SYSTEMATIC SPEEDUP OF ENERGY SPECTRA CALCULATIONS FOR MANY-BODY SYSTEMS

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We present an application of a recently developed method for accelerated Monte Carlo computations of path integrals to the problem of energy spectra calculation of generic many-particle systems. We calculate the energy spectra of a two-particle two dimensional system in a quartic potential using the hierarchy of discretized effective actions, and demonstrate agreement with analytical results governing the increase in efficiency of the new method.

Keywords: Path integral; Effective action; Many-body system; Energy spectra.

In addition to their key position in the analytical approach to quantum theory, path integrals also play an important role in the computational simulations of realistic many-body systems. The starting point in these calculations is the time-sliced expression for the general quantum-mechanical amplitude,[1]

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

where N is the number of time slices $\varepsilon = T/N$ and S_N is the naively discretized action for a system of M nonrelativistic particles in d spatial dimensions. The $N \to \infty$ limit of the above discretized amplitude gives the continuum amplitude $A(a,b;T)$.

The performance of the numerical algorithms for the calculation of path integrals is directly determined by the efficiency of the applied integration technique, as well as by the speed of convergence of the discretized amplitudes to the continuum. The first problem has been essentially solved through the development of modern efficient integration techniques. Im-

provement of performance now only depends on improved convergence of discretized expressions to the continuum.

In a recent series of papers[2–5] we focused on the systematic analytical construction of effective actions $S_N^{(p)}$ that improve convergence of discretized transition amplitudes, partition functions and expectation values to the continuum limit for one-particle one-dimensional systems. More recently[6] we have extended this to general many-particle non-relativistic systems, with the convergence of discretized amplitudes

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

with $p \leq 12$, where $p = 1$ corresponds to naive discretization. This improved convergence translates directly into significant speedup of numerical calculations.

In this paper we focus on the benefits of the above improved convergence of amplitudes for the evaluation of energy spectra of many-body systems. The speedup in the calculation of amplitudes leads to the same improvement in the convergence of partition functions, owing to the relation

$$Z_N(\beta) = \int dq A_N(q,q;\beta) \ , \tag{3}$$

where β is the inverse temperature. The partition function is the central object for obtaining information about various thermodynamical quantities.

The numerical results of a series of Monte Carlo (MC) simulations performed clearly demonstrate the analytically derived speedup. Figure 1 shows increase in convergence of discretized free energy $F_N(\beta) = -\log Z_N(\beta)/\beta$ as the level p of the used effective action $S_N^{(p)}$ increases. This is illustrated on the case of a two-dimensional system of two distinguishable particles interacting through a quartic potential

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

The convergence of discretized free energies, presented by solid lines in Fig. 1, is governed by a $1/N^p$ term, corresponding to the analog of the equation Eq. (2) for F_N.

The partition function offers a straightforward way for extracting information about the energy spectrum,[7] since

$$Z(\beta) = \sum_{n=0}^{\infty} d_n e^{-\beta E_n} \ , \tag{5}$$

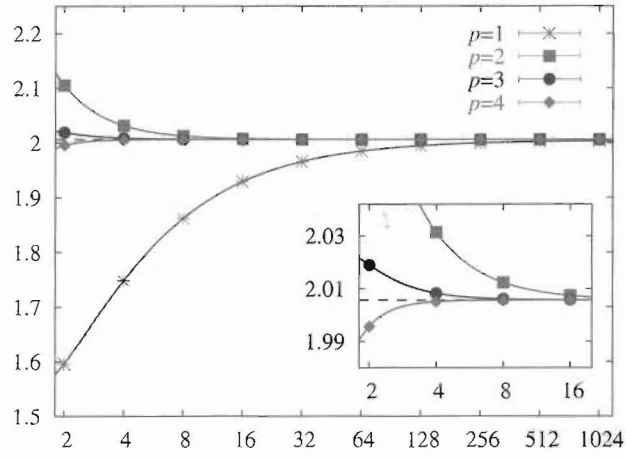

Fig. 1. Convergence of discretized free energies $F_N(\beta)$ to the continuum as a function of N for the quartic potential ($g_1 = 1$, $g_2 = 1$, $\beta = 1$). Number of MC samples is 10^7.

where E_n and d_n denote corresponding energy levels and degeneracies. Similarly to the free energy, we can introduce a set of auxiliary functions

$$f_n(\beta) = -\frac{1}{\beta} \ln \frac{Z(\beta) - \sum_{i=0}^{n-1} d_i e^{-\beta E_i}}{d_n}, \tag{6}$$

which can be fitted for large β to

$$f_n(\beta) \approx E_n - \frac{1}{\beta} \ln(1 + a e^{-\beta b}), \tag{7}$$

and which tend to the corresponding energy levels E_n. In this way, by studying the large β behavior of the functions f_n, one can obtain the energy spectrum of the model.

In numerical simulations we are inevitably limited to the finite range of inverse temperatures. In addition, the above procedure for the construction of the auxiliary functions f_n is recursive, i.e. in order to construct f_n we need to know all the energy levels below E_n. This leads to the accumulation of errors as n increases, and practically limits the number of energy levels that can be calculated. Note that the orders of magnitude increase in precision of the presented method reduces the magnitude of the accumulated error and thus allows us to extract viable information about a larger number of energy levels.

Table 1. Energy levels of the quartic potential, $g_2 = 1/9$. The corresponding 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_0^{pert}	E_1	E_2	E_3
0	1.8857(1)	1.88562	2.3571(6)	2.83(1)	3.3(2)
0.1	1.9019(2)	1.90187	2.374(2)	2.82(1)	—
1	2.0228(2)	2.03384	2.497(3)	2.94(3)	—
10	2.6327(6)	—	3.098(4)	3.57(3)	—

Table 1 gives the calculated energy levels for quartic coupling from $g_1 = 0$ (free theory) to $g_1 = 10$ (strongly interacting theory), obtained using the $p = 5$ effective action. The number of MC samples was 10^9 with discretization coarseness $N = 64$, chosen so that $F_N(\beta) = F(\beta)$ within the statistical error over the range $1 \leq \beta \leq 11$, yielding four decimal places precision for the ground energy level. The employment of higher level effective actions makes it possible to use much coarser discretization, thus substantially reducing the CPU time. For comparison, the table also contains values of the ground state energy E_0^{pert} obtained using perturbation expansion up to third order in g_1.

To conclude, we have applied the recently derived many-particle discretized effective actions to the calculation of low-lying energy spectra. Numerical results confirm the analytically derived increase in convergence of discretized expressions, resulting in substantially more efficient simulations.

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