M} \varepsilon \, \delta_{n,i}^2 \, g(\bar{q}_{n,i}) \,,$$

where g is regular function when $\varepsilon \to 0$, does not change the continuum physics since it goes over into

$$\varepsilon^2 \sum_{i=1}^{M} \int_0^T \mathrm{d}t \, \dot{q}_i^2 \, g(q_i) \,,$$

i.e. it vanishes as ε^2. Although such additional terms do not change the continuum physics they do affect the speed of convergence to that continuum limit.

In a previous series of publications [26, 27, 28] we had constructed the effective actions $S^{(p)}$ through a study of the relation between discretizations of different coarseness. This investigation was limited to one-dimensional one-particle models with Hamiltonians of the form

$\hat{H} = \frac{1}{2}\hat{p}^2 + V(\hat{q})$. In the next section we present a new, more general approach which can be applied to more complex systems (many particles, higher dimensions, general Hamiltonian). Where applicable, the two methods are equivalent: $S^{(p)}$ is just the solution of equation (5) truncated to ε^p.

Before going into further details about the new method, we give a brief overview of earlier results related to the speeding up of the convergence of path integral calculations. Key results regarding numerical evaluation of path integrals are presented in the reviews of Barker and Henderson [14], Kalos and Whitlock [12], and Ceperley [13], as well as in the papers by Pollock and Ceperley [15]. More recent results regarding the efficient implementation of PIMC algorithms are available in refs. [41, 42, 43, 44, 45]

As already stated, the mid-point prescription using the naively discretized action gives

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

for all a and b. On the other hand, in the naive left prescription the diagonal amplitude for $a \to a$ transitions converges much faster

$$A_N(a,a;T)^{left} = A(a,a;T) + O(1/N^2)\,.$$

This behavior can be easily shown both analytically and numerically. We note in passing that this is strongly related to the well known result for the partition function evaluated using naive discretization in the left prescription [25], which follows directly from the above amplitude by integrating over a (to get the trace) and writing the time of propagation T as the inverse temperature β,

$$Z_N(\beta)^{left} = Z(\beta) + O(1/N^2)\,.$$

However, going back to the language of amplitudes, it is also easy to show that the amplitudes for different initial and final states converge slower, i.e. for $a \neq b$ we have again

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

Note that the $1/N^2$ speed of convergence of off-diagonal amplitudes in the left prescription can be recovered very easily. It was shown in ref. [27] that for all a and b we have

$$\frac{1 + e^{\varepsilon(V(a)-V(b))}}{2}\, A_N(a,b;T)^{left} = A(a,b;T) + O(1/N^2)\,.$$

For a long time the state of the art result was $1/N^4$ convergence of discretized partition functions obtained by Takahashi and Imada [17], and Li and Broughton [18]. In these papers the authors used a generalized form [16] of the Trotter formula to increase the speed of convergence of the discretized partition function. Their final result is a derivation of a formula for the effective potential

$$V^{eff} = V + \frac{1}{24}\varepsilon^2 (V')^2\,.$$

The authors showed that by using this effective potential (in the left prescription) one gets

$$Z_N(\beta)^{eff} = Z(\beta) + O(1/N^4)\,.$$

Let us note that the crucial step in the derivation of the above effective potential from the generalized Trotter formula uses the cyclic property of the trace, i.e. the above increase in the speed of convergence only holds for the partition function and not the amplitudes. A direct numerical simulation shows that amplitudes calculated using this effective potential converge just as fast as the amplitudes in the naive left prescription, i.e. as $1/N$. Said another way, it is only the integral over all the diagonal amplitudes that has the $O(1/N^4)$ behavior and not any individual amplitude.

