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Vanishing of the negative-sign problem of quantum Monte Carlo simulations in one-dimensional frustrated spin systems

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We have solved the negative-sign problem in a general frustrated double-spin-chain system, namely the J_0-J_1-J_2-J_3 model. This is made possible by changing the representation basis from the conventional s^z basis to a dimer basis that has the spin-reversal symmetry. The necessary condition for the problem to disappear in this new basis is $J_0+J_1 \leqslant J_3$. Frustration is the origin only in the conventional s^z basis. We demonstrate the efficiency of this new basis at the transition point between the gapless spin-fluid phase and the gapped dimer phase. [S0163-1829(98)51506-8]

The class of low-dimensional quantum spin systems is now attracting interest both theoretically and experimentally. This interest originates in the possibility of the superconductivity upon doping carriers to an insulator that has a spin gap above the ground state.[1,2] Spin-ladder models, or more generally double-spin-chain models, are known as such candidates. Progress of this field is stimulated by syntheses of various corresponding materials.[3–7] For example, the magnetic susceptibility of $KCuCl_3$ (Ref. 5) shows a spin-gap behavior, which can be explained by a frustrated double-spin-chain model. In the analysis of such an experiment, it is necessary to estimate the strength of interaction bonds of the model Hamiltonian.[8–11] This inverse problem is generally difficult both analytically and numerically.

Numerical methods may serve as a powerful tool of calculating the thermodynamic quantities. All the eigenvalues of a finite system can be obtained by the numerical diagonalization technique. Then, any quantity at any temperature is calculated, however, the size of the system is seriously restricted, e.g., up to sixteen $S=1/2$ spins. One is sometimes misled to the wrong conclusion by the spurious finite-size effect or by an improper choice of the numerical method.[12] It is desired to develop a reliable method that is free from the finite-size effect. The quantum Monte Carlo (QMC) method can handle much larger systems, if there does not exist the negative-sign problem.[1,10] Because of this difficulty, the application of the QMC method is also restricted. This problem appears in the frustrated spin systems and in the electron systems. Here, we only deal with the spin case.

The local Boltzmann weight may take a negative value in the simulations with the negative-sign problem. Thus, one uses its absolute value for the spin update. The problem occurs when the original system is not equivalent to the system defined by taking the absolute value of the local weights. In such a case, we must reweight both the number of steps and the sum of the physical quantity to obtain the correct expectation value. The reweighting becomes difficult at low temperatures or for large system sizes, and then the QMC measurements break down. Though several techniques have already been proposed to relax the negative-sign problem,[13–15] the problem still remains. The negative-sign problem should be overcome completely to get meaningful numerical data that can be compared directly with the experiment.

In this paper, we demonstrate that the negative-sign problem is *completely* removed for the first time in a nontrivial frustrated spin system. The key idea is the use of the spin-reversal symmetry applied to the restructuring method.[15] The representation basis is changed from the conventional s^z basis to the dimer basis as will be explained below. The change of the basis has been rather ignored until quite recently, since the basis is sufficient if it is normal, orthogonal, and complete in principle. We focus on this degree of freedom. There, a guide to a proper choice is the symmetry of the system.

We consider the generalized double-spin-chain system defined by its next-nearest-neighbor interactions, J_0 and J_1, and by the alternating nearest-neighbor interactions, J_2 and J_3, as depicted in Fig. 1. This model can describe various systems. For example, the dimer-fluid transition point, where the spin-Peierls material $CuGeO_3$ (Ref. 3) is suggested to realize,[8,9] is $(J_0,J_1,J_2,J_3)=(0.2411,0.2411,1,1)$.[16] We divide this Hamiltonian into two parts for the Suzuki-Trotter decomposition.

$$\mathcal{H}_1=\sum_{n=1}^{(N+1)/2} h_{2n-1}, \quad \mathcal{H}_2=\sum_{n=1}^{N/2} h_{2n}, \tag{1}$$

$$h_n=J_0\boldsymbol{\sigma}_n\cdot\boldsymbol{\sigma}_{n+1}+J_1\boldsymbol{\tau}_n\cdot\boldsymbol{\tau}_{n+1}+\frac{J_2}{2}\boldsymbol{\sigma}_n\cdot\boldsymbol{\tau}_n+\frac{J_2}{2}\boldsymbol{\sigma}_{n+1}\cdot\boldsymbol{\tau}_{n+1}+J_3\boldsymbol{\tau}_n\cdot\boldsymbol{\sigma}_{n+1}. \tag{2}$$

Then, the total Boltzmann weight, $\langle\psi|\exp[-\beta\mathcal{H}]|\psi\rangle$, is decomposed into the product of the local weights as $\exp[-\beta\mathcal{H}]\simeq(\exp[-\beta\mathcal{H}_1/m]\exp[-\beta\mathcal{H}_2/m])^m$.

