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Ning Cai(蔡凝), Yuan Gao(高源), Wei Li(李伟), and Yang Qi(戚扬)

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RAPID COMMUNICATION

Auxiliary-field Monte Carlo method for frustrated spin systems

Ning Cai(蔡凝)[1], Yuan Gao(高源)[2,3], Wei Li(李伟)[3,4,†], and Yang Qi(戚扬)[1,‡]

[1] *State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai* 200433, *China*
[2] *School of Physics, Beihang University, Beijing* 100191, *China*
[3] *Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing* 100190, *China*
[4] *Peng Huanwu Collaborative Center for Research and Education, Beihang University, Beijing* 100191, *China*

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We extend a semiclassical numerical method, bosonic auxiliary-field Monte Carlo, to quantum spin systems. This method breaks the lattice into clusters, solves each cluster precisely and couples them with classical auxiliary fields through classical Monte Carlo simulation. We test the method with antiferromagnetic spin models in one-dimensional chains, square lattices and triangular lattices, and obtain reasonable results at finite temperatures. This algorithm builds a bridge between classical Monte Carlo method and quantum methods. The algorithm can be improved with either progress in classical Monte Carlo sampling or the development of quantum solvers, and can also be further applied to systems with different lattices or interactions.

Keywords: Monte Carlo, quantum many-body system, frustrated magnets

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1. Introduction

Frustration, which describes the situation that competing magnetic exchange interactions are unable to be satisfied simultaneously, plays a vital role in quantum magnets. The frustration-induced quantum fluctuation could avoid classical spin ordering,[1] and lead to unconventional magnetic ordering like supersolidity[2] and fractional magnetization plateau state,[3] as well as disordered spin states such as quantum spin liquid,[4–7] spin ice[8–10] and quantum Ising spins.[11–14]

A significant method for solving the strongly correlated quantum lattice is numerical methods with high efficiency and accuracy. Although several analytical techniques have been proposed and numerical methods have been applied, frustrated quantum systems still stay challenging because of their extreme complexity. A wide range of large-scale numerical approaches are based on quantum Monte Carlo (QMC) calculations.[15,16] However, the presence of frustrated couplings in the Hamiltonian often leads to the sign problem for QMC,[17] although the sign problem may be reduced for certain frustrated models.[18] Several numerical renormalization group (RG) approaches have been developed, where the density matrix renormalization group (DMRG)[19,20] and its finite temperature variant, the transfer matrix renormalization group[21,22] have solved one-dimensional (1D) systems well, but DMRG could not solve problems in two-dimensional (2D) systems or in even higher dimensions. Generalizing the RG-based algorithms to 2D systems brought several new approaches with success. For instance, the projected entangle pair state (PEPS),[23,24] the tree tensor network,[25,26] the multiscale entanglement renormalization ansatz state,[27,28] the infinite PEPS,[29,30] the tensor renormalization group[31–34] and so on have already obtained interesting results.[35–37] However, most of these algorithms are effective for the ground state properties and the thermodynamics of 2D quantum systems remains hard to be studied. Only several algorithms, like the exact diagonalization (ED), theoretically could solve nearly all the quantum systems, including the thermodynamics of 2D quantum systems, but they suffer from the Hilbert space which will increase exponentially with the lattice size and thus result in exponentially increased time and space consumption, leading to the impossibility of calculation with a large scale. The algorithm for the thermodynamics of frustrated 2D quantum models still needs to be developed.

