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Test of variational approximation for ϕ^4 quantum chain by Monte Carlo simulation

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Abstract

We report results of a Monte Carlo simulation of the ϕ^4 quantum chain. In order to enhance the efficiency of the simulation we combine multigrid simulation techniques with a refined discretization scheme. The resulting accuracy of our data allows for a significant test of an analytical approximation based on a variational ansatz. While the variational approximation is well reproduced for a large range of parameters we find significant deviations for low temperatures and large couplings.

1. Introduction

The physics of one-dimensional quantum systems has attracted considerable attention, both experimental and theoretical, for a long time. Among the methods to treat these systems analytically the variational approximation [1–5] has been shown to be a very powerful and useful one [6]. Since, however, it is hard to give precise inherent error estimates for the variational approach it is therefore desirable to check the method against independently obtained data. For the ϕ^4 chain which has been investigated both as a classical [7–9] and as a quantum system [5,10] apparently no such independent data exist up to this date.

Precise Monte Carlo simulations of many-particle quantum systems based on a path-integral representation of the partition function would provide just such an independent approach for these systems [11]. The difficulty here is to achieve sufficient accuracy. Standard path-integral simulations suffer from well-known drawbacks, such as appreciable systematic errors due to the necessary discretization and severe slowing down in the continuum limit. In order to overcome these problems a Fourier Monte Carlo simulation was tried some time ago for the closely related sine-Gordon chain [12]. Even though preliminary data seemed to reproduce the variational approximation [4] quite well similar results for the ϕ^4 chain were not obtained. Unfortunately, a full account of these investigations was never published [13]. A disadvantage of the method used in Ref. [12] is that it is not based on importance sampling, which is a problem particularly for unbounded potentials such as the ϕ^4 double well.

In view of these difficulties it is therefore gratifying that recently some algorithmic improvements developed for spin systems and lattice field theories could successfully be transferred to path-integral simulations [14]. Multigrid simulation techniques [15] in particular have been shown to eliminate slowing down in the continuum limit for one-particle systems [16]. It seemed therefore worthwhile to investigate whether

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these algorithmic improvements may now render path-integral simulations of quantum chains sufficiently accurate to allow for a significant comparison with the variational approximation. In this Letter we will report simulation data for the ϕ^4 quantum chain obtained by combining multigrid simulation techniques with a refined discretization scheme. It will be shown that the accuracy of the data does allow for a qualified judgement about the validity of the variational approximation.

2. The model and variational approximation

The system we are going to discuss is defined by the partition function

$$\mathcal{Z} = \mathrm{e}^{-\beta F} = \prod_{i=1}^{N} \int_{\phi_i(0)=\phi_i(\hbar\beta)} \mathcal{D}[\{\phi_i(u)\}] \times \exp(-\mathcal{H}[\{\phi_i(u)\}]/\hbar), \tag{1}$$

with a Hamiltonian

$$\mathcal{H}[\{\phi_i(u)\}] = \int_0^{\hbar\beta} \mathrm{d}u \left(Aa \sum_{i=1}^{N} \tfrac{1}{2}\dot{\phi}_i^2(u) + V(\{\phi_i(u)\}) \right), \tag{2}$$

where the potential is given by

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

Here $\beta = 1/k_{\mathrm{B}}T$ denotes the inverse temperature, $\dot{\phi}_i \equiv \mathrm{d}\phi_i/\mathrm{d}u$, and $\mathcal{D}[\{\phi_i(u)\}]$ is the usual path-integral measure. The partition function describes a set of N harmonically coupled oscillators of mass Aa separated by a distance a, with each oscillator moving in a double-well potential. As usual, we assume periodic boundary conditions, $\phi_0 \equiv \phi_N$.

