First-order phase transition of the exchange-interaction model studied by the Handscomb quantum Monte Carlo method

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Thermodynamic properties of the ferromagnetic spin-S exchange-interaction model are studied by the Handscomb quantum Monte Carlo method. We have studied simple cubic lattices with sizes up to $12\times12\times12$. We show numerical evidence of hysteresis effects for $S\geqslant2$ that supports the prediction of a first-order transition in mean-field theory. These results are further confirmed by using the histogram analysis of Monte Carlo data. [S0163-1829(98)01209-0]

The Handscomb quantum Monte Carlo (HQMC) method[1] was introduced by Handscomb 30 years ago in the study of the ferromagnetic Heisenberg model. Later in the 1980's this method was revised independently by Lyklema[2] and Chakravarty and Stein.[3] They proved that more accurate results for ferromagnetic quantum spin system can be obtained by using HQMC as compared with the Suzuki-Trotter quantum Monte Carlo method.[4] An important improvement of this method was put forward by Lee *et al.*[5] who generalized the method to study antiferromagnetic Heisenberg model. Inspired by Anderson's suggestion[6] of the importance of antiferromagnetic interaction in the superconducting mechanism of high-temperature superconductors, HQMC has been applied to study the low-energy properties of the two-dimensional antiferromagnetic Heisenberg model.[7] Recently, Sandvik *et al.* proposed a generalized scheme of HQMC to study the one-dimensional spin-S antiferromagnetic Heisenberg model[8] and Hubbard model.[9] It is important to note that progress along this direction is worthy of more attention.

In this paper we apply HQMC to study the thermodynamic properties of spin-S exchange interaction model[10] (EIM) in a three-dimensional (3D) simple cubic lattice. The Hamiltonian describing the EIM with N spins and M $(=3N)$ bonds is given by

$$H=-J\sum_{\langle i,j\rangle} P_{ij}, \tag{1}$$

where P_{ij} is the exchange operator, which exchanges two spin coordinates of $\mathbf{S}_i$ and $\mathbf{S}_j$, i.e., $P_{ij}|\mathbf{S}_i,\mathbf{S}_j\rangle=|\mathbf{S}_j,\mathbf{S}_i\rangle$. For $S=\frac{1}{2}$, P_{ij} is the Dirac exchange operator. Hence EIM is identical to the $S=\frac{1}{2}$ Heisenberg model. For higher spin, Shröedinger proved that P_{ij} can be expressed as a polynomial of $(\mathbf{S}_i\cdot\mathbf{S}_j)$. Therefore one can learn the effect of nonlinear term $(\mathbf{S}_i\cdot\mathbf{S}_j)^n$ on the critical properties of a spin system with EIM. In this paper we will consider the ferromagnetic EIM, i.e., $J>0$.

We have applied HQMC to study the one-dimensional EIM (Ref. 11) and obtained results in good agreement with the Bethe ansatz and spin-wave analysis. For 3D EIM there are many studies by using different methods. Chen and Joseph[10] applied high-temperature series expansion to study this model. Assuming the existence of a second-order phase transition in all spins they found the critical temperatures and exponents for spin $S\leqslant2$. However, in a mean-field approximation Chen *et al.*[12] obtained first-order phase transitions for spin $S\geqslant1$. A similar conclusion of first-order phase transition was also obtained for $S=1$ EIM by using a Greens-function decoupling method.[13] This discrepancy motivates us to apply HQMC to investigate the nature of the transition in 3D EIM. An important advantage of employing HQMC is that due to the symmetric properties of exchange operators in the Hamiltonian, the calculations can be easily implemented in the computing program.

