

# Effective Actions for Path Integral Monte Carlo Calculations

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**Abstract.** Effective action approach for path integral Monte Carlo calculations is introduced and the derivation of the corresponding effective actions, improving the convergence of discretized quantum mechanical amplitudes, partition functions and expectation values from  $1/N$  to  $1/N^p$ , is presented. Applicability of previously developed method is extended to multidimensional many-particle systems. The presented results of numerical simulations demonstrate the expected increase in the speed of convergence.

## INTRODUCTION

Path Integral Monte Carlo (PIMC) simulations are very important, general tool for numerical calculations of properties of complex quantum and statistical systems that cannot be solved analytically or treated satisfactorily using approximative techniques. Considerable effort has been devoted to the development of approaches that will enable faster convergence of discretized path-integral expressions [1]. Recent series of papers [2, 3] has focused on systematic analytical construction of effective actions that improve convergence of discretized transition amplitudes, partition functions and expectation values to the continuum limit for one-particle one-dimensional systems. This new analytical input has allowed significant speedup of several orders of magnitude in numerical calculations. Originally, effective actions have been derived considering  $N$ -fold and  $2N$ -fold discretizations of the same theory. In this paper we present different way of derivation of effective actions, which is applicable to general non-relativistic many-body systems whose lagrangian is of the form  $L = \frac{1}{2}\dot{q}^2 - V(q)$ , where  $q$  denotes vector of all coordinates of all particles in the system.

## DERIVATION OF EFFECTIVE ACTIONS

Basic property of the general quantum mechanical amplitude  $A(a, b; T)$  describing the transition of the system from the initial state  $|a\rangle$  to the final state  $|b\rangle$  during the time interval  $T$  is linearity: if the time interval  $T$  is subdivided into  $N$  equal time steps,  $\epsilon = T/N$ , the amplitude satisfies

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

When deriving path integral expression in the standard manner [4, 5] we proceed with approximate evaluation of amplitudes  $A(q_n, q_{n+1}; \varepsilon)$  for short times of propagation  $\varepsilon$ , leading to the well-known result for discretized amplitude in imaginary time

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

where  $S_N$  is naively discretized action  $S_N = \sum_{n=0}^{N-1} \varepsilon \left( \frac{1}{2} \left( \frac{\delta_n}{\varepsilon} \right)^2 + V(\bar{q}_n) \right)$  and  $\delta_n = q_{n+1} - q_n$ ,  $\bar{q}_n = \frac{1}{2}(q_n + q_{n+1})$ . In the continuum limit  $N \rightarrow \infty$  the discretized value of amplitude converges to the continuum amplitude  $A(a, b; T)$ , which is symbolically written as

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

The convergence to the continuum limit is slow if naively discretized action is used, typically  $O(1/N)$ . Our aim is to construct a series of effective actions  $S_N^{(p)}$  which will improve the convergence of discretized expressions to the desired order  $p$ ,  $A_N^{(p)}(a, b; T) = A(a, b; T) + O(1/N^p)$ .

Following approach described in [5], we calculate  $A(q_n, q_{n+1}; \varepsilon)$  approximately to the order  $\varepsilon^p$  using expansion around some referent trajectory; this way we would obtain sought-after discretized effective actions of level  $p$ . To simplify the derivation, we use new time variable  $s = t - \varepsilon/2$ . We also introduce new trajectories variable  $y(s)$  by relation  $x(s) = y(s) + \xi(s)$ , where  $x(s)$  are trajectories that we integrate over and  $\xi(s)$  is some fixed referent trajectory satisfying the same boundary conditions as  $x(s)$ . This results in  $y(-\varepsilon/2) = y(\varepsilon/2) = 0$ . Since the measure is invariant under the previous transformations, we have:

$$A(q_n, q_{n+1}; \varepsilon) = e^{-S(\xi)} \int_{y(-\varepsilon/2)=0}^{y(\varepsilon/2)=0} [dy] e^{-\int_{-\varepsilon/2}^{\varepsilon/2} ds \left( \frac{1}{2} \dot{y}^2 + U(y; \xi) \right)}, \quad (4)$$

$U(y; \xi) = V(\xi + y) - V(\xi) - y\ddot{\xi}$ . In order to calculate the remaining functional integral in (4), we introduce the expectation value with respect to the free particle action:

$$\langle F[y] \rangle = \frac{\int [dy] F[y] e^{-\int_{-\varepsilon/2}^{\varepsilon/2} ds \frac{1}{2} \dot{y}^2}}{\int [dy] e^{-\int_{-\varepsilon/2}^{\varepsilon/2} ds \frac{1}{2} \dot{y}^2}}. \quad (5)$$

Using this notation and expression for the free-particle transition amplitude, we obtain

$$A(q_n, q_{n+1}; \varepsilon) = \left( \frac{1}{2\pi\varepsilon} \right)^{Md/2} e^{-S[\xi]} \langle e^{-\int ds U(y; \xi)} \rangle, \quad (6)$$

where  $M$  is the number of particles and  $d$  is the number of spatial dimensions. In order to proceed, we use the following series expansion:

$$\langle e^{-\int ds U(y; \xi)} \rangle = 1 - \int ds \langle U(y; \xi) \rangle + \frac{1}{2} \int \int ds ds' \langle U(y; \xi) U(y'; \xi') \rangle + O(\langle U^3 \rangle), \quad (7)$$

with shorthand notation  $y' = y(t')$ ,  $\xi' = \xi(t')$ , and also

$$U(y, \xi) = y_i(\partial_i V(\xi) - \ddot{\xi}_i) + \frac{1}{2} y_i y_j \partial_i \partial_j V(\xi) + O(y^3). \quad (8)$$

