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Energy levels and expectation values via accelerated path integral Monte Carlo

D Stojiljković, A Bogojević and A Balaž

Scientific Computing Laboratory, Institute of Physics, Belgrade, Serbia

E-mail: danica@phy.bg.ac.yu

Abstract. A recently developed method systematically improved 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 level number p and converging to the continuum limit as $1/N^p$. Here we apply the above general method to numerical calculations using Metropolis Monte Carlo simulations of energy expectation values and energy spectra. We analyze and compare the ensuing increase in efficiency of several orders of magnitude.

Keywords: Path integral, Effective action, Monte Carlo

1. Introduction

In the middle of the last century Feynman introduced an alternate approach to quantum mechanics known as the path integral formalism [1, 2, 3]. This approach provided us with a new intuitive picture for understanding quantum mechanics, it enabled us to make connections and analogies between different areas of physics, and it also provided a new mathematical framework for calculating properties of physical systems. In particular, the formalism made it easy to generalize quantum theories from one particle to many particles and finally to fields in a relatively straightforward way. Unfortunately, the new formalism did not increase the number of analytically solvable systems [4, 5]. The fact that it enabled us to treat models that were previously inaccessible is due to its formulation in terms of discretized quantities, making it directly amenable to numerical treatment.

In numerical simulations, our poor understanding of the inherent mathematical structure of path integrals translates into the slow convergence of the sought-after physical quantities. Substantial increase in efficiency of numerical algorithms for calculating path integrals, can, therefore, come only through the input of new analytical information about path integrals into the calculation schemes. A recent series of papers [6, 7, 8] has investigated the relationship between discretizations of different coarseness in the case of a general quantum theory. The new found analytical results were then used to construct a more efficient Path Integral Monte Carlo (PIMC) SPEEDUP code [9] which increased convergence of generic path integrals from $1/N$ to $1/N^p$. For computational reasons, the level p is currently limited to $p = 13$, however, there are no fundamental barriers to going to even higher levels. This substantial increase in efficiency results in speedup of path integral calculations and has been applied to calculations of

amplitudes, partition functions, expectation values, as well as low lying energy spectra [10, 11]. Direct numerical calculations of a variety of different models have confirmed the analytically derived results.

All of the key properties of path integrals can be seen already on the example of one particle systems in one dimension. For this reason the current paper limits itself to systems of this kind. Let us note however that the generalization to more complex systems has also been investigated and confirms that the previously derived increase in efficiency holds for general many particle systems as well [12].

PIMC algorithms can be made more efficient either by getting better convergence to the continuum limit through the use of above mentioned hierarchy of discretized effective actions, or through better generation of relevant trajectories in the MC method. So far all the numerical verifications of improved $1/N^p$ convergence have been implemented using a PIMC code in which paths were generated through a Levy construction. In this paper we numerically investigate the derived speedup using Metropolis [13, 14, 15] method for generating relevant paths. In general the Metropolis technique is optimally suited for calculating expectation values. We have numerically verified the $1/N^p$ convergence, showing explicitly coexistence of improvements obtained through the use of effective actions and the Metropolis path generation method.

2. Path integrals

As previously stated, we focus on the motion of one particle in one dimension. The central object is the (Euclidean) amplitude for the quantum system to go from initial position a to final position b in imaginary time T. Feynman gave us three basic rules for calculating this transition amplitude:

(i) the contribution of each path is determined by the action functional $S[q]$, and is proportional to $e^{-S[q]}$,

(ii) one needs to take into account the contributions of all paths consistent with the boundary conditions,

(iii) contributions of different paths add up linearly, and the ensuing sum is called the part integral.