In Handscomb's approach, the partition function is written as

$$Z=\sum_{r=0}^{\infty}\frac{K^r}{r!}\mathrm{Tr}\left[\sum_{\langle i,j\rangle} P_{ij}\right]^r=\sum_{r=0}^{\infty}\sum_{\alpha=1}^{M^r}\frac{K^r}{r!}\mathrm{Tr}C_{r,\alpha}, \tag{2}$$

where $K=J/k_BT$. The expansion of $(\Sigma_{\langle i,j\rangle}P_{ij})^r$ contains M^r terms and each term is a product of a sequence of r exchange operators P_{ij}. The αth sequence is denoted as $C_{r,\alpha}$. Similarly, the thermal average of a physical observable A of the model

$$\langle A\rangle=[\mathrm{Tr}A\ \exp(-H/k_BT)]/Z,$$

can also be expressed as

$$\langle A\rangle=\frac{1}{Z}\sum_{r=0}^{\infty}\sum_{\alpha=1}^{M^r}\frac{K^r}{r!}\mathrm{Tr}AC_{r,\alpha}=\sum_{r}\sum_{\alpha}\left[\frac{\mathrm{Tr}AC_{r,\alpha}}{\mathrm{Tr}C_{r,\alpha}}\right]\pi_{r,\alpha}$$
$$=\sum_{r}\sum_{\alpha}A_{r,\alpha}\pi_{r,\alpha}, \tag{3}$$

where

$$\pi_{r,\alpha}=\frac{1}{Z}\frac{K^r}{r!}\mathrm{Tr}C_{r,\alpha}, \tag{4}$$

$$A_{r,\alpha}=(\mathrm{Tr}AC_{r,\alpha})/(\mathrm{Tr}C_{r,\alpha}). \tag{5}$$

Equation (3) indicates that $\langle A\rangle$ is the average of $A_{r,\alpha}$ over $C_{r,\alpha}$'s with the weight $\pi_{r,\alpha}$, provided that all $\pi_{r,\alpha}\geqslant0$, as in our case with $J>0$. Details of the Markov chain can be found in Ref. 14.

Accordingly, the total energy per spin E, can be expressed as

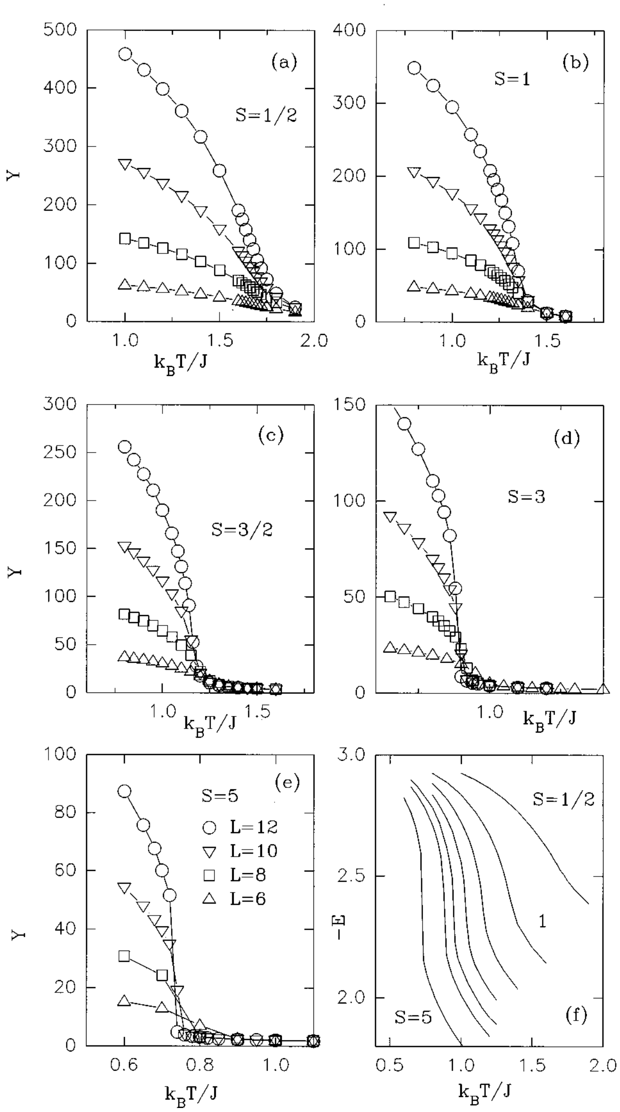

FIG. 1. (a)–(e) Temperature dependence of the magnetic second moment for $S=\frac{1}{2}$, 1, $\frac{3}{2}$, 3, and 5, respectively. For each spin, the lattice size L ranges from 6 to 12 as indicated in (e). Error bars are less than the size of symbols except those close to the transition. (f) Temperature dependence of energy for $S=\frac{1}{2}$, 1, $\frac{3}{2}$, 2, $\frac{5}{2}$, 3, and 5 with a fixed lattice size $L=12$.

