Quantum Monte Carlo study of the spin-$\frac{1}{2}$ Heisenberg model

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Thermodynamic properties of the spin-$\frac{1}{2}$ Heisenberg ferromagnet are calculated by using Handscomb's Monte Carlo method. Several methods of analyses are used to determine critical properties of the model. For a square lattice we find that the susceptibility diverges exponentially at zero temperature. That is, $\chi \sim \exp[b(J/k_B T)]$ with the constant $b=4.5\pm0.5$, which is lower than the prediction ($b=2\pi$) of a modified spin-wave theory. For the simple-cubic lattice, we find that the critical temperature $k_B T_c/J=1.68\pm0.01$, and the ratio of the exponents $\gamma/\nu=2.0\pm0.05$, which are in good agreement with the estimates of the high-temperature series-expansion method.

I. INTRODUCTION

The Monte Carlo method is a powerful tool for many branches of statistical physics.[1-4] It especially provides the most useful and accurate estimates of the critical properties of systems which can be described by classical spin models.[1,2] Monte Carlo studies of the critical properties for quantum spin models, however, are more complicated and less fruitful.[3,4]

The are several Monte Carlo methods for quantum spin models. One approach proposed by Handscomb[5] and restudied by Lyklema[4] makes use of the permutation property of the Heisenberg exchange interactions, and expresses the partition function as a sum of traces of all possible products of the interactions. A method developed by Suzuki[6] uses the generalized Trotter formula[7] and transforms a d-dimensional quantum spin model into a $(d+1)$-dimensional classical spin model, which contains multispin interactions as well as pair interactions. Another method proposed by Suzuki, called the thermofield Monte Carlo method,[8] calculates the thermal states as a diffusion process by extending the Kuti-Blankenbecler-Sugar Monte Carlo method at zero temperature[9,10] to finite temperatures. A completely different method suggested by Kadowaki and Ueda[11] calculates high-temperature series coefficients of the partition functions for finite systems by the Monte Carlo method. Thermodynamic properties at various temperatures are then evaluated from the high-temperature series expansions.

The Monte Carlo methods have been applied to study critical properties of the one-dimensional spin-$\frac{1}{2}$ Heisenberg ferromagnet. By using the Suzuki-Trotter method, Cullen and Landau[12] predict that the susceptibility exponent γ is 1.32, while Marcu *et al.*[13] obtain $\gamma=1.55$. On the other hand, a study of Handscomb's approach by Lyklema[14] gives $\gamma=1.75$. These values are lower than the estimates of other methods. The finite-size extrapolation of Bonner and Fisher[15] predicts $\gamma=1.8$. Both the Bethe ansatz approach of Schlottmann[16] and the modified spin-wave theory of Takahasi and Yamada[17] give $\gamma=2$. Recently we have studied the one-dimensional spin-S exchange-interaction model by using Handscomb's method.[18] When $S=\frac{1}{2}$ this model is identical to the Heisenberg model. With more data and by using a method of analysis we find that γ is equal to 2, and is independent of the spin.

Monte Carlo studies of critical properties of quantum spin models on two- and three-dimensional lattices are sparse. For the spin-$\frac{1}{2}$ ferromagnetic Heisenberg model, thermodynamic properties for finite systems on the square and the simple-cubic lattices have been calculated by using the Suzuki-Trotter method[19] and Handscomb's method,[20] respectively. These studies, however, have not determined critical properties of the model from the Monte Carlo data. In this article we calculate thermodynamic properties of the model by using Handscomb's approach, which will be described in Sec. II. Several methods of analyses are used to estimate critical properties from the Monte Carlo data. Our methods of analyses and the main results obtained are shown in Sec. III for the square lattice, and in Sec. IV for the simple-cubic lattice. Summary and discussion are given in Sec. V.