For a majority of physically interesting cases the action is of the form

$$S = \int_0^T dt \left(\frac{1}{2}\dot{q}^2 + V(q) \right) . \tag{1}$$

Note that for simplicity we are working in units where $\hbar$ and particle mass have been set to unity. The only problem in the outlined procedure is the enumeration of all possible paths. This is done by discretizing the time of propagation T into N equal time steps $\varepsilon = T/N$. The contribution of each piecewise linear trajectory is then determined by a discretized action of the form

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

wherethe potential is evaluated at $\bar{q}_n = (q_n + q_{n+1})/2$, corresponding to the mid-point or Weyl ordering prescription of the usual operator formalism. The final transition amplitude is given $A(a, b; T)$ is given as $N \to \infty$ limit of the discretized amplitude $A_N(a, b; T)$

$$A(a, b; T) = (2\pi\varepsilon)^{-N/2} \int dq_1 \cdots dq_{N-1} e^{-S_N[q]} , \tag{3}$$

where q_n are the positions at discrete times $n\varepsilon$, $q_0 = a$, $q_N = b$, and $(2\pi\varepsilon)^{-N/2}$ is the appropriate normalization factor.

The above discretized expression represents an $N-1$-fold integral and is directly amenable to numerical treatment. In general, for large N, such expressions are nest handled using Monte Carlo techniques [13, 14, 15]. Before we proceed with this, however, let us note that the transition from continuum to discrete theory is far from unique. Said another way, there exists an infinity of discretized actions that, in the continuum limit, give the same transition amplitude. The naively discretized action given in equation (2) is just the simplest representative. While the choice of different discretized actions does not affect the final continuum amplitude, it may substantially affect the speed of convergence to that continuum limit. The naive action typically leads to $1/N$ convergence. In a previous series of papers [6, 7, 8] we have constructed an explicit procedure for determining a hierarchy of equivalent discretized actions $S^{(p)}$ which lead to improved convergence of generic amplitudes as $1/N^p$. Explicit expression for elements of the hierarchy has so far been obtained for $p \leq 13$ and are available on our web site [9]. There are no practical impediments to going to higher values of p, the problem of determining the appropriate effective actions just gets algebraically more complex and requires the use of some package for symbolic calculus (e.g. MATHEMATICA).

Most often, however, one is interested in calculating not amplitudes but partition functions. The relation between the two is made apparent in the coordinate basis. As a result, the partition function can directly be written as a path integral. It is now an $N \to \infty$ limit of discretized partition function

$$Z_N(T) = \int dq_0 A_N(q_0, q_0; T)\,. \tag{4}$$

Note therefore that $Z(T)$ is given as a limit of an N-fold integral over periodic piecewise linear trajectories. The partition function contains all thee information about the statistical properties of the system. In particular, we can use it to determine thermodynamic potentials, such as the free energy $F = -\frac{1}{T}\ln Z$. The free energy is also the ideal starting point for evaluating the energy spectrum of a given theory. From evaluating the partition function in the energy eigenbasis it follows that, in the large T limit, the free energy tends to the ground state energy E_0. Similarly, one can introduce auxiliary functions $F^{(n)}$

$$F^{(n)} = -\frac{1}{T}\ln\left(Z - \sum_{i=0}^{n-1} d_i\ e^{-TE_i}\right)\,. \tag{5}$$

Note that $F^{(n)}$ tends to E_n in the large T limit. In this way, it is possible to use the free energy and the above auxiliary functions to numerically evaluate the low lying energy levels. The fact that $F^{(n)}$ depends on all the lower energy levels and degeneracies results in an accumulation of numerical error as one looks at higher and higher energy levels. This is illustrated in figure 1 on the case of a particle moving in the quartic potential $V(q) = q^2/2 + gq^4/24$.