This paper extends a semiclassical numerical method, the bosonic auxiliary-field Monte Carlo (bAFMC), which focuses on the difference in the scales between classical and quantum fluctuations at finite temperature. bAFMC, which was first proposed for bosons,[38] breaks the lattice into clusters. Each cluster is solved precisely using a quantum algorithm (such as ED), and the clusters are coupled together via auxiliary fields (AF) fluctuating classically, which are simulated via a classical Monte Carlo (MC) process. Quantum fluctuations depend on the length scale of a cluster, while the classical MC treatment could link them together to partly simulate the thermal fluctu-

†Corresponding author. E-mail: w.li@itp.ac.cn
‡Corresponding author. E-mail: qiyang@fudan.edu.cn

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ations at all length scales. Though the break of the system sets an artificial cutoff in the wavelength of quantum fluctuation, an extrapolation of the cluster size could remove the cutoff and lead to arbitrary cluster size. We test our approach in 1D antiferromagnetic chain and 2D antiferromagnetic square lattice compared with the exact result calculated by stochastic series expansion (SSE), and further apply it to frustrated triangular lattice with antiferromagnets.

2. Models

To be concrete, we will focus on the Heisenberg model

$$\hat{H} = \sum_{i<j} J_{ij}^x \hat{S}_i^x \hat{S}_j^x + J_{ij}^y \hat{S}_i^y \hat{S}_j^y + J_{ij}^z \hat{S}_i^z \hat{S}_j^z, \tag{1}$$

where the indices i and j run over the sites of the lattice. J_{ij} is the coupling constant between the sites i and j. A positive (negative) J_{ij} indicates an antiferromagnetic (ferromagnetic) interaction. The two types of interactions need to be treated differently in the Hubbard–Stratonovich (HS) transformation introduced later to ensure the convergence of the functional integral over the auxiliary fields.

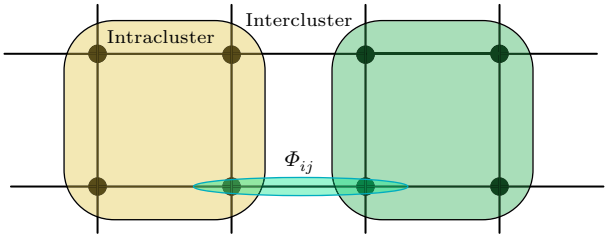


Fig. 1. The clusters, intercluster and intracluster bonds.

We start by decomposing the lattice into N_c clusters, and divide the bonds into two groups: intercluster bonds and intracluster bonds, as shown in Fig. 1. We decouple the clusters via HS transformations on the intercluster couplings, which introduces an imaginary-time-dependent, complex auxiliary field $\Phi_{ij}(\tau)$ for each intercluster bond (ij). This leads to the following form of the partition function:

$$Z = \mathrm{tr}\, \mathrm{e}^{-\beta \hat{H}} = \int \prod_{k\in xyz,(ij)} \mathcal{D}\Phi_{ij}^k \mathrm{e}^{-S[\Phi_{ij}^k(\tau)]} \prod_{m=1}^{N_c} Z_m^C[\Phi_{ij}^k(\tau)], \tag{2}$$

where the partition function is expressed as a functional integral over the auxiliary fields Φ_{ij}^k. In the weights of the functional integral, $S[\Phi_{ij}^k(\tau)] = \int \frac{1}{2}|J_{ij}^k|\Phi_{ij}^k(\tau)^2 \mathrm{d}\tau$ is the Gaussian term for the auxiliary field Φ_{ij}^k, and Z_m^C is the partition function for the m-th cluster:

$$Z_m^C[\Phi_{ij}^k(\tau)] = \mathrm{tr}\left\{ T_\tau \mathrm{e}^{-\int \mathrm{d}\tau \hat{H}_m^C[\Phi_{ij}^k(\tau)]} \right\}. \tag{3}$$