II. HANDSCOMB'S MONTE CARLO METHOD

Consider a Hamiltonian of the form

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

where J is the coupling constant, ε_{ij} is the interaction operator which depends on the spin variables $\mathbf{S}_i$ and $\mathbf{S}_j$, and the summation is over all nearest-neighbor pairs of spins. For the model on a lattice of N sites, having the coordination number q, there are $Nq/2$ nearest-neighbor pairs of interactions. (We use the periodic boundary conditions.) In the Handscomb's approach, the partition function is written as

$$\begin{aligned} Z&=\sum_{r=0}^{\infty}\frac{K^r}{r!}\mathrm{Tr}\left[\sum_{\langle i,j\rangle}\varepsilon_{ij}\right]^r \\ &=\sum_{r=0}^{\infty}\sum_{\alpha=1}^{(Nq/2)^r}\frac{K^r}{r!}\mathrm{Tr}C_{r,\alpha}\ , \end{aligned} \tag{2}$$

where $K=J/k_BT$. The expansion of $(\sum_{\langle i,j\rangle}\varepsilon_{ij})^r$ contains $(Nq/2)^r$ terms. Each term is a product of a sequence of r operators ε_{ij} The αth sequence, which has r operators ε_{ij}, is denoted as $C_{r,\alpha}$.

If we define

$$\pi_{r,\alpha}=\frac{1}{Z}\frac{K^r}{r!}\mathrm{Tr}C_{r,\alpha}\ , \tag{3}$$

it is clear from Eq. (2) that

$$\sum_{r,\alpha}\pi_{r,\alpha}=1\ . \tag{4}$$

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

$$\begin{aligned}\langle A\rangle&=\frac{1}{Z}\sum_{r=0}^{\infty}\sum_{\alpha=1}^{(Nq/2)^r}\frac{K^r}{r!}\mathrm{Tr}AC_{r,\alpha}\\&=\sum_r\sum_\alpha\left[\frac{\mathrm{Tr}AC_{r,\alpha}}{\mathrm{Tr}C_{r,\alpha}}\right]\pi_{r,\alpha}\\&=\sum_r\sum_\alpha A_{r,\alpha}\pi_{r,\alpha}\ ,\end{aligned} \tag{5}$$

where $A_{r,\alpha}=(\mathrm{Tr}AC_{r,\alpha})/\mathrm{Tr}C_{r,\alpha})$. If $\pi_{r,\alpha}\geq 0$ for all $C_{r,\alpha}$ sequences, Eqs. (4) and (5) indicate that $\langle A\rangle$ is nothing but the average of $A_{r,\alpha}$ for all $C_{r,\alpha}$ which have the weights $\pi_{r,\alpha}$.

In Handscomb's approach, all $C_{r,\alpha}$ sequences form the elements of the sampling space in which the Markov chain is generated in the Monte Carlo calculation. In each Monte Carlo step we select a new $C_{r',\alpha'}$ sequence randomly. If the original sequence is $C_{r,\alpha}$, the most convenient way is to select $r'=r-1$ or $r+1$ with equal probability ($\frac{1}{2}$ each). When $r'=r-1$, $C_{r-1,\alpha'}$ is obtained by randomly removing one operator ε_{ij} from the $C_{r,\alpha}$ sequence. When $r'=r+1$, $C_{r+1,\alpha'}$ is obtained by inserting one operator $\varepsilon_{i'j'}$ randomly to any of the $(r+1)$ positions of the $C_{r,\alpha}$ sequence. The operator to be inserted into $C_{r,\alpha}$ is selected randomly from the $Nq/2$ operators ε_{ij}.

The transition probability for the Markov chain to walk from $C_{r,\alpha}$ to $C_{r',\alpha'}$ is chosen as

$$\tau(C_{r,\alpha}\rightarrow C_{r',\alpha'})=\min\{1,\pi_{r',\alpha'}/\pi_{r,\alpha}\}\ , \tag{6}$$

where $\pi_{r,\alpha}$ are given by Eq. (3). The Markov chain generated in this way will have the equilibrium distribution of $C_{r,\alpha}$ sequences described by Eq. (3).