In addition to amplitudes and partition functions, path integrals are also used to evaluate expectation values of physical variables. The thermal expectation values of an observable $\mathcal{O}$ is given by

$$\langle\mathcal{O}\rangle = \mathrm{Tr}\left(e^{-T\hat{H}}\hat{\mathcal{O}}\right) / \mathrm{Tr}\, e^{-T\hat{H}}\,. \tag{6}$$

This can be directly written in the form of path integrals as the $N \to \infty$ limit of the discretized expectation values

$$\langle\mathcal{O}\rangle_N = (2\pi\varepsilon Z_N(T))^{-N/2} \int dq_0 dq_1 \ldots dq_{N-1} \mathcal{O}_N e^{-S_N[q]}\,. \tag{7}$$

In the above expression $\mathcal{O}_N$ stands for the discretized estimator of the corresponding physical variable. One needs to be careful in how one chooses estimators. They are not just simple discretizations of the continuum expressions. In addition, the estimator must be consistently

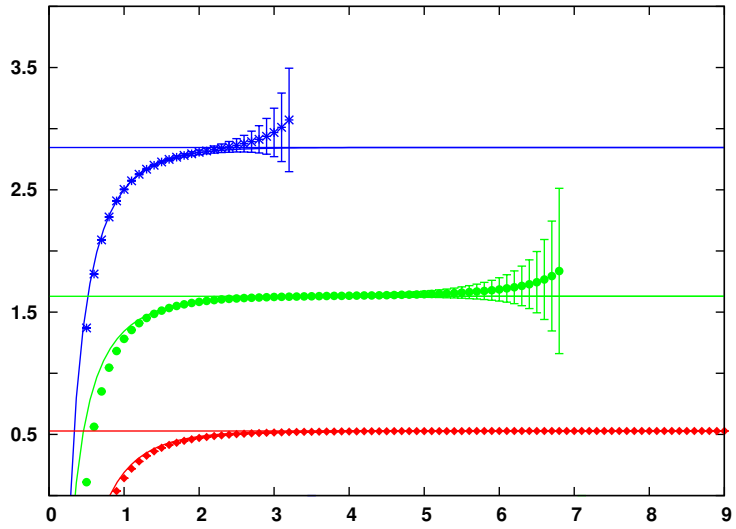

Figure 1. Metropolis implementation of PIMC algorithm for the calculation of low lying energy levels of a quartic potential. The plot shows the dependence of the free energy and the auxiliary function $F^{(1)}$ and $F^{(2)}$ as functions of T. The asymptotes are the corresponding energy levels E_0, E_1 and E_2. The parameters of the theory are $g = 1$, $N_{MC} = 10^7$, $N = 256$. The simulations were performed with $p = 9$ level improved effective actions.

paired with the discretized effective action used in order for expectation values to profit from the same increase in convergence as transition amplitudes. As a particular example, let us look at energy estimators. The continuum expression $\mathcal{E} = \dot{q}^2/2 + V(q)$ would naively be discretized as $\mathcal{E}_N = (q_{n+1} - q_n)^2/2\varepsilon^2 + V(\bar{q}_n$ for any n. Al alternate, more symmetrical estimator would be $\mathcal{E}_N = N^{-1} \sum \left[(q_{n+1} - q_n)^2/2\varepsilon^2 + V(\bar{q}_n)\right]$, where we have made use of the fact that the energy is a conserved quantity. Both of these estimators lead to problems in the continuum limit and give divergent results. This is easily understood if we recall that for short times of propagation each theory is well approximated by a free particle (random walker), satisfying the diffusion relation $\langle (q_{n+1} - q_n)^2 \rangle \sim \varepsilon$. As a result, the above naive estimators have a dominant term diverging as $1/\varepsilon$. The source of the problem is in the T-dependence of the normalization of the above expectation value. A better way to derive the energy estimator is to use the relation

$$\langle \mathcal{E} \rangle = -\frac{\partial}{\partial T} \ln Z(T) \,. \tag{8}$$

If we define the discretized energy expectation value to satisfy the same kind of relation with the discretized partition function, it follows that the consistent energy estimator is given by

$$\mathcal{E}_N = \frac{N}{2T} - \frac{1}{N} \sum_{n=0}^{N-1} \frac{(q_{n+1} - q_n)^2}{2\varepsilon^2} + \frac{1}{N} \sum_{n=0}^{N-1} V(\bar{q}_n) \,. \tag{9}$$

