Devil's-staircase behavior of a simple spin model

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The Ising model considered by von Boehm and Bak [Phys. Rev. Lett. 42, 122 (1979)] is studied in a spin-$\frac{1}{2}$ version with the spins arrayed on a simple cubic lattice. The model is uniaxial with ferromagnetic interaction between nearest-neighbor spins in the xy planes and competing interactions between nearest-neighbor and next-nearest-neighbor spins in the z direction. The phase transitions of the model are studied by mean-field and Monte Carlo calculations for the same set of interaction parameters as chosen by von Boehm and Bak. The mean-field calculations suggest that the wave vector q, as a function of temperature, picks up every rational number from $\frac{1}{4}$ at low temperature to $q_0 \simeq 0.3036$ at T_N, the transition temperature to the paramagnetic phase. Monte Carlo calculations with periodic boundary conditions are performed on lattices with $M \times M \times L$ spins with M ranging from 4 to 10. Two values of L, 56 and 280, are considered. The calculations show 4 and 16 sinusoidal phases in the two cases, respectively. The transitions between the ordered phases appear to be first order. The number and value of the wave vectors in the two cases agree with the pattern from the mean-field calculations. Monte Carlo calculations with free surfaces for $L = 56$ lead to a pattern similar to that of the corresponding calculations with periodic boundary conditions. It is argued that the temperature dependence of the wave vector is consistent with the devil's-staircase type of behavior. The values of T_N and q_0 determined from the Monte Carlo calculations are in good agreement with the results of an analysis of the ordering susceptibility obtained from known general series.

I. INTRODUCTION

Neutron-diffraction experiments on certain magnetic materials such as Er, Tm, and CeSb exhibit temperature-dependent wave vectors, $q(T)$, of the magnetic structure. In Er (Refs. 1 and 2) and Tm (Refs. 3 and 4) it seems that $q(T)$ varies continuously with temperature. In contrast, in CeSb $q(T)$ apparently attains a finite set of values.[5–7] Pronounced hysteresis is present in all three materials.

The temperature variation of the wave vector has been described by a spin model which includes interactions between spin pairs in various distances.[8,9] Selke and Fisher[10] (SF) consider an Ising analog of this model using Monte Carlo (MC) calculations to study the magnetic phases appearing for various values of the model parameters. In some cases SF find a rather dramatic change of the wave vector in a comparatively small temperature range. However, the study does not answer the question whether, for an infinite system, the change is continuous or not.[10]

Von Boehm and Bak[11] (BB) use a mean-field approach to study the same model with parameters reasonable for CeSb. They find a large number of commensurate phases, some of which are stable only in a very small temperature range. BB discuss their findings in terms of the devil's-staircase behavior,[12] which is a variation where q locks in an infinity of rational (commensurate) values. Between any two q values there is always an infinity of additional q values. The temperature variation of q is continuous but nonanalytic.

In principle, it is impossible to establish experimentally that the wave vector exhibits the devil's-staircase behavior. However, the finite size of the system used in MC calculations offers an advantage in testing whether a given model is consistent with the devil's staircase or not. Suppose the MC calculations on a given lattice size show that all commensurate wave vectors in a range are observed. An increase in lattice size will increase the number of commensurate wave vectors in the range. If *all* these commensurate wave vectors are observed for the larger system then the model is consistent with the devil's staircase. This approach is used in the present article to investigate the same model as studied by BB. These authors consider a spin system with $S = \frac{5}{2}$ (relevant for CeSb). We study the somewhat simpler case of $S = \frac{1}{2}$ expecting the basic feactures of $q(T)$ to be rather independent of the value of S. However, it turns out, that there are some distinct differences between the results for the different values of S.

The article is organized as follows: In Sec. II we present the microscopic Hamiltonian, which is the object of our calculations. In Sec. III we describe the results of mean-field calculations on the model. We describe the MC technique and present the results of the MC calculations in Sec. IV. It turns out that the model has a large number of sinusoidal phases and that all commensutate wave vectors are indeed observed. Section V briefly lists the results of an analysis of the high-temperature series for the ordering susceptibility. The series is obtained from general series derived by Redner and Stanley.[13] The values obtained for the temperature, T_N, where the system becomes paramagnetic, and the corresponding wave vector, q_0, agree with those estimated from the MC calculations. In Sec. VI we summarize and discuss our results in relation to those of BB and SF.