The thermal average of the physical observable A can then be evaluated as

$$\langle A\rangle=\frac{1}{M}\sum_{i=1}^{M}A_{r_i,\alpha_i}\equiv\overline{A(r,\alpha)}\ , \tag{7}$$

where $A_{r_i,\alpha_i}=(\mathrm{Tr}AC_{r_i,\alpha_i})/(\mathrm{Tr}C_{r_i,\alpha_i})$, and C_{r_i,α_i} are M sequences ($M\gg 1$) chosen randomly from the Markov chain which has reached the equilibrium distribution at the given temperature.

The procedure described above can be applied to any quantum or classical spin model. But this method is useful only if $\mathrm{Tr}AC_{r,\alpha}$ and $\mathrm{Tr}C_{r,\alpha}$ can be determined easily by a computer. For the spin-$\frac{1}{2}$ Heisenberg model, the operators ε_{ij} in Eq. (1) are the exchange operators

$$\varepsilon_{ij}=2\mathbf{S}_i\cdot\mathbf{S}_j+\tfrac{1}{2}\ . \tag{8}$$

The operators ε_{ij}, which exchange the spin coordinates $\mathbf{S}_i$ and $\mathbf{S}_j$, are elements of the symmetric group of degree N. By using properties of the symmetric group, $\mathrm{Tr}C_{r,\alpha}$ and $\mathrm{Tr}AC_{r,\alpha}$ can be calculated rather easily.

A $C_{r,\alpha}$ sequence is a product of r transpositions. It can also be expressed as a product of independent cycles.[21] The number of cycles of $C_{r,\alpha}$ will be denoted as $k(r,\alpha)$, and the number of objects (spins) in the jth cycle will be denoted as $a_j(r,\alpha)$. As an example consider the sequence

$$c_{5,\alpha}=(13)(36)(46)(14)(15)$$

for a system of six spins [(ij) is a shorthand notation for ε_{ij}]. In terms of independent cycles, $C_{5,\alpha}=(15)(2)(364)$. The number of cycles is $k(5,\alpha)=3$ and the numbers of objects of these cycles is $a_1(5,\alpha)=2$, $a_2(5,\alpha)=1$, and $a_3(5,\alpha)=3$.

For the spin-$\frac{1}{2}$ Heisenberg ferromagnet, we have calculated the internal energy (per spin)

$$E=-(J/N)(\partial\ln Z/\partial K)\ ,$$

the specific heat per spin $C=\partial E/\partial T$ and the second moment per spin

$$Y=(1/N)\left\langle\left[\sum_i S_{iz}\right]^2\right\rangle\ ,$$

where S_{iz} are z components of $\mathbf{S}_i$ and the summation is over all lattice sites. From properties of the symmetric group it can be shown that $\mathrm{Tr}C_{r,\alpha}=2^{k(r,\alpha)}$ and the thermodynamic functions are[4,5]

$$E/J=-\bar{r}/NK\ , \tag{9}$$

$$C/k_B=[\overline{r^2}-(\bar{r})^2-\bar{r}]/N\ , \tag{10}$$

and

$$Y=(4N)^{-1}\overline{\sum_j a_j^2(r,\alpha)}\ . \tag{11}$$

Here r is the number of operators ε_{ij}, $k(r,\alpha)$ is the number of cycles, $a_j(r,\alpha)$ are the numbers of spins of the jth cycles of the $C_{r,\alpha}$ sequence, and the averages $\overline{f(r,\alpha)}$ are taken over the $C_{r,\alpha}$ sequences generated in the Markov chain as defined by Eq. (7).

For a given lattice at a given temperature, typically 5×10^5 to 5×10^6 Monte Carlo steps are performed (more steps for larger systems at lower temperatures). The initial 10% of the data in each simulation are discarded in taking the average over the $C_{r,\alpha}$. The uncertainties in the calculations of E and Y are within a few percent. Critical properties of the model can be determined from the Monte Carlo data of the second moment. The uncertainties of the specific-heat data are much larger. Precise estimates of the critical properties cannot be obtained. In

the following sections only the analyses of the second moment are presented.

