Computer Simulations of Quantum Chains

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Abstract

We report recent progress in computer simulations of quantum systems described in the path-integral formulation. For the example of the $\phi^4$ quantum chain we show that the accuracy of the simulation may greatly be enhanced by a combination of multigrid update techniques with a refined discretization scheme. This allows us to assess the accuracy of a variational approximation.

1 Introduction

Monte Carlo (MC) simulations of many-particle quantum systems based on a path-integral representation of the partition function provide a numerical approach to these systems which in principle is free of any approximations [1]. The difficulty here is to achieve sufficient accuracy. Standard path-integral MC simulations suffer from well-known drawbacks, such as systematic errors due to the necessary discretization and severe slowing down in the continuum limit. These problems clearly ask for the development of refined simulation techniques.

A Fourier MC simulation of the Sine-Gordon quantum chain was tried some time ago [2]. Preliminary data seemed to be quite promising, but the method did not work quite so well for the related $\phi^4$ chain. The reason is that the Fourier MC method is not based on importance sampling which is a problem particularly for unbounded potentials such as the $\phi^4$ double well.

In view of these difficulties it is gratifying that recently algorithmic improvements developed for spin systems and lattice field theories could successfully be transferred to path-integral simulations [3]. Multigrid techniques and the staging algorithm have been shown to eliminate slowing down in the continuum limit for one-particle systems [4, 5]. It seemed therefore worthwhile to investigate whether these refinements may now render simulations of quantum chains sufficiently accurate to allow for a significant test of analytical approximations.
2 Simulation techniques

The $N$-particle quantum systems we want to investigate are defined in any dimension $D$ by the partition function

$$Z = e^{-\beta F} = \prod_{i=1}^{N} \int \mathcal{D}[[\phi_i(u)]] \exp \left[ - \int_0^{\hbar \beta} du \left( Aa \sum_{i=1}^{N} \frac{1}{2} \dot{\phi}_i^2(u) + V(\{\phi_i(u)\}) \right) / \hbar \right], \quad (1)$$

where $\beta = 1/k_B T$ is the inverse temperature, $\dot{\phi}_i \equiv d\phi_i/du$, and $\mathcal{D}[[\phi_i(u)]]$ denotes the functional measure for periodic paths, $\phi_i(0) = \phi_i(\hbar \beta)$.

For a simulation of these systems the partition function (1) needs to be discretized. Standard discretization schemes based on the Trotter formula $e^A + B = \lim_{L \to \infty} [e^{A/2L} e^{B/L} e^{A/2L}]^L$ for operators $A$ and $B$ entail a systematic error of the order $\epsilon^2$ where $\epsilon \equiv \hbar \beta / L$ and $L$ is the Trotter number. A more rapidly converging discretization scheme of the order $\epsilon^4$ was proposed by Takahashi and Imada [6]. The only modification with respect to the standard discretization is that the potential $V$ is replaced by an “improved” potential,

$$V_{TI}(\{\phi_{i,k}\}) = V(\{\phi_{i,k}\}) + \beta^2 \hbar^2 \frac{24 Aa L^2}{2} \sum_{i=1}^{N} \left( \frac{\partial V}{\partial \phi_{i,k}} \right)^2, \quad (2)$$

where $k$ denotes the additional index for the Trotter discretization at each site.

As far as the statistical error of the simulations is concerned we expect a quadratic slowing down in the continuum limit of large Trotter numbers $L$ for standard local update algorithms such as the Metropolis algorithm [3–5]. It is therefore desirable to apply refined update techniques which reduce autocorrelations in the MC process. Fortunately, even though the discretized partition function effectively represents a $(D+1)$-dimensional classical system, in many applications it is sufficient to apply one-dimensional refined update schemes since we are approaching the continuum limit only in the Trotter direction. We may therefore use improved update schemes developed for one-particle systems at each site along the discretized time axis such as one-dimensional multigrid cycles [4] or the staging algorithm [5].

The observables of interest are the internal energy and the specific heat. It is well-known that the definition of the internal energy $U$ gives rise to an estimator $U_k$ of the energy by differentiating the discretized partition function, $U = -\partial \ln Z / \partial \beta \approx U_k$, where $U_k$ denotes the arithmetic mean over $N_m$ measurements of $U_k$ in the MC process. Applying a simple scaling argument one can also derive a different but equivalent energy estimator $U_v$ based on the virial theorem with the same mean but different variance. In order to further reduce the statistical error of the energy estimation we may then use an optimized linear combination of these two estimators [7]. Note that the energy estimators differ for the standard and the improved discretization schemes since the correction term in $V_{TI}$ is $\beta$-dependent. For the estimation of the specific heat analogous considerations apply. A full account of the technical details discussing various systematic algorithmic refinements of path-integral MC simulations will be given elsewhere [7].
3 Results for the $\phi^4$ quantum chain

In the following we will present simulation results for the $\phi^4$ quantum chain [8] where the potential $V$ in (1) is given by

$$V(\{\phi_i\}) = Aa \sum_{i=1}^{N} \left[ \frac{\omega_0^2}{2}(\phi_i - \phi_{i-1})^2 + \frac{\omega_1^2}{8}(\phi_i^2 - 1)^2 \right]. \quad (3)$$

The partition function describes a set of $N$ harmonically coupled oscillators of mass $Aa$ moving in double-well potentials separated by a distance $a$. Following Ref. [9] we assume periodic boundary conditions, $\phi_0 \equiv \phi_N$, and introduce dimensionless parameters $R = \omega_0/\omega_1$, $Q = \hbar\omega_1/E_s$, and $t \equiv k_B T/E_s$, where $E_s = (2/3)Aa\omega_0\omega_1$ is the energy of the classical static kink and $R$ is its length in units of the lattice spacing $a$. The latter two parameters were kept fixed at $E_s = 1$ and $R = 5$. The coupling constant $Q$ controls the quantum character of the system by determining whether the kinks are “heavy” enough (small $Q$) to be treated semiclassically.