Following the notation of Ref. [5] we introduce dimensionless parameters and define a coupling constant $Q = \hbar\omega_1/E_{\mathrm{s}}$ which controls the quantum character of the system by determining whether the kinks are "heavy" enough to be treated semiclassically. In our simulations we will fix the energy scale by setting the energy of the classical static kink $E_{\mathrm{s}} = \frac{2}{3}Aa\omega_0\omega_1 = 1$. We also introduce the parameter $R = \omega_0/\omega_1$, which measures the length of the classical kink in units of the lattice spacing a. The reduced temperature will be denoted by $t \equiv k_{\mathrm{B}}T/E_{\mathrm{s}}$.

The variational approach for one-dimensional quantum systems [2,4,5] starts from a quadratic trial Hamiltonian. The parameters in this trial Hamiltonian are determined by optimizing the Jensen–Peierls inequality for the free energy. A numerical solution of the resulting set of $\frac{1}{2}N(N+1)$ self-consistent equations is extremely complicated. Therefore only the limiting cases of high and low temperatures and for small coupling Q have been treated in the literature. For the latter case, which seems to be the most useful one, the final result reads [5]

$$\beta F = \sum_{i=1}^{N} \ln \frac{\mathrm{sh}\, F_k}{F_k} - \beta \times \tfrac{3}{4}NAa\omega_1^2 D^2 - \ln\left[\left(\frac{\hat{A}a}{2\pi\hbar^2\beta} \right)^{N/2} \prod_{i=1}^{N} \int \mathrm{d}\phi_i \times \exp\left(-\beta\hat{A}a \sum_{i=1}^{N} [\tfrac{1}{2}\omega_0^2(\phi_i - \phi_{i-1})^2 + \tfrac{1}{8}\hat{\omega}_1^2(\phi_i^2 - 1)^2] \right) \right], \tag{4}$$

where $\hat{A} \equiv A(1-3D)$, $\hat{\omega}_1^2 \equiv \omega_1^2(1-3D)$, and

$$D = \sum_{i=1}^{N} \left(\frac{\hbar^2\beta}{4AaF_k} (\mathrm{cth}\, F_k - 1/F_k) \right),$$

with $F_k = \beta\hbar\omega_k/2$ and $\omega_k^2 = 4\omega_0^2 \sin^2(k\pi/N) + \omega_1^2$.

In the sequel the thermodynamic observables of interest will be the internal energy per site $u = U/N = (1/N)(F - T\partial F/\partial T)$ and the specific heat per site c given by $c = C/N = (1/N)\partial U/\partial T$. More precisely, we will be interested only in the anharmonic contribution to these quantities. For the free energy this is given by $\mathrm{d}F \equiv F - F_{\mathrm{harmon}} = F - (1/\beta)\sum \ln(2\,\mathrm{sh}\, F_k)$. Therefore the last two terms of Eq. (4) give the anharmonic contribution to the quantum free energy after subtracting the corresponding classical contribution $F_{\mathrm{class}} = (1/\beta)\sum \ln(2F_k)$. In order to obtain analytical data for a comparison with our Monte Carlo results we

therefore have to evaluate the configurational integral (4).

This can be achieved by employing standard transfer integral techniques [7]. Here we have to find the eigenvalues of the transfer integral equation associated with Eq. (4). In the thermodynamic limit $N \to \infty$ only the lowest eigenvalue survives but in order to control finite-size effects we need to compute all eigenvalues. With decreasing temperature more and more eigenvalues have to be taken into account. In particular, we observe that for low temperatures the two lowest eigenvalues are almost degenerate.

3. Simulation techniques

The partition function (1)–(3) was discretized using the Takahashi–Imada scheme [17]. The discretized version of the partition function here reads

$$\mathcal{Z} = \prod_{i=1}^{N}\prod_{k=1}^{L}\int \frac{\mathrm{d}\phi_{i,k}}{\sqrt{2\pi\beta\hbar^2/LAa}} \times \exp\left[-\frac{\beta}{L}Aa\sum_{i=1}^{N}\sum_{k=1}^{L}\frac{1}{2}\left(\frac{L}{\hbar\beta}\right)^2(\phi_{i,k}-\phi_{i,k-1})^2 - \frac{\beta}{L}V_{\mathrm{TI}}(\{\phi_{i,k}\})\right], \tag{5}$$

where the potential is given by

$$V_{\mathrm{TI}}(\{\phi_{i,k}\}) = \sum_{k=1}^{L}\left[V(\{\phi_{i,k}\}) + \frac{\beta^2\hbar^2}{24AaL^2}\sum_{i=1}^{N}\left(\frac{\partial V}{\partial\phi_{i,k}}\right)^2\right]. \tag{6}$$