3. New approach

As already outlined, the standard definition of path integrals as limits of time-sliced discretized expressions is based on the completeness relation (4). As we have seen, the next step is the approximate calculation of short-time amplitudes $A(q_n, q_{n+1}; \varepsilon)$ as a power series in ε. The use of the naive action in equation (1) corresponds to keeping only the dominant term for the short-time amplitude. This is what gives the $1/N$ convergence to standard path integral expressions[3]. Calculating the short time amplitudes exactly we find

$$A(q_n, q_{n+1}; \varepsilon) = (2\pi\varepsilon)^{-\frac{Md}{2}} \, e^{-S_n^*(q_n, q_{n+1}; \varepsilon)}, \tag{7}$$

where the ideal discretized effective action equals

$$S_N^* = \sum_{n=0}^{N-1} S_n^*(q_n, q_{n+1}; \varepsilon) \, .$$

$1/N^p$ convergence of path integrals is obtained by evaluating amplitudes up to order ε^p,

$$A(q_n, q_{n+1}; \varepsilon) = (2\pi\varepsilon)^{-\frac{Md}{2}} \left(e^{-S_n^{(p)}(q_n, q_{n+1}; \varepsilon)} + O(\varepsilon^{(p+1)}) \right) . \tag{8}$$

Inserting the above result into the formula for S_N^*, we obtain the level p effective action $S_N^{(p)}$ as

$$S_N^{(p)} = \sum_n S_n^{(p)}(q_n, q_{n+1}; \varepsilon) \, . \tag{9}$$

A simple shift of integration variable $q = \xi + x$ about a fixed referent trajectory ξ gives

$$A(q_n, q_{n+1}; \varepsilon) = e^{-S_n[\xi]} \int_{x(-\varepsilon/2)=0}^{x(\varepsilon/2)=0} [\mathrm{d}x] \; e^{-\int_{-\varepsilon/2}^{\varepsilon/2} \mathrm{d}s \left(\frac{1}{2}\dot{x}^2 + U(x;\xi) \right)} . \tag{10}$$

Note that we have also shifted the time from $t \in [n\varepsilon, (n+1)\varepsilon]$ to $s \in [-\varepsilon/2, \varepsilon/2]$. The referent trajectory ξ satisfies the same boundary conditions as q. As a result, the new integration variable x vanishes at the boundaries. The action $S_n[\xi]$ is defined as

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

and $U(x;\xi) = V(\xi+x) - V(\xi) - x\ddot{\xi}$, with dots representing derivatives over time s. The amplitude may now be written as

$$A(q_n, q_{n+1}; \varepsilon) = \frac{e^{-S_n[\xi]}}{(2\pi\varepsilon)^{\frac{Md}{2}}} \left\langle e^{-\int_{-\varepsilon/2}^{\varepsilon/2} \mathrm{d}s \; U(x;\xi)} \right\rangle , \tag{11}$$

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.

The class of theories considered is free of ordering ambiguities, i.e. different ordering prescriptions yield the same continuum results. We will present a derivation of the discretized effective actions in the midpoint prescription. We stress that the same calculation can be done just as easily in any other ordering prescription. Since we are using series expansion in small

[3] When calculating partition functions in the left prescription one has an additional symmetry which gets rid of odd powers in ε. As a result, in this case naive discretization converges as $1/N^2$.

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 $\delta_{n,i}^2 \propto \varepsilon$. Therefore, keeping all terms proportional to $\varepsilon^k \delta_{n,i}^{2l}$ with $k+l \leq p$ will be sufficient for obtaining the desired precision.

The free particle expectation value in equation (11) is calculated using the series expansion

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

with shorthand notation $x' = x(s'), \xi' = \xi(s')$. By expanding $U(x;\xi)$ around the referent trajectory ξ, we get

$$U(x;\xi) = x_i(\partial_i V(\xi) - \ddot{\xi}_i) + \frac{1}{2} x_i x_j \partial_i \partial_j V(\xi) + \dots \,. \tag{12}$$