The first two terms in the above estimator (9) both diverge in the continuum limit. However, taken together divergences cancel out and one obtains a finite result. Irrespective of this, the above (so called kinetic) estimator does not represent a good choice, as it contains within it the difference of two large numbers, making its standard deviation divergent and such numerical calculations nontractable. The standard way around this problem is to use the virial theorem

$$\left\langle \frac{\hat{p}^2}{2} \right\rangle = \left\langle \frac{1}{2} \hat{x} V'(\hat{x}) \right\rangle \,. \tag{10}$$

Using it we obtain what is called the virial energy estimator [16]

$$\mathcal{E}_N^{vir} = \frac{1}{2N}\sum_{n=0}^{N-1}\bar{q}_n V'(\bar{q}_n) + \frac{1}{N}\sum_{n=0}^{N-1} V(\bar{q}_n)\,. \tag{11}$$

Each term of this estimator is well behaved and has finite continuum limit and finite standard deviation. It is important to note that the final form of the energy estimator used follows directly from the form of the discretized action. As a result, by changing the discretized action to $S_N^{(p)}$ we immediately obtain the appropriate p-level generalization of the energy estimator. These generalized estimators have been derived and studied in [11], where it was shown that they have the correct improved $1/N^p$ convergence.

3. Metropolis implementation

PIMC algorithms can be made more efficient either by getting better convergence to the continuum limit through the use of above mentioned hierarchy of discretized effective actions, or through better generation of relevant trajectories in the MC method. So far all the numerical verifications of improved $1/N^p$ convergence have been implemented using a PIMC code in which paths were generated through a Levy construction. The Levy construction [15] samples paths with 2^s time steps through a recursive halving, starting with some boundary conditions (representing the trajectory with 2^0 time steps). In the first step we generate one new node at the moment $T/2$ and get a new trajectory, with 2^1 time steps. The procedure is then repeated recursively for each segment of the trajectory. The new nodes are generated using the free particle approximation: if the coordinates of the boundaries of the segment are R_1 and R_2, and if the current time step is ε, the new node is selected from a Gaussian distribution centered at $(R_1 + R_2)/2$ and with the standard deviation $\sigma^2 = \varepsilon/2$. This method, although powerful and simple, can sometimes require very long runs in order to give results with the desired precision. The generated paths are sampled using a free particle approximation, and for models with strong interactions this way of sampling is far from optimal.

In this section we investigate the analytically derived speedup of path integral calculations within the framework of a PIMC code based on the Metropolis algorithm [13, 14, 15], a path generating technique optimally suited for calculating expectation values. Metropolis rejection algorithm is a special type of Markov process, enabling sampling of arbitrary probability distributions. The desired probability distribution $\pi(q)$ is obtained asymptotically, using a series of transformations (Metropolis moves) of the state of the system. The transformations are characterized by a transition matrix $T(q \to q')$, and the trial configuration q' is accepted according to the following probability

$$A(q \to q') = \min\left\{1, \frac{T(q' \to q)\pi(q')}{T(q \to q')\pi(q)}\right\}\,. \tag{12}$$

Metropolis moves in PIMC implementations are usually chosen to represent random local displacements (of given size) of individual nodes. The trajectories generated by the Metropolis technique are not independent, and we can have large correlations between consecutive paths. The correlations, however, depend on the physical quantity which is being calculated. The measure of such correlations is described through the correlation coefficient

$$c_k = \frac{\langle (O_0 - \langle O\rangle)(O_k - \langle O\rangle)\rangle}{\langle (O_0 - \langle O\rangle)^2\rangle}\,, \tag{13}$$

where O_k is the expectation values of the physical quantity calculated using each k-th configuration. The correlation length is defined as a minimal value of k for which the correlation