Here k denotes the additional index for the Trotter discretization at each site. The convergence of this discretization is of the order ϵ^4 where $\epsilon \equiv \hbar\beta/L$ and L is the Trotter number. The standard, quadratically convergent discretization scheme is recovered by dropping the second term in Eq. (6).

Since for local update algorithms we expect a quadratic slowing down in the continuum limit of large Trotter numbers L [16] we applied a multigrid W-cycle with piecewise constant interpolation [15] at each site along the Trotter direction. Note that since we are approximating the continuum limit only for the Trotter discretization we do not need to apply two-dimensional multigrid coarsening. Also note that the interactions between the oscillators enter the multigrid coarsening only as constants for the polynomial expression for the energy on the finest grid.

The observables of interest are the internal energy and the specific heat. As to the question of energy estimators we remark that the discretized partition function (5) gives rise to a so-called kinetic estimator of the energy U_{k} [18] by differentiating $\langle U\rangle = -\partial \ln \mathcal{Z}/\partial\beta \approx \overline{U_{\mathrm{k}}}$ where $\overline{U_{\mathrm{k}}}$ denotes the simple arithmetic mean over N_m measurements of U_{k} in the Monte Carlo process. Applying a simple scaling argument one can find a different but equivalent energy estimator U_{v} [19] based on the virial theorem with different variance. In order to reduce the variance of the energy estimation we may then use a linear combination of these two estimators. In doing so it should be noted that the optimal combination of the two estimators has to take into account the individual variances *and* the covariance of the (blocked) individual estimators [20]. Note that the energy estimators differ for the standard discretization scheme and the improved discretization since the correction term in V_{TI} is β-dependent. For the evaluation of the anharmonic contributions the discretization error was further reduced by subtracting the exact values for the harmonic contribution at finite Trotter number L. For the standard discretization this improvement was already made use of in Ref. [21]. Since we are only dealing with Gaussian integrals the exact harmonic contribution can, however, also readily be found for the Takahashi–Imada scheme [20]. A full account of the simulational details discussing various systematic algorithmic refinements of path-integral Monte Carlo simulations will be given elsewhere [20].

4. Results

We have performed simulations of the partition function (1)–(3) using the improved discretization scheme (5), (6) for different values of N, Q, and t. The parameter R was kept fixed at $R = 5$ for all simulations. The update was performed using a multigrid W-cycle with piecewise constant interpolation in the Trotter direction at each site with single-hit Metropo-

lis updating and $n_1 = 1$ pre-, $n_2 = 0$ postsweeps. For each data point we have measured the internal energy using the optimally combined estimator with $N_m = 200000$ measurements taken every second sweep, i.e. $n_e = 2$, after discarding $n_e \times 1000$ 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-kniving the data on the basis of 500 blocks.

Comparing the jack-knife error with the canonical variance of the individual measurements we find that the integrated autocorrelation time for both the kinetic energy estimator and the virial estimator never exceeded a value of $\tau^{\mathrm{int}}/n_e \leqslant 2$. Within these bounds we noticed that the autocorrelation times tended to be larger for low temperatures and large coupling constants. This observation is also reflected in the fact that the acceptance rates were roughly constant on all levels for high temperatures and small couplings but tended to decrease for lower t and larger Q. We conclude that in our simulations the measurements of the energies were more or less statistically decorrelated.