From now on, indices i and j go over all Md components of positions of particles, and we assume summation over repeated indices. Expectation values of products $\langle x_i(s) \dots x_j(s') \rangle$ can be calculated in the usual way, by introducing a generating functional for the free-particle theory whose propagator is given by:

$$\begin{aligned} \Delta(s,s')_{i,j} = & \quad \frac{\delta_{ij}}{\varepsilon} \theta(s-s') \left(\frac{\varepsilon}{2} - s \right) \left(\frac{\varepsilon}{2} + s' \right) \\ + & \quad \frac{\delta_{ij}}{\varepsilon} \theta(s'-s) \left(\frac{\varepsilon}{2} + s \right) \left(\frac{\varepsilon}{2} - s' \right). \end{aligned} \tag{13}$$

Using Wick's theorem, one easily finds $\langle x_i(s) \rangle = 0$, $\langle x_i(s) x_j(s') \rangle = \Delta(s,s')_{i,j}$, 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 (13). 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 leads to short-time expansion.

In order to perform the remaining integrations over s in (11), due to the explicit dependence of the referent trajectory on s, we first expand the potential and all its derivatives in (12) 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 in (11) 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:

$$S_n[\xi] = \varepsilon \left(\frac{1}{2} \frac{\delta_n^2}{\varepsilon^2} + V(\bar{q}_n) + \frac{\delta_{n,i} \delta_{n,j}}{24} \partial_{i,j}^2 V(\bar{q}_n) \right) + O(\varepsilon^3) \,, \tag{14}$$

$$\left\langle e^{-\int \mathrm{d}s\ U(x;\xi)} \right\rangle = 1 - \frac{\varepsilon^2}{12} \Delta V(\bar{q}_n) + O(\varepsilon^3) = e^{-\frac{\varepsilon^2}{12} \Delta V(\bar{q}_n)} + O(\varepsilon^3) \,. \tag{15}$$

From these expressions we see that the level $p = 2$ discretized effective action is

$$S_N^{(p=2)} = \sum_{n=0}^{N-1} \varepsilon \left(\frac{1}{2} \left(\frac{\delta_n}{\varepsilon} \right)^2 + V(\bar{q}_n) + \frac{\varepsilon}{12} \Delta V(\bar{q}_n) + \frac{\delta_{n,i} \delta_{n,j}}{24} \partial_{i,j}^2 V(\bar{q}_n) \right). \tag{16}$$

In the above equation, the Laplacian operator consists of the sum of second partial derivatives over all Md components of vectors of particle positions. The explicit analytical expression for

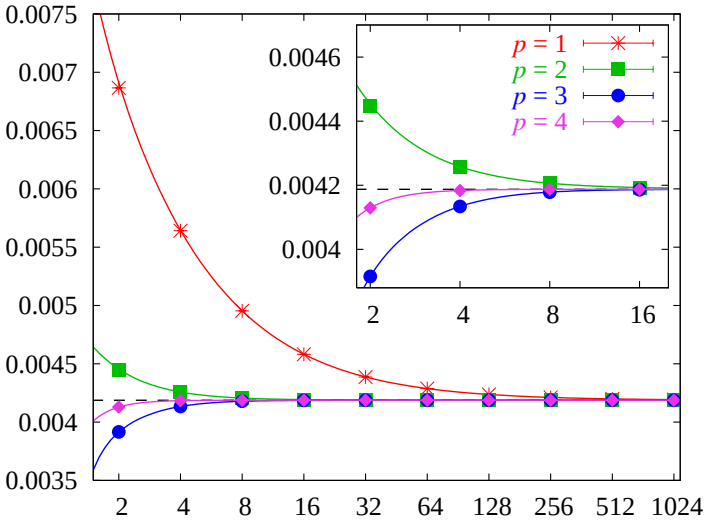

Figure 1. Convergence of the discretized amplitudes $A_N^{(p)}$ to the continuum as functions of N for $p = 1, 2, 3, 4$ for the system of two particles in two dimensions in a quartic potential (17), $g_1 = 10$, $g_2 = 0$, with time of propagation $T = 1$ and initial and final states $a = (0, 0; 0.2, 0.5)$, $b = (1, 1; 0.3, 0.6)$. The number of MC samples was 10^6. Horizontal black line represents the continuum limit, while solid lines correspond to the fitted functions given by (18).

the many-particle discretized effective action at level $p = 5$ is given in the Appendix. There are no obstacles in going to higher values of p. The derived expressions become algebraically more complex, and the calculations are best conducted using some of the available packages for symbolic calculus (e.g. Mathematica). Higher level effective actions can be found on our web site [33].