II. MODEL

We consider a spin-$\frac{1}{2}$ Ising model on a simple cubic lattice. The interaction between the spins is given by the Hamiltonian[8–11,13]

$$H=-J\left[\sum_{\langle j,k\rangle}^{(\mathrm{NN})'}\sigma_j\sigma_k+J_1\sum_{\langle j,k\rangle}^{(\mathrm{NN})_z}\sigma_j\sigma_k+J_2\sum_{\langle j,k\rangle}^{(\mathrm{NNN})_z}\sigma_j\sigma_k\right], \tag{2.1}$$

where $(\mathrm{NN})_z$ and $(\mathrm{NNN})_z$ indicate nearest- and next-nearest neighbors of spins placed along a fourfold axis (z axis), respectively. Similarly $(\mathrm{NN})'$ indicates nearest neighbors of spins in planes orthogonal to the z axis. J is taken to be positive and the Ising spin variable σ_j, $j=1,\ldots,N$, attains the values ±1. The coupling parameters J, J_1, and J_2 are temperature independent. We have set $J_1=-4$ and $J_2=-2.819$ corresponding to the values chosen by BB.[11] SF[10] studies the model with $J_1=1$ (corresponding to an isotropic nearest-neighbor interaction) and various negative values for J_2. The phase diagram of the model has been calculated by SF as function J_2/J_1 at zero temperature. The ground state for our choice of parameters may be described by

$$\sigma_j=\sqrt{2}\cos(\vec{q}\cdot\vec{r}_j+\pi/4), \tag{2.2}$$

where the wave vector $\vec{q}$ is given by

$$\vec{q}=\frac{2\pi}{r_0}(0,0,q)=\frac{2\pi}{r_0}(0,0,\tfrac{1}{4}), \tag{2.3}$$

and r_0 is the lattice parameter of the unit cell.

III. MEAN-FIELD CALCULATIONS

In our mean-field approach we follow the procedure of BB.[11] The mean-field Hamiltonian is

$$H_{\mathrm{MF}}=-\sum_j h_j\sigma_j+\tfrac{1}{2}\sum_j h_j\langle\sigma_j\rangle, \tag{3.1}$$

where the summations are over all xy layers and $\langle\sigma_j\rangle$ denotes the thermal average of one of the equivalent spins in a xy layer. The corresponding effective field h_j is

$$h_j=-J\left[\sum_k^{(\mathrm{NN})'}\langle\sigma_k\rangle+J_1\sum_k^{(\mathrm{NN})_z}\langle\sigma_k\rangle+J_2\sum_k^{(\mathrm{NNN})_z}\langle\sigma_k\rangle\right], \tag{3.2}$$

where the summations are over the spins interacting with the jth spin [cf. Eq. (2.1)]. The mean-field approach for a spin-$\frac{1}{2}$ system relates $\langle\sigma_j\rangle$ and h_j through

$$\langle\sigma_j\rangle=\tanh(h_j/k_BT). \tag{3.3}$$

Equations (3.2) and (3.3) are solved self-consistently by numerical iteration. In this calculation we impose periodic boundary conditions, i.e., $\langle\sigma_j\rangle=\langle\sigma_{j+L}\rangle$, where L is the number of xy layers.

The free energy per spin $F(L,T)$ is obtained from the self-consistent solution as

$$F(L,T)=\frac{1}{L}\sum_{j=1}^{L}-k_BT\ln\mathrm{Tr}_j\left[\exp\left(\frac{-H_{\mathrm{MF}}}{k_BT}\right)\right], \tag{3.4}$$

where Tr_j denotes the trace over the two spin states for the jth spin. $F(L,T)$ is calculated for $L=3,4,\ldots,23$ and for a number of temperatures. At a given temperature the spin structure with the lowest free energy per spin is the stable one.

The wave vector describing a stable structure has been obtained from Fourier analysis (see Sec. IV) of $\langle\sigma_j\rangle$, $j=1,\ldots,L$. The stable structures turn out to be approximately sinusoidal, i.e.,

$$\langle\sigma_j\rangle=\Phi\cos(\vec{q}\cdot\vec{r}_j+\phi), \tag{3.5}$$

$$\vec{q}=\frac{2\pi}{r_0}(0,0,q). \tag{3.6}$$

Figure 1 shows the equilibrium wave vector versus temperature. With increasing temperature the wave vector varies stepwise picking up every value n/L (n is an integer and $L=3,4,\ldots,23$) in the interval from $q=\frac{1}{4}$ at $T=0$ to q_0^{MF} at the temperature T_N^{MF}, where the system becomes paramagnetic. Within the mean-field approximation T_N^{MF} and the corresponding q_0^{MF} are given by[13,14]

$$q_0^{\mathrm{MF}}=\frac{1}{2\pi}\cos^{-1}\left[-\frac{J_1}{4J_2}\right]=0.3077\approx\tfrac{4}{13} \tag{3.7}$$

and

$$\begin{aligned}k_BT_N^{\mathrm{MF}}/J&=4+2J_1\cos(2\pi q_0^{\mathrm{MF}})+2J_2\cos(4\pi q_0^{\mathrm{MF}})\\&=11.06\,.\end{aligned} \tag{3.8}$$