We note that, in Z_m^C, the original Hamiltonian is modified as $H_m^C[\Phi_{ij}^k(\tau)]$ such that the spin on a lattice site is coupled to the auxiliary fields associated with the intercluster bond connecting to that site,

$$\begin{aligned} &H_m^C[\Phi_{ij}^k(\tau)] \\ &= \sum_{i,j\in C_m,k} J_{ij}^k \hat{S}_i^k \hat{S}_j^k + \sum_{i\in C_m, j\notin C_m,k} \eta_{(ij);i} J_{ij}^k \Phi_{ij}^k(\tau) \hat{S}_i^k, \end{aligned} \tag{4}$$

where the first term resembles the original Heisenberg Hamiltonian (1) as it contains intracluster couplings, and the second is the coupling between spins and the auxiliary fields, where $\eta_{(ij);i} = \pm 1$ is a parameter that arises in the HS transformation: On the two sites of an FM bond ($J_{ij}^k < 0$), $\lambda_{(ij);i} = +1$. On the two sites of an AFM bond ($J_{ij}^k > 0$), we need to set $\eta_{(ij);i} = +1$ on one site and $\eta_{(ij);j} = -1$ on the other site. The difference between antiferromagnet and ferromagnetic cases comes from the different HS transformations we choose to make the action $S[\Phi_{ij}^k(\tau)]$ positive definite.

The HS transformation and consequently Eq. (1) are exact but impractical for Monte Carlo sampling since the single-cluster partition functions Z_m^C are generally complex and still lead to the sign problem.[39] To make the bAFMC more practical for numerical calculations, the partition functions Z_m^C should be positive real numbers. Therefore, we make the approximation of ignoring the imaginary-time fluctuation of the auxiliary fields $\Phi_{ij}^k(\tau)$, and treat them as classical fields $\Phi_{ij}^k(\tau) = \phi_{ij}^k$. Under this approximation, the partition function becomes

$$Z \approx \int \prod_{(ij),k} \mathrm{d}\phi_{ij}^k \mathrm{e}^{-S_{\mathrm{eff}}[\phi]}, \tag{5}$$

where the effective action is given by

$$S_{\mathrm{eff}}[\phi] = \beta \sum_{(ij),k} \frac{1}{2} J_{ij}^k (\phi_{ij}^k)^2 - \sum_{m=1}^{N_c} \log Z_m^C[\phi]. \tag{6}$$

The partition function for each cluster now takes a simpler form $Z_m^C[\phi] = \mathrm{tr}\exp(-\beta H_m^C[\phi])$, and it is therefore positive definite, because the Hamiltonian $H_m^C[\phi]$ becomes independent of the imaginary time. The sign problem is hence avoided as the partition function in Eq. (5) can be simulated by a classical Monte Carlo algorithm.

Such an approximation will partly decouple clusters in the imaginary-time fluctuations, and the cluster size can be viewed as an upper bound of wavelengths of quantum fluctuations in the approximated partition function (5). Using the picture of real-space renormalization group transformations, the upper bond could be seen as a moving cutoff and it describes the discrepancy between fully quantum and classical views of the system. Consequently, to obtain an accurate result, we should extrapolate to infinite cluster size, or the upper bound of the wavelength of quantum fluctuation. This extrapolation of the upper bond could be achieved using the ratio

$\lambda = N_{\rm ext}/(N_{\rm int}+N_{\rm ext})$, where $N_{\rm ext}$ is the number of bonds connecting different clusters and $N_{\rm int}$ is the number of bonds inside each cluster. Considering that the intracluster bonds are close to the exact result, the extrapolation should be done to make $\lambda = 0$,[38] equivalent to that all bonds are intracluster and the whole system is in a whole cluster as the case in exact solutions.

The physical quantity could be measured through the common way in quantum statistics:

$$\langle A\rangle = \frac{1}{Z}\int D\phi \langle A\rangle^C[\phi]\, {\rm e}^{-S_{\rm eff}[\phi]}, \tag{7}$$

which means first getting the expected value of the physical quantity in the cluster through a quantum computation:

$$\langle A\rangle^C[\phi] = \frac{{\rm tr}\left[\hat{A}\,{\rm e}^{-\beta\hat{H}^C[\phi]}\right]}{{\rm tr}\left[{\rm e}^{-\beta\hat{H}^C[\phi]}\right]},$$

and then getting the average value from the importance sampling of classical MC method.