4. Numerical results

In this section we present results of numerical PIMC simulations that confirm the analytically derived speedup in convergence of discretized path integrals. To do this, we have conducted a series of PIMC simulations of transition amplitudes for a two-dimensional system of two particles interacting through potential

$$V(\vec{r}_1, \vec{r}_2) = \frac{1}{2}(\vec{r}_1 - \vec{r}_2)^2 + \frac{g_1}{24}(\vec{r}_1 - \vec{r}_2)^4 + \frac{g_2}{2}(\vec{r}_1 + \vec{r}_2)^2 \,. \tag{17}$$

Numerical simulations, based on our SPEEDUP [33] PIMC code, have been performed for different values of couplings g_1 and g_2 and for 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 (6):

$$A_N^{(p)} = A^{(p)} + \frac{B^{(p)}}{N^p} + \frac{C^{(p)}}{N^{p+1}} + \dots \,. \tag{18}$$

For all values of p the fitted continuum values $A^{(p)}$ agree within the error bars. The obtained $1/N$ dependence gives explicit verification of the analytically derived increase in convergence. The typical case is illustrated in Figure 1. The expected $1/N^p$ convergence may be most easily discerned from Figure 2, the plot of the deviations of discretized amplitudes from the continuum limit. As can be seen, the increase of level p leads to an ever faster approach to the continuum.

As a result of the newly presented method, the usual simulations (in which one calculates specific physical quantities such as the one in Figure 1) proceed much faster than by using standard methods. On the other hand, Figure 2 is itself time consuming since it illustrates subdominant behavior. For this reason the figures contain only results obtained by effective action to level $p = 4$. Note, however, that the $p = 4$ curve corresponds to a precision of four decimal places even for an extremely coarse discretization such as $N = 2$.

In usual PIMC calculations one always chooses the number of MC samples so that the stochastic error of numerical results is of the order of deviations from the continuum limit. In Figure 2 the number of MC samples had to be much larger, in order for deviations from the continuum limit to be clearly visible.

5. Energy spectra

The improved convergence of path integral expressions for amplitudes leads directly to the same kind of improvement in the convergence of discretized partition functions, owing to the relation

$$Z_N(\beta) = \int \mathrm{d}q A_N(q, q; \beta)\,, \tag{19}$$

where the inverse temperature β plays the role of the time of propagation T. The partition function is the central object for obtaining information about statistical systems. In addition, the partition function offers a straightforward way for extracting information about low lying energy levels of a system. This follows from evaluating the trace in the definition of the partition function in the energy eigen-basis