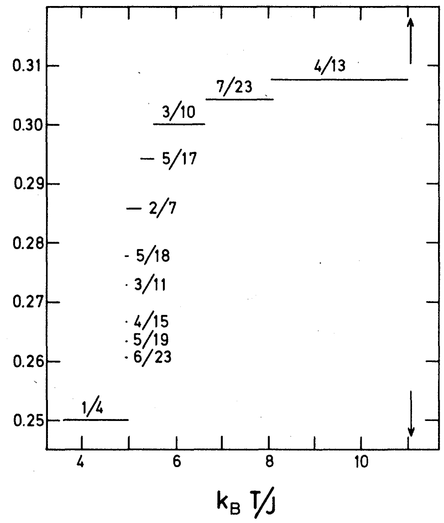

FIG. 1. Temperature dependence of the wave vector $q(T)$, derived from mean-field calculations on the model in Eq. (2.1). The used lattice length ranges from 3 to 23. Periodic boundary conditions are used. The arrows indicate the temperature, where the mean-field theory predicts a transition from a sinusoidal phase to the paramagnetic phase.

For $k_B T/J \sim 5$ the wave vector varies very abruptly and for instance the phase with $q=\frac{6}{23}$ is only stable in a temperature interval $\Delta T = 10^{-10} T_N^{\mathrm{MF}}$.

In principle, the lattice length L should be allowed to assume every value from 3 up to infinity, but the results from the calculation with $L=3,4,\ldots,23$ show a clear pattern, which we believe is unchanged by including higher values of L in the calculation. The pattern is the following: *With increasing temperature from zero to* T_N^{MF} *the wave vector increases continuously from* $\frac{1}{4}$ *to the* q_0^{MF} *picking up every rational value in that interval.*

IV. MONTE CARLO CALCULATIONS

Mean-field calculations do not include fluctuations. It is therefore possible that an incorporation of fluctuations may lead to a destruction of the stability of some of the phases found in Sec. III. In order to investigate if this is actually the case, we have performed extensive Monte Carlo calculations, which allow for fluctuations. In the following we shall describe these calculations.

A. Computational techniques

We have applied a conventional Monte Carlo (MC) importance-sampling technique to calculate at a prescribed temperature a canonical ensemble corresponding to the Hamiltonian in Eq (2.1).

Simple cubic lattices with $N=M\times M\times L$ sites are considered. L is taken to be fairly large, $L=56$ and 280 ($=5\times 56$), since we are interested in studying the spatial modulation of the spin structure along the z axis. The choice of the L values is discussed later in this section. For $L=56$ we have used lattices with $M=10$, and for $L=280$ we have used values of M ranging from 4 at low temperature to 10 at temperature close to T_N, the temperature for the transition to paramagnetism. Although we do not know the correlation length for the system, we do not expect the rather small values of M (compared with the L values) to substantially affect our results far from T_N. We always use periodic boundary conditions along the x and y direction. In the majority of the calculations we apply periodic boundary conditions along the z direction, but we have also performed a set of calculations using free surfaces in the case $L=56$. Each system in the ensemble consists of a certain configuration of the N spins. As a starting configuration at a given temperature we always use a spin configuration typical for a lower nearby temperature. We follow the equilibirum evolution of the ensembles with $L=56$ and 280 for at least 10^4 and 2.5×10^4 MCS/site respectively (MCS/site ≡ Monte Carlo steps per site).

In order to determine the internal energy per spin, $E=\langle H\rangle/N$, we have calculated coarse-grained averages for Δj systems

$$\langle E\rangle_j = \frac{1}{\Delta j}\sum_i E_i' \ , \tag{4.1}$$

where E_i' is the contribution to the internal energy per spin from the ith system in the ensemble. The evolution of the ensemble may be followed using "consecutive coarse-grained" averages

$$E_j = \frac{1}{k}\sum_{i=j}^{j+k}\langle E\rangle_i \ . \tag{4.2}$$

These averages are useful in detecting metastable states close to first-order transitions. A typical evolution of the E_j values during a MC calculation is shown in Fig. 2. For the first 2.5×10^3 MCS/site the E_j values are considered as a set of fluctuations around a certain mean value, and for the last 9.5×10^3 MCS/site they are considered as a set of fluctuations around a different mean value. We interpret the abrupt shift between the two sets as an indication of a first-order phase transition. The ensemble averages of the energy for the two phases are derived from the two sets of coarse-grained averages using the backward summation technique described in Ref. 15. In some cases, for $k_B T/J > 4.3$, the evolution of the ensemble may involve shifts back and forth between two or perhaps three or more phases.