3. Results

3.1. The 1D-antiferromagnetic chain

To validate the bAFMC approach, we test it in the cases of 1D antiferromagnetic spin-1/2 and spin-1 Heisenberg models. Figures 2 and 4 show the temperature dependence of the internal energy of the whole system with spin-1/2 and spin-1 through two different methods: (a) the exact result of SSE and (b) the result of bAFMC with the cluster size growing from a single site to half of the system. At finite cluster sizes, the results of bAFMC remain different from the SSE ones but exhibit a trend towards the latter upon the growing size of each cluster. As the internal energy of the system consists of the product of spins and there are two different kinds of products just as the bonds do, the intracluster ones and the intercluster one, we make a linear extrapolation in the ratio λ to get the result with all products being intracluster ones, as shown in Fig. 3. The linear form is also justified by the boundary chemical potential shift which might affect the thermodynamics linearly in λ within a single cluster. For the spin-1/2 chain, the extrapolated values of energy match well with the exact result of SSE.[40–42] For the spin-1 chain, the extrapolation matches well with SSE at high temperatures while it gives a higher energy at low temperatures, showing that the approximation of ignoring the temporal fluctuation of the auxiliary fields works better at higher temperatures.

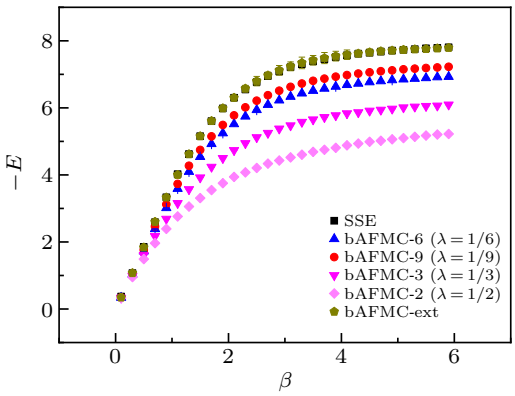


Fig. 2. Result for a spin-1/2 chain with 18 sites. The symbols labeled with "bAFMC-n" are data points produced using the bAFMC approach with cluster size n. The corresponding λ values are also noted in the legends.

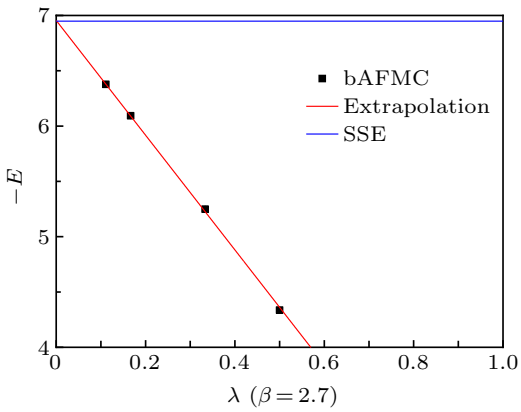


Fig. 3. The extrapolation of bAFMC with spin-1/2 chain.

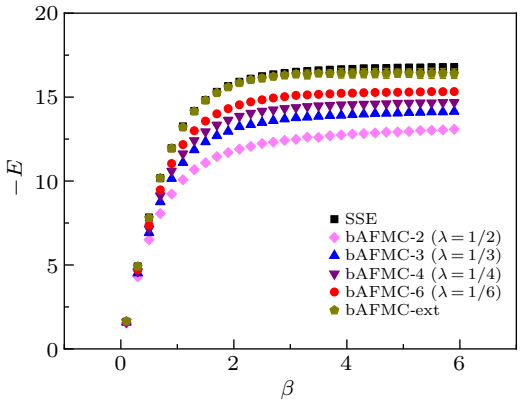


Fig. 4. Result for a spin-1 chain with 12 sites. The symbols labeled with "bAFMC-n" are data points produced using the bAFMC approach with cluster size n. The corresponding λ values are also noted in the legends.