III. LOW-TEMPERATURE PROPERTIES OF THE SQUARE LATTICE

For the square lattice we study $L\times L$ lattices with periodic boundary conditions for L up to 40. Thermal variations of the second moment Y for some values of L are shown in Fig. 1. For a finite system the behavior of $Y(T,L)$ at high temperatures is the same as that of $Y(T,\infty)$. $Y(T,L)$ deviates from $Y(T,\infty)$ at the temperature where the correlation length of the system is of the order of L.

Above the critical temperature T_c, the susceptibility χ is related to the second moment $\chi=\mu^2 Y/k_B T$ ($\mu/2$ is the magnetization per spin at $T=0$). The analysis of high-temperature series expansions by Stanley and Kaplan[22] suggests that χ has a power-law singularity at a finite temperature for a two-dimensional Heisenberg ferromagnet. On the other hand, it has been shown that the system cannot have a spontaneous magnetization at nonzero temperatures.[23] Recently, a modified spin-wave theory studied by Takahasi[17] also predicts that the susceptibility diverges at the zero temperature.

We first assume that the susceptibility has a power-law singularity and analyze the Monte Carlo data by using the phenomenological renormalization approach.[24] This approach was first introduced by Nightingale.[25] A renormalization of the temperature is defined through the correlation length $\xi(T,L)$ by setting

$$\xi(T,L)/L=\xi(T',L')/L' .$$

Barber and Selke[24] generalized the approach of Nightingale by using the second moment (or other quantities which are easy to calculate) to define the renormalization of the temperature. That is, they define the transformation by

$$Y(T,L)=(L/L')^{\omega}Y(T',L') . \tag{12}$$

The fixed point T^* of the transformation gives the estimate of the critical temperature T_c, while the exponent ω is determined through

$$(L/L')^{\omega}=Y(T_c,L)/Y(T_c,L') . \tag{13}$$

If we define

$$\zeta(T,L,L')=\ln[Y(T,L)/Y(T,L')]\ln(L/L') , \tag{14}$$

the plots of $\zeta(T,L,L')$ against T for several sets of (L,L') will intersect approximately at $\zeta=\omega$ and $T=T_c$. For the square lattice our results are shown in Fig. 2. These curves do not intersect in the temperature range which we have studied ($k_B T/J\geq 0.2$). At $T=0$ it can be shown that $Y(T=0,L)=L^2/12$ for the square lattice and for $L\gg 1$. Therefore, these curves are expected to intersect at $T=0$ and $\zeta=2$. That is, the susceptibility diverges at $T_c=0$ and the exponent $\omega=2$.

If the susceptibility has a power-law singularity $\chi\sim T^{-\gamma}$, the exponent can be estimated from

$$\chi(T)=\mu^2 Y(T,\infty)/k_B T .$$

We regard γ as a function of the temperature and define $\gamma(T)=-\partial\ln\chi/\partial\ln T$. Then the extrapolation of $\gamma(T)$ to $T=0$ gives the estimate of γ. This method has successfully determined $\gamma=2$ for the one-dimensional lattice. For each temperature, $Y(T,\infty)$ can be obtained by extrapolating the $Y(T,L)$ versus L^{-1} plot to $L^{-1}=0$. From our data of the square lattice for $L\leq 40$, we can determine $Y(T,\infty)$ for $k_B T/J>0.6$. When $k_B T/J\leq 0.6$, accurate estimates of $Y(T,\infty)$ cannot be obtained unless larger values of L are considered. For two nearby temperatures T_1 and T_2 we calculate $\gamma(T)$ by