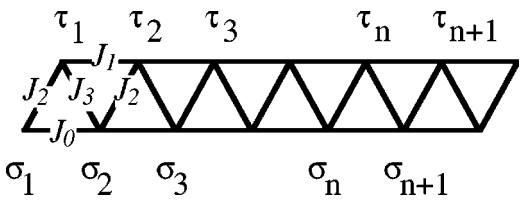

FIG. 1. Shape of the general double-spin-chain model we treat in this paper.

We propose the representation basis $|\psi\rangle$ in the following manner. Two spins of $\boldsymbol{\sigma}_n$ and $\boldsymbol{\tau}_n$ are coupled and considered as a unit. This dimer unit takes four states associated with the s^z eigenvalues of each spin, $|\sigma^z,\tau^z\rangle$. Then, these four states are restructured so as to become eigenstates of the spin-reversal operator R:

$$v_1=(|\uparrow,\uparrow\rangle+|\downarrow,\downarrow\rangle)/\sqrt{2}, \tag{3}$$

$$v_2=(|\uparrow,\uparrow\rangle-|\downarrow,\downarrow\rangle)/\sqrt{2}, \tag{4}$$

$$v_3=(|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle)/\sqrt{2}, \tag{5}$$

$$v_4=(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle)/\sqrt{2}. \tag{6}$$

Here, $\uparrow$ and $\downarrow$ denote the s^z eigenstates. Direct product of these four states spans the whole phase space. In this new basis, three interaction bonds, J_0, J_1, and J_3, become a single effective bond connecting the neighboring dimer units, and the J_2 bonds only contribute to the inner energy of the dimer units. It is quite striking that this basis transformation alone removes the negative-sign problem. Let us call this basis a ''dimer-R'' basis hereafter.

We first write down the matrix element of h_n. The 16×16 square matrix is block-diagonalized by the spin-reversal symmetry into four 4×4 sub-blocks:

$$\begin{array}{c} \\ \langle v_1,v_1| \\ \langle v_2,v_2| \\ \langle v_3,v_3| \\ \langle v_4,v_4| \end{array} \begin{array}{c} \begin{array}{cccc} |v_1,v_1\rangle & |v_2,v_2\rangle & |v_3,v_3\rangle & |v_4,v_4\rangle \end{array} \\ \begin{pmatrix} -J_2 & -a & -a & -d \\ -a & -J_2 & a & d \\ -a & a & -J_2 & d \\ -d & d & d & 3J_2 \end{pmatrix} \end{array} \times\frac{-1}{4},$$

$$\begin{array}{c} \\ \langle v_2,v_1| \\ \langle v_1,v_2| \\ \langle v_3,v_4| \\ \langle v_4,v_3| \end{array} \begin{array}{c} \begin{array}{cccc} |v_2,v_1\rangle & |v_1,v_2\rangle & |v_3,v_4\rangle & |v_4,v_3\rangle \end{array} \\ \begin{pmatrix} -J_2 & -a & -b & -c \\ -a & -J_2 & b & c \\ -b & b & J_2 & d \\ -c & c & d & J_2 \end{pmatrix} \end{array} \times\frac{-1}{4},$$

$$\begin{array}{c} \\ \langle v_1,v_3| \\ \langle v_3,v_1| \\ \langle v_2,v_4| \\ \langle v_4,v_2| \end{array} \begin{array}{c} \begin{array}{cccc} |v_1,v_3\rangle & |v_3,v_1\rangle & |v_2,v_4\rangle & |v_4,v_2\rangle \end{array} \\ \begin{pmatrix} -J_2 & -a & -b & -c \\ -a & -J_2 & b & c \\ -b & b & J_2 & d \\ -c & c & d & J_2 \end{pmatrix} \end{array} \times\frac{-1}{4},$$