Fig. 1 shows the measured anharmonic contributions to the internal energy per site for $Q = 0.1$ and $t = 0.1, 0.2, 0.3$, and 0.4 as a function of the number of oscillators N. Here the Trotter number L was set to $L = 16$ for all temperatures. The solid lines show the variational approximation for finite N, and the dotted horizontal lines show the corresponding values in the thermodynamic limit $N \to \infty$. We see that the Monte Carlo data fully confirm the variational approximation within the statistical uncertainty. For high temperatures the finite-size effects are quite appreciable but die off rapidly with increasing N. For low temperatures on the other hand the finite-size data approach the thermodynamic limit rather slowly but the absolute values differ only by a small amount from the asymptotic value.

Let us now look at the temperature dependence of the internal energy. Fig. 2 shows the measured anharmonic contributions to the internal energy per site as a function of the temperature t for various couplings Q. Here 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 $t \geqslant 0.20$, $L = 32$ for $t = 0.15$, $L = 64$ for $t = 0.10$, and $L = 128$ for $t = 0.05$. Regarding a comparison with the variational data we observe that the approximation again 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. The situation is differ-

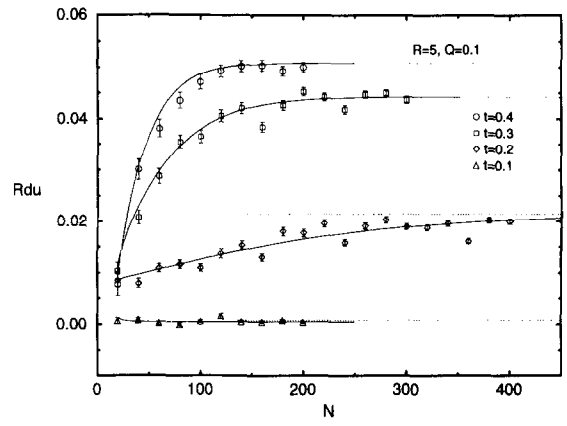

Fig. 1. Finite-size dependence for the measured anharmonic contributions to the internal energy per site. Solid lines show the variational approximation for finite N and dotted lines show the thermodynamic limit.

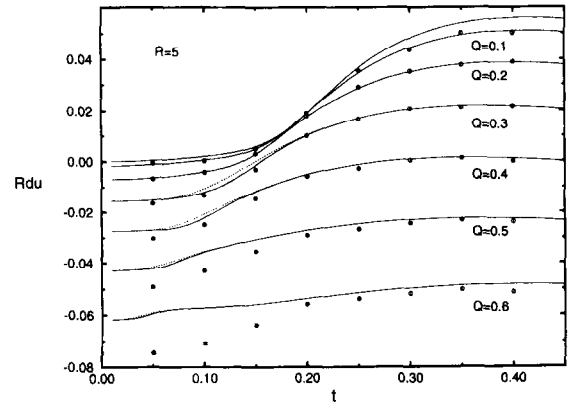

Fig. 2. Anharmonic contributions to the internal energy per site as a function of the temperature t for various coupling parameters Q. Solid lines show the variational approximation for $N = 300$. Dotted lines show the variational approximation for $N = \infty$.

ent, however, for low temperatures and large couplings as can be clearly seen in Fig. 2. 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 confirmed within our statistical error estimate. But already for $Q = 0.3$ we find a statistically significant discrepancy between our measured value of $Rdu = 0.01641(21)$ and the variational approximation which predicts a value of $Rdu = -0.01512$ for both $N = 200$ and $N = \infty$. This discrepancy increases if we go to larger couplings. For the worst case, $Q = 0.6$, the variational approximation gives a value of $Rdu = -0.05898$ for $N = \infty$ and $Rdu = -0.05982$ for $N = 200$. The simulation on the other hand yields a value of $Rdu = -0.07447(26)$, i.e., the variational approximation deviates from the Monte Carlo results by 56 statistical error bars even if finite-size corrections are fully taken into account.

In order to check whether for the Monte Carlo data systematic errors due to the discretization would still play a role we have checked our data for $t = 0.1$ against simulations with smaller Trotter numbers, $L = 16$ and $L = 32$. For $Q = 0.1$ and $Q = 0.2$ we found no significant differences but we did observe finite ϵ effects for larger couplings Q. Their sizes, however, were small enough and in view of the fact that our discretization converges with the fourth order in ϵ we believe that the remaining discretization error for small t and large Q is at most of the same order as the statistical errors. In any case, we observed that going to a larger Trotter number would push the values *down*, i.e. would further increase the difference to the variational approximation.