$$Z(\beta) = \sum_{n=0}^{\infty} d_n e^{-\beta E_n}\,, \tag{20}$$

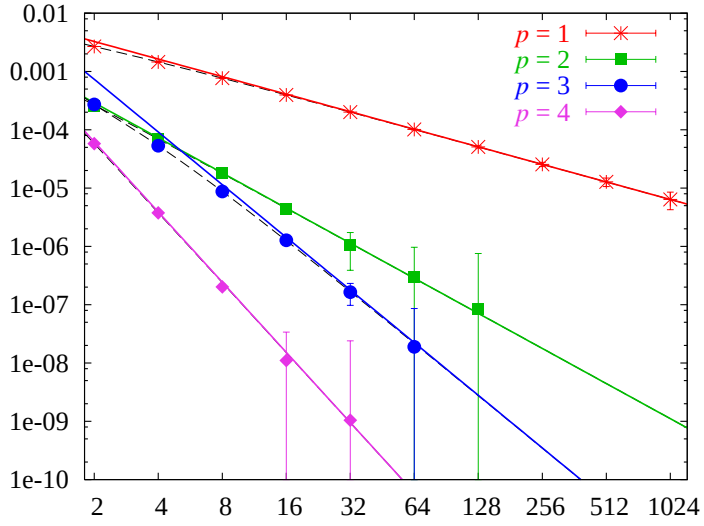

Figure 2. Deviations from the continuum limit $|A_N^{(p)} - A|$ as functions of N for $p = 1, 2, 3, 4$ for the system of two particles in two dimensions in quartic potential $g_1 = 10$, $g_2 = 0$, with time of propagation $T = 1$ and initial and final states $a = (0, 0; 0.2, 0.5)$, $b = (1, 1; 0.3, 0.6)$. The number of MC samples was 10^6 ($p = 1$), 10^7 ($p = 2$), 10^9 ($p = 3$), and 10^{10} ($p = 4$). Solid lines give the leading $1/N^p$ behavior, while dashed lines correspond to the fitted functions given by (18).

where E_n and d_n denote corresponding energy levels and degeneracies. A detailed description of the procedure for extracting energy levels from the partition function is given in [31, 32]. The free energy of the system, given by

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta)\,, \tag{21}$$

tends to the ground state energy E_0 in the large β limit. Similarly, we introduce auxiliary functions

$$F^{(n)}(\beta) = -\frac{1}{\beta} \ln \frac{Z(\beta) - \sum_{i=0}^{n-1} d_i\ e^{-\beta E_i}}{d_n}\,, \tag{22}$$

which can be fitted for large β to

$$f^{(n)}(\beta) = E_n - \frac{1}{\beta} \ln(1 + ae^{-\beta b})\,. \tag{23}$$

and which tend to the corresponding energy level E_n.

In this way, by studying the large β behavior of the free energy and the corresponding auxiliary functions, one obtains the low lying energy spectrum of the model. Note that the procedure for the construction of the auxiliary function $f^{(n)}$ is recursive, i.e. in order to construct $f^{(n)}$ we need to now all the energy levels below E_n. This leads to the accumulation of errors as n increases, and limits the number of levels that can be calculated. The practical limit on how high in the spectrum we can go depends on the precision with which we calculate path integrals. The orders of magnitude increase in precision of the presented method for calculating path integrals can therefore be used to extract numerical information about a larger number of energy levels.

Figures 3 and 4 illustrate the calculation of low lying energy levels using the more efficient PIMC formalism presented in this paper on the case of a two-dimensional system of two distinguishable particles interacting through a quartic potential (17).

Figure 3 demonstrates that the improved convergence of free energies is the same as in the case of amplitudes. Figure 4 illustrates the calculation of the low lying energy levels of the

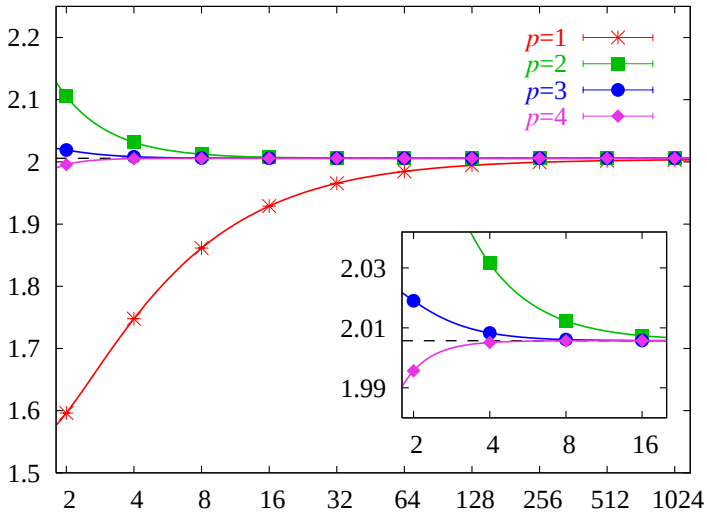

Figure 3. Convergence of discretized free energies $F_N(\beta)$ to the continuum as functions of N for $p = 1, 2, 3, 4$ for the system of two particles in two dimensions in a potential (17), $g_1 = 1$, $g_2 = 1$, $\beta = 1$. The number of MC samples was 10^7.