Here  $i$  and  $j$  count  $Md$  degrees of freedom and we assume summation over repeated indices. After expanding  $V(\xi)$  and all its derivatives in (8) around  $\bar{q}_n$  in order to do the remaining integrations, from (7) and (8) it is obvious that it is sufficient to calculate  $\langle y_i(s) \rangle$ ,  $\langle y_i(s) y_j(s') \rangle$ , etc. This is achieved by introducing generating functional for the free-particle theory whose propagator in this particular case is:

$$\Delta(s, s')_{i,j} = \frac{\delta_{i,j}}{\varepsilon} \left[ \theta(s - s') \left( \frac{\varepsilon}{2} - s \right) \left( \frac{\varepsilon}{2} + s' \right) + \theta(s' - s) \left( \frac{\varepsilon}{2} + s \right) \left( \frac{\varepsilon}{2} - s' \right) \right]. \quad (9)$$

We easily see that  $\langle y_i(s) \rangle = 0$ ,  $\langle y_i(s) y_j(s') \rangle = \Delta(s, s')_{i,j}$ , etc. The calculation of the generating functional (and also of the expectation values) is the same irrespective of the choice of  $\xi$ . In all cases the action and the boundary conditions for the field  $y$  are the same, and so the propagator is always given by formula (9).

In order to achieve  $1/N^p$  convergence of  $A_N^{(p)}(a, b, T)$  we have to keep all the terms proportional to  $\varepsilon^p$  when calculating  $A(q_n, q_{n+1}; \varepsilon)$  taking into account that  $\delta_i^2 \sim \varepsilon$ . For example, choosing linear referent trajectory  $\xi(s) = \bar{q}_n + \frac{\delta_n}{\varepsilon} s$  and keeping terms up to the  $\varepsilon^2$  we obtain:

$$A(q_n, q_{n+1}; \varepsilon) = \left( \frac{1}{2\pi\varepsilon} \right)^{Md/2} \left( e^{-\varepsilon \left( \frac{\delta_n^2}{2\varepsilon^2} + V(\bar{q}_n) + \frac{\varepsilon}{12} \Delta V(\bar{q}_n) + \frac{\delta_{n,i} \delta_{n,j}}{24} \partial_{i,j}^2 V(\bar{q}_n) \right)} + o(\varepsilon^2) \right) \quad (10)$$

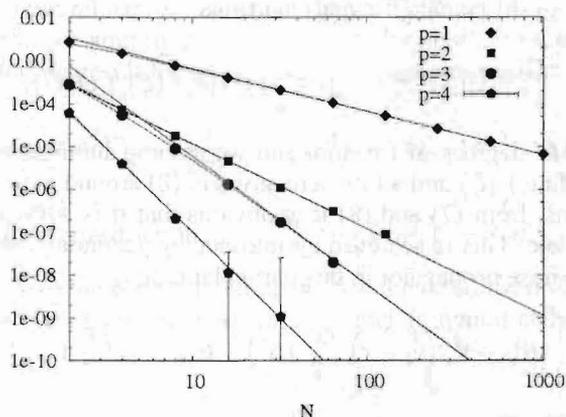
( $\Delta = \sum_{i=1}^{Md} \partial_{i,i}^2$ ). From the above formula we read off  $p = 2$  discretized effective action:

$$S_N^{(p)} = \sum_{n=0}^{N-1} \left( \frac{\delta_n^2}{2\varepsilon^2} + V(\bar{q}_n) + \frac{\varepsilon}{12} \Delta V(\bar{q}_n) + \frac{\delta_{n,i} \delta_{n,j}}{24} \partial_{i,j}^2 V(\bar{q}_n) \right) \quad (11)$$

## RESULTS AND CONCLUSIONS

Previously, for one-particle one-dimensional systems effective actions up to  $p = 12$  have been derived and applied for efficient PIMC calculations [2, 3, 7, 8]. By now, using the above outlined procedure, we have derived effective actions for general many-particle systems up to the level  $p = 5$ .

In order to verify our analytical results, Monte Carlo simulation for many-particle system of distinguishable bosons in  $d$  spatial dimensions is developed. Deviations of discretized amplitudes from the continuum limit for system of two particles in two dimensions are shown on log-log scale in Figure 1. Slopes of solid lines clearly indicate expected improved convergence governed by  $1/N^p$  term. As level  $p$  increases discretized amplitudes approach continuum limit ever faster, so for higher values of  $p$  it is possible to use much smaller values of  $N$  to obtain results of the same quality. Since the CPU



**FIGURE 1.** 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 potential  $V(\vec{q}_1, \vec{q}_2) = \frac{1}{2}(\vec{q}_1 - \vec{q}_2)^2 + \frac{g}{24}(\vec{q}_1 - \vec{q}_2)^4$ ,  $g = 10$ , with the time of propagation  $T = 1$  and initial and final states  $\vec{a} = (0, 0; 0.2, 0.5)$ ,  $\vec{b} = (1, 1; 0.3, 0.6)$ . Number of Monte Carlo samples used is  $N_{MC} = 10^6$  ( $p = 1$ ),  $N_{MC} = 10^7$  ( $p = 2$ ),  $N_{MC} = 10^9$  ( $p = 3$ ) and  $N_{MC} = 10^{10}$  ( $p = 4$ ). Solid lines give the leading  $1/N^p$  behaviour.

time of PIMC calculation depends linearly in  $N$ , this leads to substantial speedup in numerical calculations.

To conclude, new approach to the derivation of effective actions for PIMC calculations is presented. Important advantage of this approach is the possibility of its straightforward generalisation to many-particle systems. This enables wide range of applications of effective action approach for efficient PIMC simulations. Numerical simulations obtained for a two-dimensional two-particle system demonstrate analytically derived results. Derivation of higher-level effective actions and applications to systems of identical particles are in progress.

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