We conclude that our data differ significantly from the variational approximation for large Q and small t. The question then arises whether these discrepancies are a consequence of the low coupling expansion or rather inherent to the variational approach at this level. In view of the fact that the data fit quite well even for large Q at high temperatures it seems more likely that the latter is the case. On the basis of the validity of the Wigner expansion Giachetti et al. [5] suggested that their expansion be valid as long as

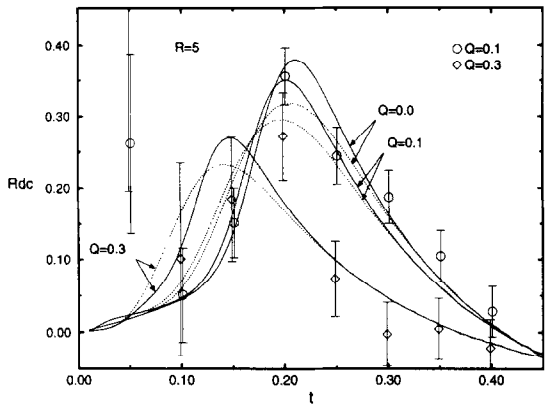

Fig. 3. Anharmonic contributions to the specific heat per site as a function of the temperature t for various coupling parameters Q. Solid lines show the variational approximation for $N = 300$. Dotted lines show the variational approximation for $N = \infty$.

$$t \gg \frac{1}{8\pi} Q^2 \ln(8R) \approx 0.1468 Q^2. \tag{7}$$

This means, for $Q = 0.3$ we have to compare $t = 0.05$ with 0.013212 to explain a discrepancy of almost 5 statistical error bars. For our worst case of $Q = 0.6$ Eq. (7) reads explicitly $t \gg 0.053$ and the discrepancy of 56 statistical error bars for $t = 0.05$ is indeed due to a violation of this condition. Looking at Fig. 2 for the largest coupling, $Q = 0.6$, we conclude that condition (7) is violated for almost all temperatures displayed in Fig. 2 only if we take the $\gg$ to mean: larger by more than one order of magnitude.

Let us finally take a look at the specific heat. Fig. 3 shows the measured anharmonic contributions to the specific heat per site. Again the solid lines are the variational approximation for $N = 300$ and the dotted lines show the corresponding thermodynamic limit. 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 our data for the specific heat do not allow for a significant falsifying test of the variational approximation. For the more interesting case of large couplings we also see that the statistical uncertainty unfortunately is even increasing, in particular for low temperatures. One therefore would have to conclude that neither a brute force increase of the statistics appears to be a reasonable way of getting more accurate data. With these restrictions we nevertheless do see, however, that the gen-

eral trend of the quantum effects as computed by the variational approximation is confirmed.

5. Discussion

Employing refined path-integral Monte Carlo techniques we have been able to considerably reduce the systematic and statistical errors of a quantum Monte Carlo simulation of the ϕ^4 chain. The resulting accuracy now allows for a significant test of the variational approximation. For small couplings we find that the variational quantum corrections to the thermodynamic quantities are fully confirmed and only for large couplings and low temperatures do we observe significant deviations from the exact Monte Carlo data. The discrepancies may be due to the additional approximation of the small coupling expansion which was used to evaluate the effective classical potential of the variational approximation. It would therefore be interesting to see whether the Monte Carlo data might be reproduced by taking into account higher-order corrections in the coupling parameter Q. The discrepancies increase both for large couplings and for low temperatures. Since it is known that the variational approximation works better at high temperatures the other possible reason for the deviations of the analytical data may be an inherent failure of the variational approximation itself (at this level of accuracy). If this should be the case it would be interesting to see whether by calculating the higher-order corrections to the variational approach [22] one would be able to account for the remaining discrepancies.

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