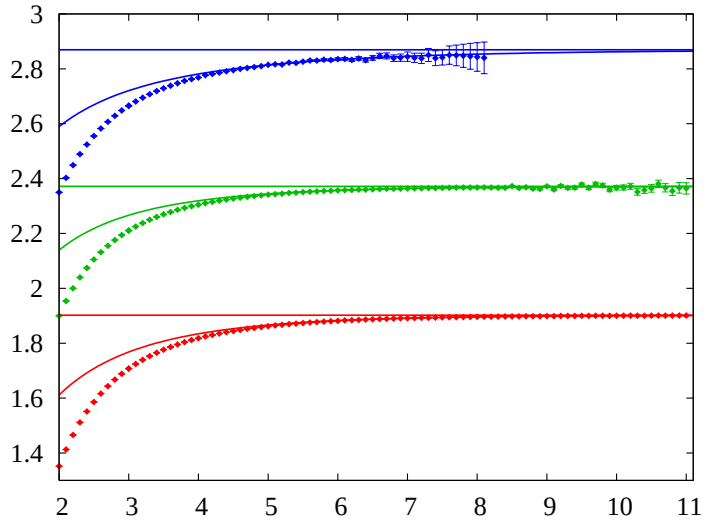

Figure 4. Dependence of the free-energy and auxiliary functions $f^{(1)}$ and $f^{(2)}$ on β for the system in the potential (17), $g_1 = 0$, $g_2 = 1/9$. Horizontal lines correspond to energy levels. Numerical simulations were performed with 10^9 MC samples, level $p = 5$ effective action and $N = 64$.

model. Table 1 gives the calculated energy levels for quartic coupling from $g_1 = 0$ (free theory) to $g_1 = 10$ (strongly interacting theory).

Table 1. Low lying energy levels of the system in the potential given by (17), $g_2 = 1/9$, calculated using $= 10^9$ MC samples, level $p = 5$ effective action and $N = 64$. The degeneracies of the calculated energy levels are found to be $d_0 = 1$, $d_1 = 2$, $d_2 = 3$, $d_3 = 6$.

g_1	E_0	E_1	E_2	E_3
0	1.8857(1)	2.3571(6)	2.83(1)	3.3(2)
0.1	1.9019(2)	2.374(2)	2.82(1)	—
1	2.0228(2)	2.497(3)	2.94(3)	—
10	2.6327(6)	3.098(4)	3.57(3)	—

6. Conclusions

We have presented a derivation of discretized effective actions that lead to substantial, systematical speedup of numerical procedures for the 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 [46], as well as for calculations of energy levels. The obtained analytical results have been numerically verified through simulations of path integrals for several multi-particle models. The developed calculation scheme has been completed and is ready for applications to relevant problems in condensed matter physics. Further analytical work will focus on the generalization of the outlined scheme to more complex quantum systems: bosonic and fermionic quantum field theory, gauge theories, topologically non-trivial spaces.

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Appendix
The effective discretized action for a general non-relativistic multi-particle system in the mid-point prescription is, to level $p = 5$, given by