$$\begin{array}{c} \\ \langle v_2,v_3| \\ \langle v_3,v_2| \\ \langle v_1,v_4| \\ \langle v_4,v_1| \end{array} \begin{array}{c} \begin{array}{cccc} |v_2,v_3\rangle & |v_3,v_2\rangle & |v_1,v_4\rangle & |v_4,v_1\rangle \end{array} \\ \begin{pmatrix} -J_2 & -a & -b & -c \\ -a & -J_2 & b & c \\ -b & b & J_2 & d \\ -c & c & d & J_2 \end{pmatrix} \end{array} \times\frac{-1}{4},$$

where $a=J_0+J_1+J_3$, $b=-J_0+J_1+J_3$, $c=J_0-J_1+J_3$, and $d=-J_0-J_1+J_3$.

These matrix elements include negative signs and the negative-sign problem still seems to exist. However, we can prove by the following nonlocal unitary transformation[17–19] that these negative signs do not cause the problem. This transformation is an adaptation of the Kennedy-Tasaki transformation[17] of the $S=1$ antiferromagnetic (AF) Heisenberg chain to the $S=1/2$ double-spin-chain systems. It transforms the hidden-AF order into the ferromagnetic order by the spin-reversal operation, and is defined by U:

$$U=\prod_{n=1}^{N} P_n^+ + P_n^- \exp[i\pi S_n^x], \tag{7}$$

$$P_n^{\pm}=\frac{1}{2}\left(1\pm\exp\left[i\pi\sum_{k=1}^{n-1} S_k^z\right]\right), \tag{8}$$

where $\mathbf{S}_n=\boldsymbol{\sigma}_n+\boldsymbol{\tau}_n$. Then, the local Hamiltonian h_n is transformed as,

$$\begin{aligned} U^{-1}h_nU=&J_0(-\sigma_n^x\tau_{n+1}^x-\tau_n^z\sigma_{n+1}^z-4\sigma_n^x\tau_{n+1}^x\tau_n^z\sigma_{n+1}^z)\\ &+J_1(-\tau_n^x\sigma_{n+1}^x-\sigma_n^z\tau_{n+1}^z-4\tau_n^x\sigma_{n+1}^x\sigma_n^z\tau_{n+1}^z)\\ &+J_3(-\tau_n^x\tau_{n+1}^x-\sigma_n^z\sigma_{n+1}^z-4\tau_n^x\tau_{n+1}^x\sigma_n^z\sigma_{n+1}^z)\\ &+\frac{J_2}{2}\boldsymbol{\sigma}_n\cdot\boldsymbol{\tau}_n+\frac{J_2}{2}\boldsymbol{\sigma}_{n+1}\cdot\boldsymbol{\tau}_{n+1}. \end{aligned} \tag{9}$$

Each matrix element of this transformed Hamiltonian becomes the one whose negative sign is taken away from the original one. Note that the signs of the interactions, J_0, J_1, and J_3, are changed. All the matrix elements become positive if all the a, b, c, and d are positive. This is when

$$d=-J_0-J_1+J_3\geqslant0 \tag{10}$$

for the AF positive values of J_0, J_1, and J_3. The above condition does not restrict the value of J_2, since it only contributes to the diagonal matrix elements.

Why does the negative-sign problem vanish by this basis change? The answer may be found by considering why it vanishes in the nonfrustrated systems in the s^z basis. This is because we can remove negative signs of the local Boltzmann weights by the following transformation. First, we decompose the system into bipartite sublattices, so that a spin on one sublattice only interacts antiferromagnetically with spins on the other sublattice. This decomposition is only possible in nonfrustrated systems. Then, we apply the 180° rotation of the spin space along the s^z axis, $s_i^x\rightarrow-s_i^x$ and $s_i^y\rightarrow-s_i^y$, for i belonging to one sublattice. This transformation does not influence the physics, but changes the negative off-diagonal matrix elements to the positive values. Therefore, the negative-sign problem does not appear, since the original system is equivalent to the system defined by the absolute values of the local weights. Here, it should be noticed that this transformation preserves the symmetry of the basis. In the present dimer-R basis, the nonlocal unitary transformation defined by Eq. (7) works the same as the rotational transformation stated above. This transformation alternatively reverses the spin state depending on the hidden-AF order, and also preserves the symmetry of the basis. The unitarity guarantees the equivalence of the origi-