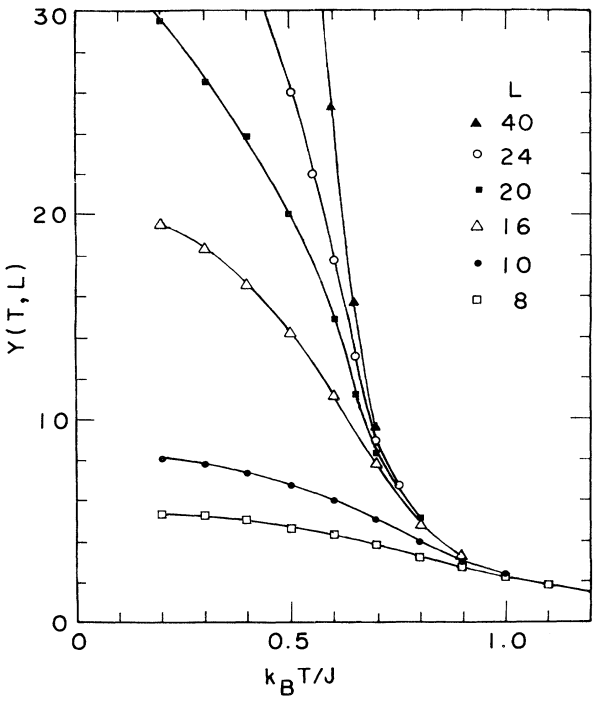

FIG. 1. The second moment $Y(T,L)$ for the Heisenberg model on the square lattice.

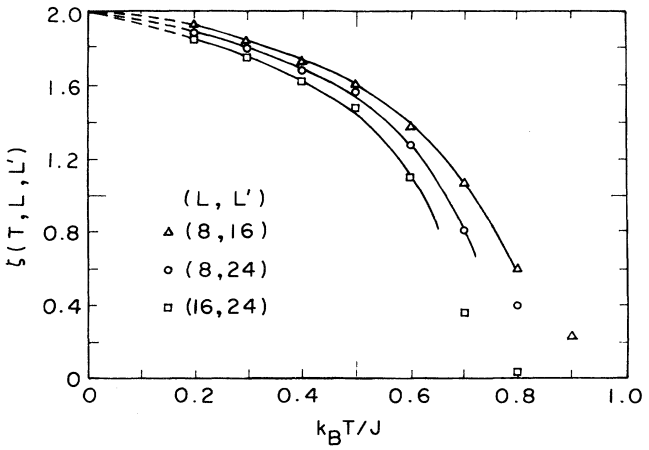

FIG. 2. Plots of $\zeta(T,L,L')$ [defined by Eq. (14)] against the temperature for the square lattice.

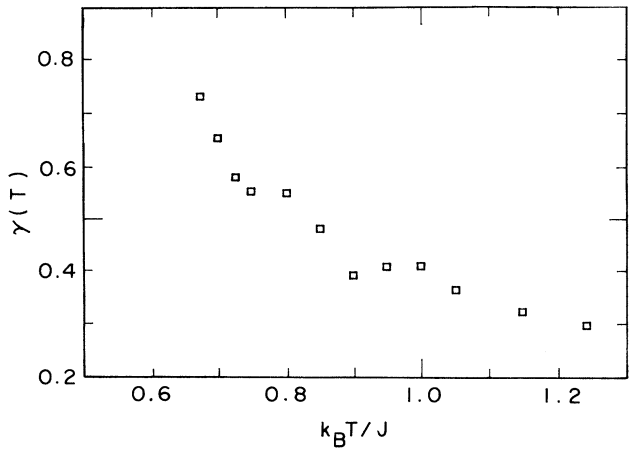

FIG. 3. A plot of $\gamma(T)$ [defined by Eq. (15)] against T for the square lattice.

$$\gamma[(T_1+T_2)/2] = -[\ln\chi(T_1)-\ln\chi(T_2)]/(\ln T_1-\ln T_2) . \quad (15)$$

A plot of $\gamma(T)$ versus T is shown in Fig. 3. We see that $\gamma(T)$ does not seem to converge to a finite value. This suggests that χ diverges exponentially.

Assume that the susceptibility at low temperatures has the form[17]

$$J\chi/\mu^2 = YJ/k_BT = A\exp[b(J/k_BT)][1+O(T)+\cdots] . \quad (16)$$

We will estimate the coefficients A and b. Equation (16) implies that

$$(k_BT/J)\ln(YJ/k_BT) = b+(k_BT/J)\ln A . \quad (17)$$

A plot of $(k_BT/J)\ln(YJ/k_BT)$ against k_BT/J approaches a straight line at small T and intersects the ordinate at b with the slope $\ln A$. From Fig. 4 we obtain $b=4.5\pm0.5$ and $A=0.027\pm0.004$. The constant b can also be determined from the slope of the $\ln(YJ/k_BT)$ versus J/k_BT plot at low temperatures. A consistent estimate ($b=4.4$) is obtained from Fig. 5.