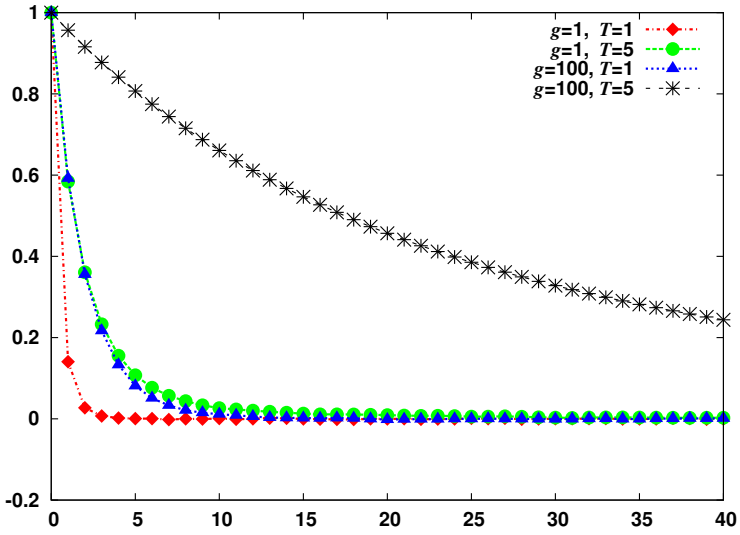

Figure 2. Correlation coefficient as a function of the correlation length k for the Metropolis implementation of the quartic anharmonic oscillator with $g = 100$, $T = 5$, $N_{MC} = 10^6$, $N = 1024$. The simulations were performed with $p = 9$ level improved effective actions.

coefficient c_k is sufficiently small (typically $c_k < 0.1$). Figure 2 illustrates the usual behavior of correlation coefficients for an anharmonic oscillator with quartic coupling.

The described method for correlation reduction is sufficiently good for accurate estimation of expectation values of physical quantities [14]. However, the estimates of MC errors of numerical results (standard deviations) can still be affected by the remaining correlations. This is caused by the deviation of the distribution of MC samples from the Gaussian: the numerically obtained

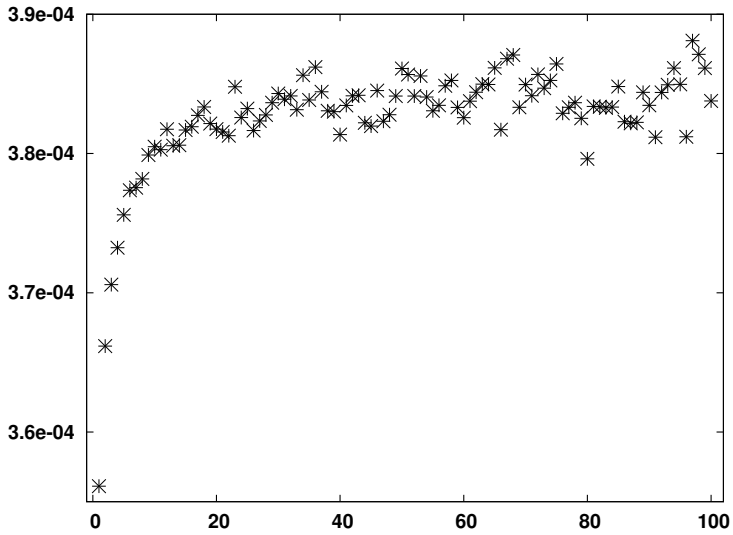

Figure 3. Standard deviation for Metropolis algorithm as a function of block size for a quartic anharmonic oscillator with $g = 1$, $T = 5$, $N_{MC} = 10^6$, $N = 1024$. The simulations were performed with $p = 5$ level improved effective actions.

distribution can be skewed, or have non-zero kurtosis, or both. This is dealt with by dividing the generated set of MC samples into blocks of a chosen size, and then by using just the averages over blocks as a new MC sample. By increasing the block size so that the skew and kurtosis of the obtained new distribution can be neglected, we may correctly estimate the value of MC errors. Note that this procedure does not affect the estimate for the expectation value. Figure 3 gives the dependence of the estimated standard deviation on the block size for a Metropolis implementation of a PIMC calculation of the energy expectation value for a quartic anharmonic oscillator. From this figure wee see that by using small enough block sizes the MC error can be substantially underestimated.