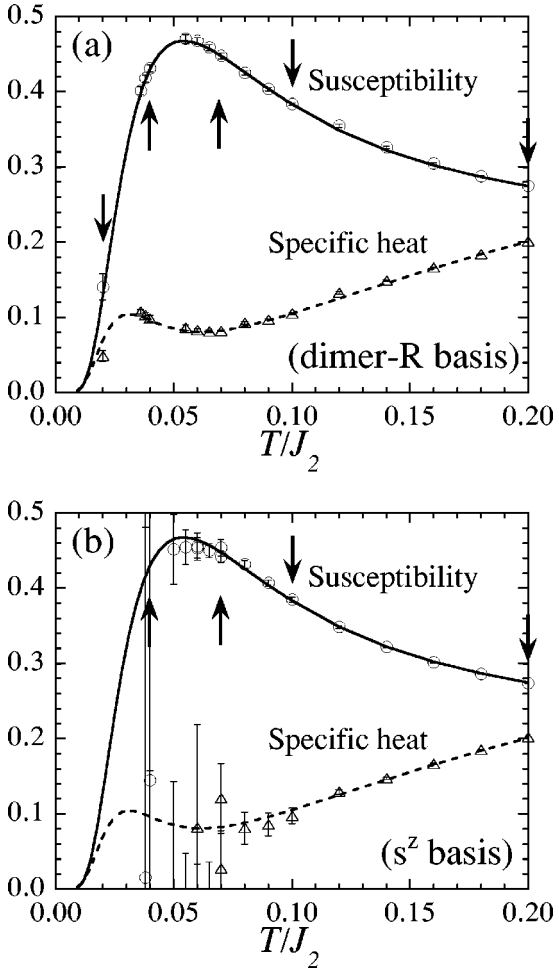

FIG. 2. (a) The susceptibility (circles) and the specific heat (triangles) for the system with ten spins calculated by using the present dimer-R basis. The exact results obtained by the numerical diagonalization are denoted by lines. (b) Those of the same system calculated by using the conventional s^z basis. Arrows indicate the temperatures at which the simulations are actually performed. The others are estimated by the reweighting method.

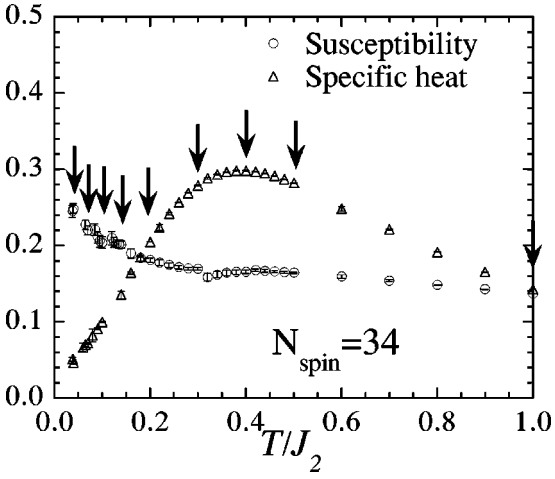

FIG. 3. The susceptibility (circles) and the specific heat (triangles) for the system with 34 spins calculated by using the dimer-R basis. Arrows indicate the temperatures at which the simulations are actually performed.

nal system to the system actually simulated. It can be said that the necessary condition for the negative-sign problem to disappear is dependent on the symmetry of the basis and its preserving transformation. The statement, ''the negative-sign problem occurs in the frustrated spin systems,'' is only valid in the conventional s^z basis. General proof of this idea is left for the future.