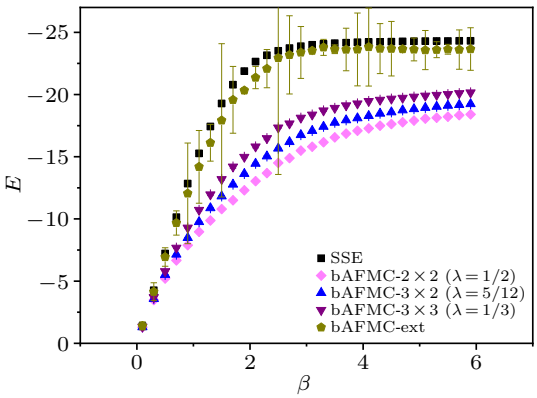


Fig. 5. Result for spin-1/2 antiferromagnetic Heisenberg model on a 6×6 square lattice. The symbols labeled with "bAFMC-$n\times m$" are data points produced using the bAFMC approach with cluster size $n\times m$. The corresponding λ values are also noted in the legends.

3.2. The 2D antiferromagnetic Heisenberg model in square lattice

We further test the bAFMC method in the case of spin-1/2 antiferromagnetic Heisenberg model in square lattice and the extrapolation matches result of SSE quite well as shown in Fig. 5 with the bar of extrapolation in the figure being the range of 95% confidence intervals.

3.3. The 2D antiferromagnetic Heisenberg model in triangle lattice

After validating the bAFMC method in models with no frustration and no sign-problem, we move on to frustrated magnets. The simplest frustrated model is antiferromagnetic Heisenberg model on triangle lattices. Figure 6 shows the temperature dependence of internal energy of the system compared with the result calculated through tangent-space approach for thermal tensor network,[43] in which the bar of extrapolation is the range of 95% confidence intervals. The agreement between results of two methods validates the bAFMC method in this frustrated model, where quantum Monte Carlo simulation is not available due to the sign problem.

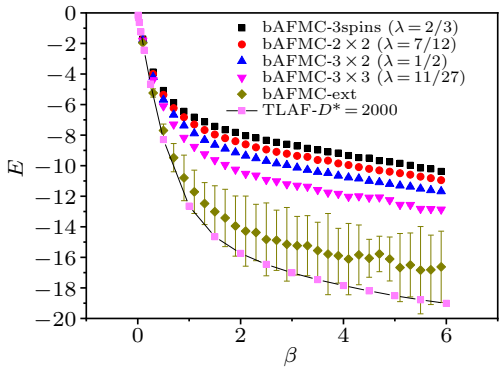


Fig. 6. Result for spin-1/2 antiferromagnetic Heisenberg model on a 6×6 triangular lattice. The symbols labeled with "bAFMC-$n \times m$" are data points produced using the bAFMC approach with cluster size $n \times m$ (the symbols labeled with "bAFMC-3spins" are calculated with clusters consisting of three spins in a triangle). The corresponding λ values are also noted in the legends.

4. Conclusion

In this work, we introduce bAFMC to frustrated magnets, which eliminates sign problems at the cost of cutting off long-range quantum correlations via cluster decoupling. The approximation is reliable due to the short-ranged quantum correlations at finite temperature and can be improved by moving the cutoff to large scales using larger cluster sizes. In our approach, we use ED for solving the quantum problem in a cluster, which encounters difficulty in clusters bigger than 16 sites at an enough high speed, and we use Metropolis algorithm to generate configurations, which costs a lot to generate uncorrelated configurations. It is natural that other algorithms for finite quantum systems, like finite-temperature Lanczos algorithm[44] or tensor-based methods,[43] can replace ED to speed up the calculation of larger clusters, which will improve the accuracy in larger systems. Besides, instead of Metropolis algorithm, methods like Hamiltonian Monte Carlo or self-learning Monte Carlo[45] might also be applied for higher efficiency in generating uncorrelated configurations. We believe the wide applicability and flexibility of our approach could solve a wide range of frustrated many-body problems.

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