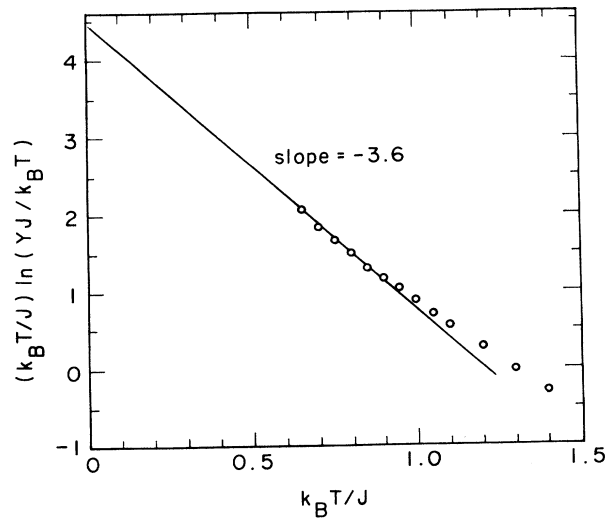

FIG. 4. A plot of $(k_BT/J)\ln(YJ/k_BT)$ vs k_BT/J for the square lattice. The slope of the line is $\ln A$.

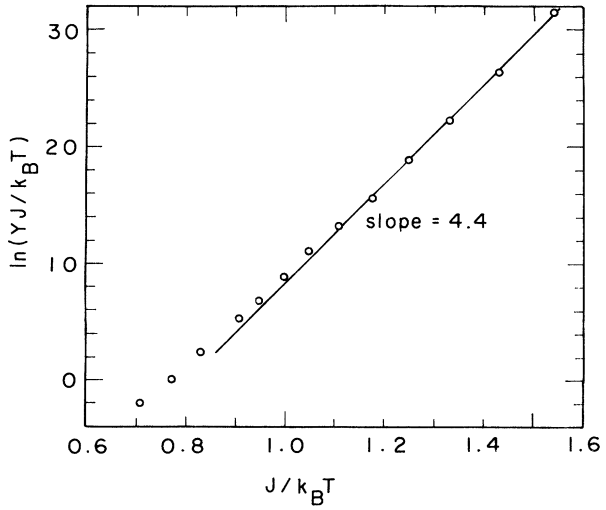

FIG. 5. A plot of $\ln(YJ/k_BT)$ against J/k_BT for the square lattice. The slope of the line is b.

IV. CRITICAL PROPERTIES OF THE SIMPLE-CUBIC LATTICE

For the simple-cubic lattice we consider $L\times L\times L$ lattice with periodic boundary conditions for $L\le 10$. We first analyze our data by the phenomenological renormalization method described in Sec. III. We find from Fig. 6 that $k_BT_c/J=1.68\pm0.01$ and $\omega=2.00\pm0.05$. It is well known that the susceptibility of a three-dimensional lattice has a power-law singularity. From the finite-size scaling theory[24] $\omega=\gamma/\nu$, where γ and ν are exponents of the susceptibility and the correlation length, respectively.

The value of $\omega=\gamma/\nu$ can also be determined from $Y(T_c,L)$, as $Y(T_c,L)\sim L^{\gamma/\nu}$. A plot of $\ln Y(T_c,L)$ against $\ln L$ is a straight line with the slope γ/ν for large L. By assuming $k_BT_c/J=1.68$ we have calculated $Y(T_c,L)$ for $L=2-10$. These data are shown in Fig. 7. The estimate of γ/ν from Fig. 7 is also 2.0. In principle, the susceptibility exponent γ can be estimated from

$$J\chi(T)/\mu^2 = Y(T,\infty)J/k_BT ,$$

if T_c is known. But our data of $Y(T,L)$ for $L\le 10$ give $\chi(T)$ precisely only for $k_BT/J\ge 2.1$. The temperature is not low enough to determine γ accurately.