In usual implementation of the Metropolis algorithm, the probability distribution that is to be sampled is given by the exponential of the naively discretized action

$$\pi_N[q(t)] \sim e^{-S_N[q(t)]} \,. \tag{14}$$

In our implementation, the naively discretized action is replaced by one of the improved effective actions in the hierarchy $S_N^{(p)}$, trial paths were sampled using Levy construction, and acceptance of new trajectories was done according to the Metropolis rule (12). Figure 4 illustrates the typical behavior that one uncovers. As expected, the implementation of the Metropolis algorithm does not interfere with the increased convergence obtained through the use of higher level effective actions. Indeed, by using p level effective actions we again find that the numerical results of a new PIMC code display improved convergence of the form $1/N^p$. In fact, far from interfering negatively, the use of higher level effective actions brings about an improved efficiency of the Metropolis algorithm per se through the generation of more relevant trajectories. This is seen through the reduction of the variance of numerical results. A mode detailed investigations of this would be reported elsewhere. In particular, there we will focus on effective actions with $p \geq 10$ and take into consideration the effects of the increased algebraic complexity of these expressions on the computation time. For levels $p \leq 10$ numerical investigations have shown that this accumulated complexity does not have significant effects on the computation time.

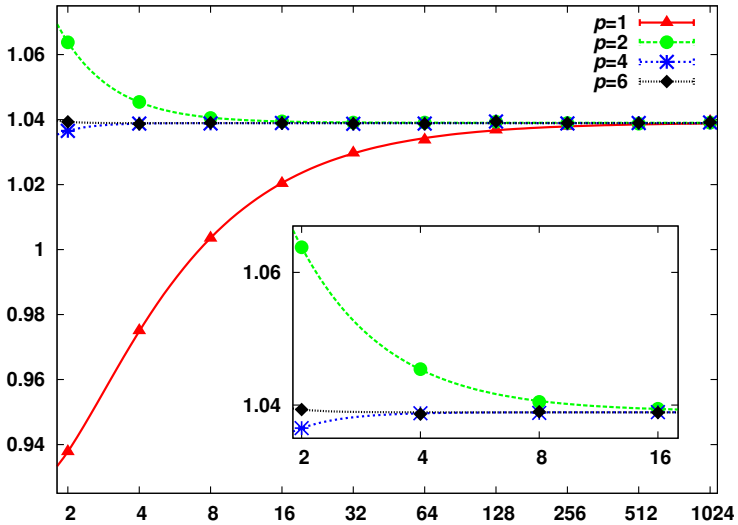

Figure 4. Metropolis implementation of the energy expectation value as a function of the discretization coarseness N for the quartic anharmonic oscillator with $g = 1$, $T = 1$, $N_{MC} = 10^7$. The simulations were performed with level $p = 1, 2, 3, 4$ improved effective actions.

4. Conclusions

We have given a brief overview of the current state of the research effort behind the construction of more efficient PIMC algorithms leading to improved convergence of path integral calculations. In particular, we have outlined how the developed hierarchy of effective actions may be used to calculate transition amplitudes, partition functions and energy spectra. Particular emphasis was given to the calculation of expectation values. We outlined a scheme for the derivation of estimators consistent with the hierarchy of effective actions, i.e. leading to the same increase in convergence. The second part of the paper centers around a new PIMC code encompassing the effective actions and derived estimators, implemented using the Metropolis algorithm. The new PIMC code displays the same $1/N^p$ increase in convergence. Moreover, the use of higher level effective actions brings about an improved efficiency of the Metropolis algorithm through the generation of more relevant trajectories. In the future work we will focus on the detailed investigation of the increase in efficiency of the Metropolis algorithm brought about by the use of higher level effective actions.

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