$$
\begin{aligned}
S_N^{p=5} &= \sum \Big\{ \frac{\delta_i \delta_i}{2\varepsilon^2} + V \Big\}_{p=1} \\
&+ \Big\{ \frac{\varepsilon}{12} \Delta V + \frac{\delta_i \delta_j}{24} \partial^2_{i,j} V \Big\}_{p=2} \\
&+ \Big\{ -\frac{\varepsilon^2}{24} \partial_i V \partial_i V + \frac{\varepsilon^2}{240} \Delta\Delta V + \frac{\varepsilon \delta_i \delta_j}{480} \partial^2_{i,j} \Delta V + \frac{\delta_i \delta_j \delta_k \delta_l}{1920} \partial^4_{i,j,k,l} V \Big\}_{p=3} \\
&+ \Big\{ \frac{\varepsilon^3}{6720} \Delta\Delta\Delta V - \frac{\varepsilon^3}{120} \partial_i V \partial_i \Delta V - \frac{\varepsilon^3}{360} \partial^2_{i,j} V \partial^2_{i,j} V \\
&- \frac{\varepsilon^2 \delta_i \delta_j}{480} \partial_k V \partial^3_{k,i,j} V + \frac{\varepsilon^2 \delta_i \delta_j}{13440} \partial^2_{i,j} \Delta\Delta V - \frac{\varepsilon^2 \delta_i \delta_j}{1440} \partial^2_{i,k} V \partial^2_{k,j} V \\
&+ \frac{\varepsilon \delta_i \delta_j \delta_k \delta_l}{53760} \partial^4_{i,j,k,l} \Delta V + \frac{\delta_i \delta_j \delta_k \delta_l \delta_m \delta_n}{322560} \partial^6_{i,j,k,l,m,n} V \Big\}_{p=4} \\
&+ \Big\{ \frac{\varepsilon^4}{241920} \Delta\Delta\Delta\Delta V - \frac{\varepsilon^4}{1680} \partial^2_{i,j} V \partial^2_{i,j} \Delta V - \frac{17\varepsilon^4}{40320} \partial_i \Delta V \partial_i \Delta V \\
&- \frac{\varepsilon^4}{2240} \partial_i V \partial_i \Delta\Delta V - \frac{\varepsilon^4}{6720} \partial^3_{i,j,k} V \partial^3_{i,j,k} V + \frac{\varepsilon^4}{240} \partial_i V \partial_j V \partial^2_{i,j} V \\
&+ \frac{\varepsilon^3 \delta_i \delta_j}{483840} \partial^2_{i,j} \Delta\Delta\Delta V - \frac{\varepsilon^3 \delta_i \delta_j}{6720} \partial_k V \partial^3_{i,j,k} \Delta V - \frac{\varepsilon^3 \delta_i \delta_j}{10080} \partial^2_{i,k} V \partial^2_{k,j} \Delta V \\
&- \frac{\varepsilon^3 \delta_i \delta_j}{10080} \partial^2_{k,l} V \partial^4_{i,j,k,l} V - \frac{\varepsilon^3 \delta_i \delta_j}{5040} \partial_k \Delta V \partial^3_{i,j,k} V - \frac{\varepsilon^3 \delta_i \delta_j}{20160} \partial^3_{i,k,l} V \partial^3_{k,l,j} V \\
&+ \frac{\varepsilon^2 \delta_i \delta_j \delta_k \delta_l}{1935360} \partial^4_{i,j,k,l} \Delta\Delta V - \frac{\varepsilon^2 \delta_i \delta_j \delta_k \delta_l}{53760} \partial_m V \partial^5_{m,i,j,k,l} V \\
&- \frac{\varepsilon^2 \delta_i \delta_j \delta_k \delta_l}{40320} \partial^2_{i,m} V \partial^4_{m,j,k,l} V - \frac{\varepsilon^2 \delta_i \delta_j \delta_k \delta_l}{32256} \partial^3_{i,j,m} V \partial^3_{m,k,l} \\
&+ \frac{\varepsilon \delta_i \delta_j \delta_k \delta_l \delta_m \delta_n}{11612260} \partial^6_{i,j,k,l,m,n} \Delta V + \frac{\delta_i \delta_j \delta_k \delta_l \delta_m \delta_n \delta_p \delta_q}{92897280} \partial^8_{i,j,k,l,m,n,p,q} V \Big\}_{p=5}
\end{aligned}
$$

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