In our simulations, the number of oscillators was $N = 300$ except for $t = 0.05$, 0.30, 0.35, and 0.40 where we simulated a chain of $N = 200$ oscillators. The Trotter number was $L = 16$ for $t \geq 0.20$, $L = 32$ for $t = 0.15$, $L = 64$ for $t = 0.10$, and $L = 128$ for $t = 0.05$. In all simulations we used the improved discretization scheme (2). The update was performed using a multigrid W-cycle with piecewise constant interpolation in Trotter direction at each site with single-hit Metropolis updating and $n_1 = 1$ pre-, $n_2 = 0$ postsweeps [4, 8]. The thermodynamic observables of interest are the internal energy per site, $u = U/N$ and the specific heat per site given by $c = C/N = \partial u/\partial T$. More precisely, we will be interested only in the anharmonic contribution to these quantities. For the free energy this is given by $dF \equiv F - F_{\text{harmon}} = F - (1/\beta) \sum_{k=1}^{N} \ln(2 \sinh F_k)$, where $F_k = \beta \hbar \omega_k/2$ and $\omega_k^2 = 4\omega_0^2 \sin^2(k\pi/N) + \omega_1^2$. For each data point we have measured the internal energy using the optimally combined estimator with $N_m = 200,000$ measurements taken every second sweep, after discarding 2000 sweeps for thermalization. The Metropolis acceptance rates were adjusted to be $\approx 40 - 60\%$ on the finest grid and the same step width was used for all multigrid levels. The specific heat was measured by simple numerical differentiation of the “combined” estimator which was reweighted in a temperature interval of $dt = 0.0001$. These estimates gave consistent values with direct measurements of the specific heat using the estimators obtained by differentiating the discrete partition function but (slightly) smaller errors. All statistical errors were computed by jack-knifing the data on the basis of 500 blocks.

In Fig. 1 we compare our simulation data with analytical results based on a variational ansatz [10] which has been shown to be a very powerful and useful method for an approximate evaluation of quantum partition functions [9–11]. The variational approach starts from a quadratic trial Hamiltonian whose parameters are determined by optimizing the Jensen-Peierls inequality for the free energy. A numerical solution of the resulting set of $N(N + 1)/2$ self-consistent equations is extremely complicated and only the limiting cases of high and low temperatures and for small coupling $Q$ have been treated in the literature. This adds another source of error to the uncertainty inherent in the variational ansatz itself. For the $\phi^4$
Let us first look at the temperature dependence of the internal energy. Figure 1 shows the measured anharmonic contributions to the internal energy per site as a function of the temperature $t$ for various couplings $Q$. Regarding a comparison with the variational data we observe that the approximation is fully confirmed for high temperatures $t$ and small couplings $Q$. For lower $t$ we still find a satisfactory agreement if we also take into account finite-size corrections in the variational approach by evaluating the effective classical partition function given in eq. (4.6) of Ref. [9] for finite $N$ with the help of the transfer matrix method [8].

The situation is different, however, for low temperatures and large couplings as can be clearly seen in Fig. 1. Here we find significant deviations from the variational approximation. Note that the error bars for the data are smaller than the data symbols. Let us take a closer look at the lowest temperature which we have investigated, $t = 0.05$. For $Q = 0.1$ and $Q = 0.2$ the variational approximation is still confirmed within the statistical errors. But already for $Q = 0.3$ we find a statistically significant discrepancy which further increases when we go to larger couplings. For the worst case, $Q = 0.6$, the variational approximation deviates from the MC results already by 56 error bars, even if finite-size corrections are fully taken into account. We emphasize that within the statistical errors our data are to be regarded exact, i.e. that the deviations are entirely due to the variational approximation.

Let us finally take a look at the plot on the r.h.s. of Fig. 1 which shows the measured anharmonic contributions to the specific heat per site. Due to the fact that the estimation of the specific heat involves a difference of statistically fluctuating variables the resulting statistical accuracy is greatly reduced compared to the estimation of energies. Therefore the accuracy of our data for the specific heat unfortunately still does not allow for a significant falsifying test of the variational approximation.
4 Conclusions

By employing refined path-integral MC techniques we have been able to drastically reduce the systematic and statistical errors of a quantum MC simulation of the $\phi^4$ chain. The resulting accuracy now allows for a significant test of the variational approximation. For small couplings $Q$ we find very good agreement. Only for large couplings and low temperatures do we observe significant deviations from the MC data. The discrepancies may be due to the limitations inherent in the variational approximation or to the additional approximation of the small coupling expansion. It would therefore be interesting to see whether the MC data can be reproduced by evaluating the variational equations to higher orders of $Q$ or by taking into account higher-order corrections to the variational approach itself [12].

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