To determine the exponents γ and ν we use the finite-size scaling theory.[26] The singular part of the susceptibility (per site) has the form

$$\chi\sim L^{\gamma/\nu}Q(tL^{1/\nu}) , \quad (18)$$

where $t=|T-T_c|/T_c$. The scaling function $Q(y)$ depends only on the scaling variable $y=tL^{1/\nu}$, rather than

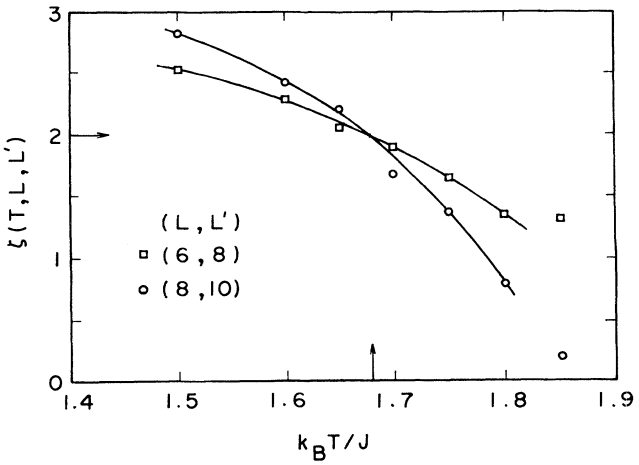

FIG. 6. Plots of $\zeta(T,L,L')$ [defined by Eq. (14)] against k_BT/J for the simple-cubic lattice.

on the variables T and L separately. Similarly, the spontaneous magnetization (per site) has the form

$$M \sim L^{-\beta/\nu} R(tL^{1/\nu}) , \tag{19}$$

where β is the magnetization exponent. $Q(y)$ and $R(y)$ are constants when the scaling variable $y \ll 1$. On the other hand, $Q(y) \sim y^{-\gamma}$ and $R(y) \sim y^{\beta}$ for $y \gg 1$.

Above the critical temperature T_c, $M=0$ and $KY=J\chi/\mu^2$. Below T_c,

$$KY = J\chi/\mu^2 + L^d K(M/\mu)^2 ,$$

where $d=3$ is the lattice dimensionality. By using the scaling relation[27] $\nu d = 2\beta+\gamma$, we obtain

$$KY \sim L^{\gamma/\nu}[Q(tL^{1/\nu}) + R^2(tL^{1/\nu})] . \tag{20}$$

If we plot $\ln(KYL^{-\gamma/\nu})$ against $\ln(tL^{1/\nu})$, all data fit two curves only. In the asymptotic region $tL^{1/\nu} \gg 1$, the curves for $T > T_c$ has the slope $-\gamma$, while the curve for $T < T_c$ has the slope 2β ($Q \ll R^2$ in this region).

We have plotted the Monte Carlo data ($1.2 \le k_BT/J \le 2.3$) in Fig. 8 by assuming $\gamma = 1.4$, $\gamma/\nu = 2.0$, and $k_BT_c/J = 1.68$. Our data actually fit two curves, and the limiting slopes of the figure are consistent with our assumption $\gamma = 1.4$ and $2\beta = \nu d - \gamma = 0.7$. This confirms that the assumed values of the exponents and T_c are correct.