$$E=-(J/N)(\partial \ln Z/\partial K)=-\frac{k_BT}{N}\sum_r \sum_\alpha r\pi_{r,\alpha}, \tag{6}$$

and the magnetic second moment per spin, Y as

$$Y=\frac{3}{NS(S+1)}\left\langle\left[\sum_i S_{iz}\right]^2\right\rangle=\sum_r \sum_\alpha \left[\sum_j a_j^2(r,\alpha)\right]\pi_{r,\alpha}, \tag{7}$$

where $a_j(r,\alpha)$ are the number of spins in the jth cycles of the $C_{r,\alpha}$ sequence.[14]

In Figs. 1(a)–1(e) we show the temperature dependence of the magnetic second moment for $S=\frac{1}{2}$, 1, $\frac{3}{2}$, 3, and 5 with lattice size ranging from 6 to 12. A periodic boundary condition is imposed. A typical result for energy is shown in Fig. 1(f). We performed $2-10\times 10^4$ Monte Carlo steps[15] (MCS) for each data point depending on temperature and lattice size. The measurements of energy have better accuracy than those of the magnetic second moment. It is interesting to note that very accurate results are obtained by moderate computation time and there is no need to do extrapolation in imaginary time.[4] As we mentioned, the mean-field theory predicts first-order phase transition for $S \geqslant 1$, in which cases a discontinuous jump in the order parameter at transition is expected. This can be seen by comparing the data for increasing values of spin. To have an intimate picture of how the transition changes qualitatively with spin, we put all energy data of $L=12$ for various spins in Fig. 1(f). It is obvious that the transition becomes sharper as spin value increases.

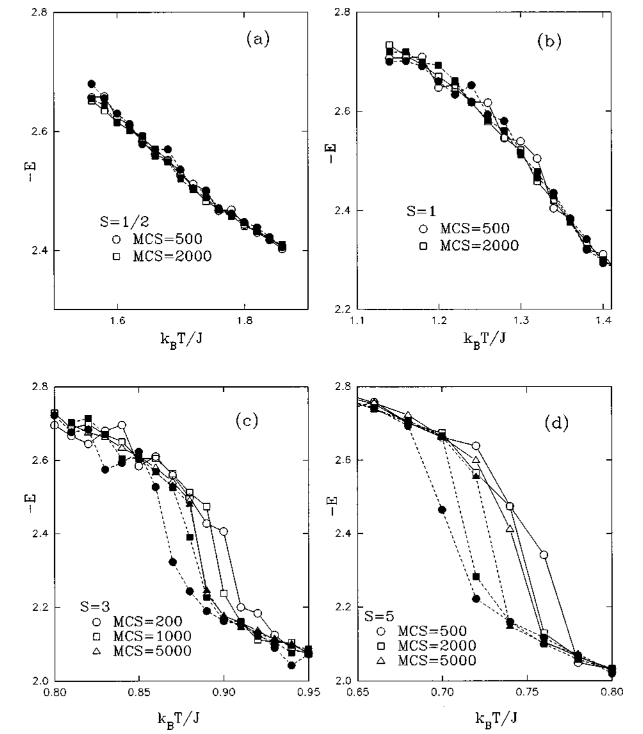

FIG. 2. (a)–(d) Hysteresis data of the energy for $S=\frac{1}{2}$, 1, 3, and 5, respectively. Open symbols connected with solid lines are heating processes and filled symbols connected with dash lines are cooling processes. The rate of heating/cooling process is indicated by the Monte Carlo steps performed between two successive temperatures with difference $\Delta T=0.2$ (a,b) and 0.1 (c,d).