Before the demonstration of the advantage of the present method, we point out several important notices briefly. Details will be reported elsewhere. Since the negative-sign problem has been removed by using the spin-reversal symmetry, we have to be careful about the operation that breaks this symmetry; the negative-sign problem appears again, if we apply the uniform magnetic field. In our new representation, the matrix element for the field H only takes the nonvanishing value between v_1 and v_2, i.e., $\langle v_1|-H(\sigma_i^z+\tau_i^z)|v_2\rangle=-H$. Another point is that we cannot observe the uniform magnetic susceptibility from the fluctuation of the magnetization, since it does not fluctuate but always remains zero. In other words, a local expectation value of the magnetization vanishes for a nonvanishing Boltzmann weight, and vice versa. Therefore, we have considered the following two different methods of calculating the susceptibility. The first one is that we take all the configurational summation over a single Trotter layer to deduce the expectation value of $(\Sigma_i S_i^z)^2$ in the measurement stage in each Monte Carlo step. This partial trace-out can be done by multiplying the 4×4 transfer matrix along the real space direction. The second one is the numerical differentiation of the magnetization when we apply the sufficiently small magnetic field. Of course, the negative-sign problem appears in this case, but the problem is not so serious if the field is small enough. For example, the typical negative-sign ratio at the temperature $T/J_2=0.04$ is only 0.5 when $H/J_2=0.02$ in the system with 34 spins. Thus, we can calculate the susceptibility without any difficulty.

We can now perform the QMC simulation without the negative-sign problem if the condition (10) is satisfied. The numerical results are presented for the system at the dimer-fluid transition point, where $J_0=J_1$, $J_2=J_3$, and $J_1/J_2=0.2411$. The boundary conditions are set open. The temperatures where we actually perform simulations are pointed out by arrows within figures. The other data are obtained by the reweighting method.[13] We have done the Trotter extrapolations by using five or six different Trotter numbers ranging from $\beta/m=0.5$ to 0.2. The number of the Monte Carlo steps is five millions divided into ten parts to estimate the deviations. The typical correlation time for the energy is about five steps for $T/J_2=0.2$ and $m=24$ and that for the susceptibility is less than 1 step.

We first check our QMC simulation in the system with ten spins. The uniform susceptibility and the specific heat are calculated. The susceptibility data are taken by using the first method. Figure 2(a) shows the data by using the dimer-R basis, and Fig. 2(b) shows those by the s^z basis. The exact results obtained by the numerical diagonalization are also plotted by lines. Agreements of the data in our method are excellent down to the temperature $T/J_2=0.02$ for both quantities. Error bars are mostly smaller than symbols On the other hand, the QMC measurement in the s^z basis begins to crash already at $T/J_2=0.1$. This reveals that the conven-

tional QMC method cannot be applied even to a small system that can be numerically diagonalized.

Figure 3 shows the results of the system with 34 spins for $T/J_2 > 0.04$, which cannot be obtained by any other method. The susceptibility was calculated both by the transfer matrix and by the numerical differentiation of the magnetization. The magnitude of the uniform magnetic field for the latter case is $H/J_2 = 0.02$. Both methods give consistent results within the error bars, and we have adopted the one whose error bar is smaller than the other one. The data of $T/J_2 \geqslant 0.2$ are obtained by the transfer matrix, and the others are by the differentiation. The susceptibility grows as the temperature decreases, i.e., the pseudogap caused by the finite size of the system seems to be smaller than the temperatures we have simulated. The specific heat was obtained in the simulation at zero field. The error bars for this value are also negligible. Rather large ones, though they are within the symbols, are solely from the reweighting error. We believe that the temperature can be still lowered below $T/J_2 = 0.04$, if one can have enough CPU time to handle the simulations of large Trotter numbers.

We have presented a new possibility of the quantum Monte Carlo simulation in the one-dimensional frustrated spin systems. The negative-sign problem is completely removed in a wide range of the parameter space by using the representation basis that has the spin-reversal symmetry. This basis change alone is responsible for solving the sign problem. The nonlocal unitary transformation of Eq. (7) is only used to prove that the negative signs disappear. The present method makes it possible to perform large-scale simulations within the restricted computational facilities. All the numerical results presented in this paper were obtained by a DEC Alpha-433 personal computer in two weeks. These data will not be obtained even by any supercomputer, if one uses the conventional s^z basis. As for the negative-sign problem in two dimensions, the necessary condition for the problem to disappear should take a different form independent from frustration, if one uses the basis with a different symmetry. In such a situation, one should take into account the relevant symmetry of the system as was successful in the present case.

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