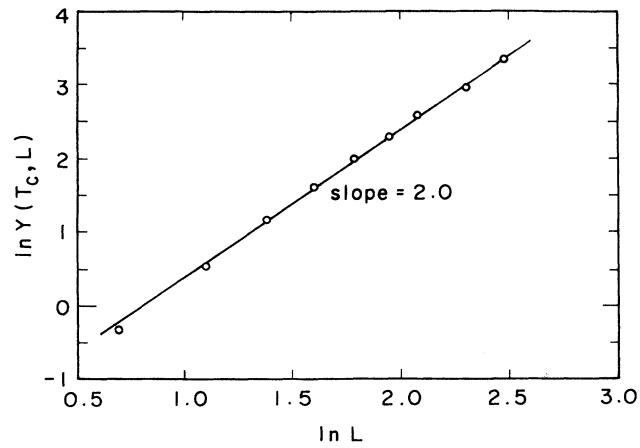

FIG. 7. $\ln Y(T_c,L)$ plotted vs $\ln L$ for the simple-cubic lattice. T_c is assumed to be $1.68J/k_B$.

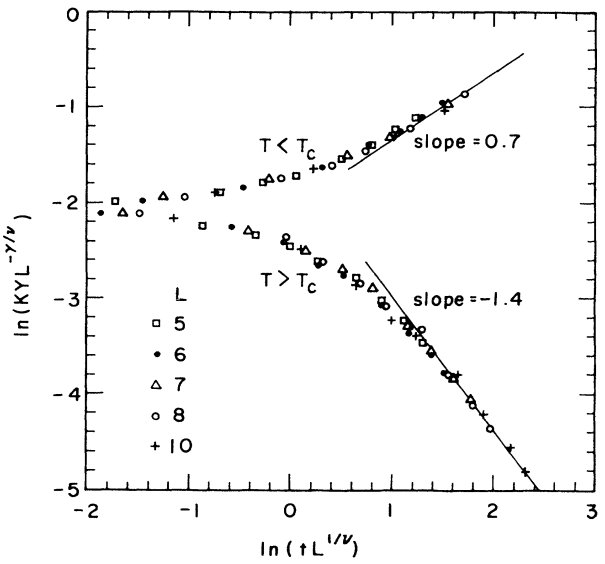

FIG. 8. $\ln(KYL^{-\gamma/\nu})$ plotted against $\ln(tL^{1/\nu})$ for the simple-cubic lattice, where $K=J/k_BT$ and $t=|T-T_c|/T_c$. We have assumed that $T_c=1.68J/k_B$, $\gamma/\nu=2.0$, and $\gamma=1.4$.

V. SUMMARY AND DISCUSSION

We have calculated thermodynamic properties of the spin-$\frac{1}{2}$ ferromagnetic Heisenberg model by using Handscomb's Monte Carlo method. Various methods of analyses are used to extract estimates of the critical temperatures and critical exponents from the Monte Carlo data.

For the square lattice we have shown that $T_c=0$ and that the susceptibility diverges exponentially. By assuming $\chi \sim \exp[b(J/k_BT)]$, we have estimated (based on the data for $L \le 40$) that $b=4.5\pm0.5$, which is lower than the result ($b=2\pi$) of a modified spin-wave theory.[17] The susceptibility may behave in a more general way,

$$\chi \sim (k_BT/J)^a \exp[b(J/k_BT)] ,$$

such as the one-dimensional Ising model (exact result[28]) and the two-dimensional classical Heisenberg model (Monte Carlo renormalization-group method[29]). The constants a and b can be estimated from the $\partial \ln(KY)/\partial K$ versus k_BT/J plot. This plot should intersect the ordinate at b with the slope $-a$. Our data of $\partial \ln(KY)/\partial K$, however, are too scattered to determine a and b accurately.

The phenomenological renormalization-group analysis for the square lattice gives $\omega=2$. From the finite-size scaling, $\omega=2$ and

$$\chi \sim (k_BT/J)^a \exp[b(J/k_BT)]$$

indicate that the correlation length ξ also diverges exponentially at the zero temperature. That is,

$$\xi \sim (k_B T/J)^c \exp[d(J/k_B T)]$$

with $b/d=\omega=2$ and $(a+1)/c=\omega=2$. For the simple-cubic lattice, our analyses using both the finite-size scaling and the phenomenological renormalization predict that $k_B T_c/J=1.68$, $\gamma/\nu=2.0$, and $\gamma=1.4$, which are in good agreement with the high-temperature series results.[30]

ACKNOWLEDGMENTS

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