Though there are indications of qualitative differences between low and high spins, it is still quite a delicate problem to determine the nature of the transition in a weak first-order transition revealed by Monte Carlo simulation. Several criteria have been proposed to determine the nature of transitions in the Potts model.[16,17] One of the signatures of first-order transition in Monte Carlo simulation is the observation of hysteresis effect.

However, the occurrence of hysteresis may depend on the rate of heating and cooling and even worse it may also be present in a second-order transition due to critical slowing down. We indeed observed hysteresis for most spins ($S \geqslant 2$) with a high enough heating/cooling rate. Typical results are shown in Figs. 2(a)–2(d) for $S=\frac{1}{2}$, 1, 3, and 5. We also show the results for different rates of heating and cooling. From these we can see that as we slow down the rate of the hysteresis loop becomes narrower and eventually merges to the curve of equilibrium (Fig. 1), in spite of the qualitative

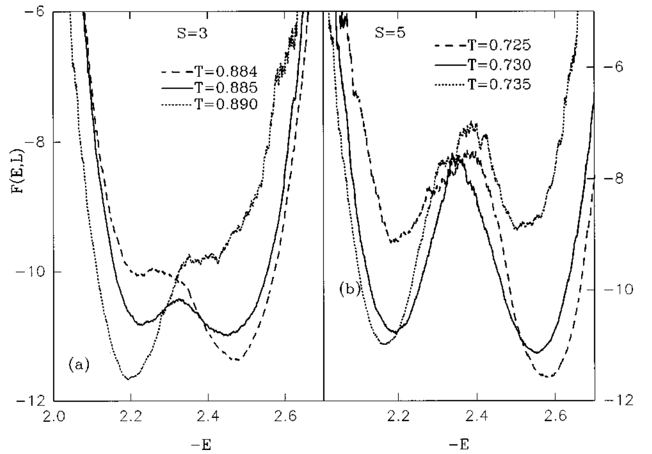

FIG. 3. Free energy $F(E,L)$ for $S=3$ (a) and 5 (b) for various temperatures around transition at fixed $L=12$.

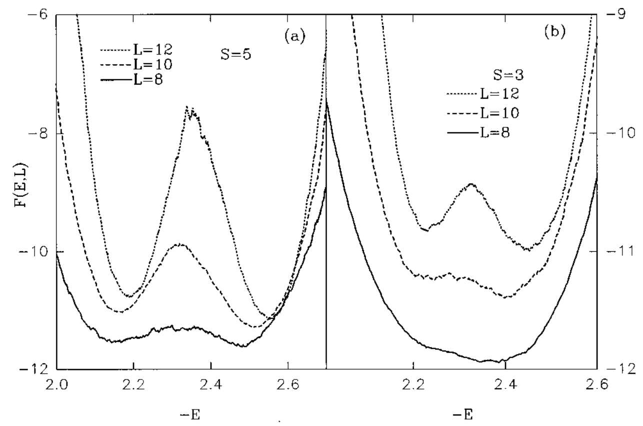

FIG. 4. Finite-size behaviors of free energy $F(E,L)$ for $S=5$ (a) and 3 (b) with temperatures fixed at $T_c(L)$.

difference between low and high spins. We have not found the clear evidence of first-order transition for $S=1$ and $\frac{3}{2}$. As compared with $\frac{1}{2}$ we have observed the enhanced fluctuations at the transition region. (With these it is sufficient to show that they are at most of a weak first-order transition for these low-spin cases.) On the other hand, the pronounced hysteresis for $S=5$ [Fig. 2(d)] suggests a strong first-order transition. To assess the issue of the nature of transition without ambiguity, we must study carefully the finite-size dependence. Fortunately, we found that the method of histogram analysis introduced by Lee and Kosterlitz[18,16] can be successfully applied to determine the nature of the transition of EIM.

Let us define the ''free energy'' in terms of probability distribution function,

$$F(E,L) = -\ln(\Pr(E,L)), \tag{8}$$

where $\Pr(E,L)$ is the probability of the configuration with energy E and lattice size L appears in the simulation. In the vicinity of transition, $F(E,L)$ has a characteristic double-minima structure, correspondingly, a double-peak structure in $Pr(E,L)$. The characteristic transition temperature for the finite lattice, $T_c(L)$, is defined as the temperature at which two minima have equal depth. Then we define the free-energy barrier, $\Delta F(L)$, as the difference between the maximum and minimum at $T_c(L)$. According to Lee and Kosterlitz, for a temperature-driven phase transition we can determine the properties of the transition by studying the finite-size behavior of $\Delta F(L)$. At a first-order transition, $\Delta F(L)$ is a monotonically increasing function of L, rather than a constant for continuous transition. This criterion has been tested for the q-state Potts model both in 2D and 3D cases.

In our HQMC, energy is proportional to the number r of the operators of sequence $C_{r,\alpha}$ [Eq. (6)]. Therefore the histogram data of the energy can be directly obtained by counting the frequency of which the number r appears in the Markov chain. In our simulations, r is updated in each step, which appears to be an excellent observable for histogram analysis. In Fig. 3 we show the histogram results for $S=2$, $\frac{5}{2}$, 3, and 5 for temperatures close to the transition region. From these we see that there are prominent double minima for higher spins in a way similar to what have been observed for the q-state Potts model. We fail to observe unambiguous double minima for $S\leqslant 2$ for lattice size $L\leqslant 12$. However we do find evidence for $S=2$ in a larger lattice with $L=14$ (not shown). To estimate the ''free-energy barrier'' $\Delta F(E,L)$, it is necessary to locate the characteristic transition temperature $T_c(L)$ accurately. These were achieved by performing a shorter run of histogram data for various temperatures around transition. From Fig. 3 we can see that the double-minima structure has a sensitive response to temperature variation. This helps in locating the characteristic temperature $T_c(L)$ for different sizes and spins. After $T_c(L)$ is set, we perform a long run of histograms at $T_c(L)$ to obtain the free-energy barrier $\Delta F(E,L)$.

In Fig. 4 we present the free energy of $S=3$ (a) and 5 (b) for $L=8$, 10, and 12 at the temperature $T_c(L)$. We can see that the free-energy barrier grows monotonically with increasing lattice size for both cases. This confirms the first-order transition for higher spins. Moreover, the rapid increase of $\Delta F(E,L)$ for $S=5$ indicates a strong first-order transition which is consistent with the hysteresis [Fig. 2(d)] observed for $S=5$ even in a slow heating and cooling rate.

For $S=1$ and $\frac{3}{2}$, due to large correlation length we are unable to determine the nature of their transition with current computational power and limited lattice size. Calculations on a larger lattice $L>12$ is necessary to detect the signals of the first-order transition. On the other hand, if we assume a second-order transition for $S=1$ and $\frac{3}{2}$, then we can apply a phenomenological renormalization method[14] to determine the critical temperatures and exponents. Using this method to analyze the data of Figs. 1(a)–1(c), we obtain the critical temperatures and exponents agreeing with the results of high-temperature series expansion. This situation resembles very much the ''pseudocritical behavior'' observed in the Potts model where the weak first-order transition is featured.[16]

In conclusion, we have applied the Handscomb quantum Monte Carlo method to investigate the thermodynamic properties of the 3D exchange interaction model. Accurate data can be obtained with moderate computer time. Pronounced hysteresis effects are observed for high spins. By the use of the histogram analysis of the energy data, we confirm the first-order transition predicted in previous mean-field theory for $S\geqslant 2$. On the other hand, it is interesting to compare these results with the critical properties of the Heisenberg model of general spins.[19] One finds that (1) they are consistent with second-order transition for all spins and (2) there is little change in the critical exponents for spins from $\frac{1}{2}$ to ∞ (classical Heisenberg model), hence universality is valid. Obviously, the appearance of a higher-order term of $(\mathbf{S}_i \cdot \mathbf{S}_j)$ in the exchange operator is the origin of the first-order transition in EIM. It is interesting to point out that the histogram method which has been successfully employed to the q-state Potts model also works well for EIM which is a quantum-spin system with continuous symmetry. It is promising that this method may be applied to study the phase separation (expected to be a first-order transition) in the t-J model[20] and other related models of strongly correlated electrons.[21,22]

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