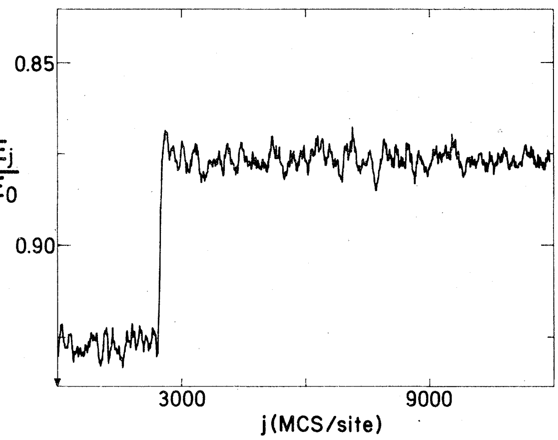

FIG. 2. Evolution of the normalized consecutive coarse-grained averages of the internal energy, Eq. (4.2). E_0 refers to the ground-state value for the internal energy. The data are obtained from a Monte Carlo calculation on a simple cubic lattice with the lattice length $L=56$. Each coarse-grained average corresponds to 10 MCS/site. The parameter k, in Eq. (4.2) is chosen as 10. The scale for j is normalized to MCS/site units.

It is therefore useful to have a precise condition for accepting a set of E_j values as representing a stable phase. As an "experimental condition" for a stable phase we adopt that the E_j values must not exhibit changes like the one in Fig. 2 during 7×10^3 MCS/site for $L=56$ and 2×10^4 MCS/site for $L=280$. The shift frequency may be reduced by increasing M.

The ordering of the different phases is determined from Fourier analysis. For every 10 ($L=56$) or 50 ($L=280$) MCS/site we take a system and calculate for each xy layer the layer magnetization

$$m_j=\frac{1}{M^2}\sum_i \sigma_i,\quad j=1,\ldots,L\ , \tag{4.3}$$

where the summation is over all spins in the jth xy layer. The Fourier coefficients are obtained from the m_j values as

$$a_k=\frac{P}{L}\sum_{j=1}^{L} m_j\cos(2\pi kj)\ , \tag{4.4}$$

$$b_k=\frac{P}{L}\sum_{j=1}^{L} m_j\sin(2\pi kj)\ , \tag{4.5}$$

where $P=2$ for $0<k<\frac{1}{2}$ and $P=1$ for $k=0,\frac{1}{2}$. If the structure is sinusoidal, then the wave vector is determined as the value of k, for which the amplitude function

$$\Phi_k=(a_k^2+b_k^2)^{1/2}\ , \tag{4.6}$$

has its maximum. The corresponding phase angle is obtained from

$$\phi_k=-\tan^{-1}(b_k/a_k)\ . \tag{4.7}$$

The ensemble values $\langle\Phi_k\rangle$ and $\langle\phi_k\rangle$ are determined as averages over the parts of the ensemble corresponding to a stable phase. We emphasize that we are averaging the Fourier-transformed layer magnetizations for single systems. SF[10] use a similar Fourier analysis but these authors average the m_j values over a certain number of steps before Fourier transforming. This technique is not appropriate in our case due to rapid changes (especially for $L=280$) in the m_j values during an MC calculation.

B. Monte Carlo results

1. *Periodic boundary conditions*

Figures 3 and 4 show for the various phases the temperature variation of the internal energy obtained from MC calculations with periodic boundary conditions. For the case $L=56$ we find four ordered

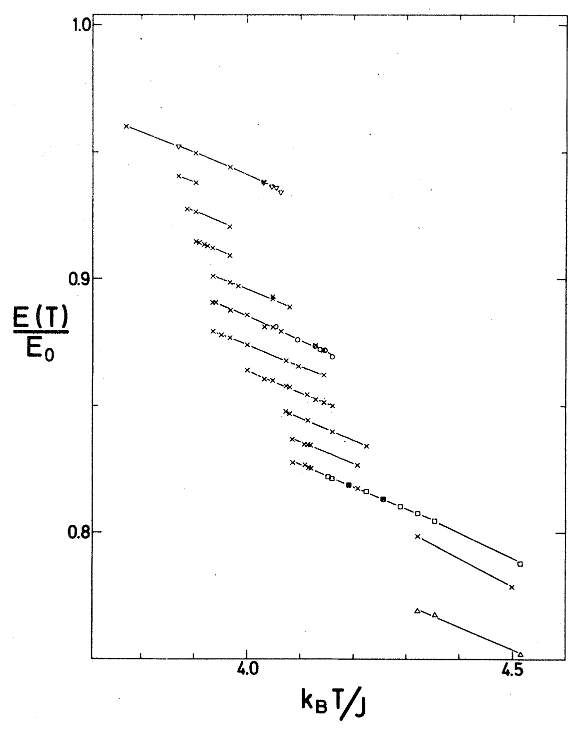

FIG. 3. Temperature dependence of the normalized internal energy $E(T)/E_0$, for the various observed phases. E_0 refers to the ground-state value. The data are obtained from Monte Carlo calculations on simple cubic lattices with the lattice length $L=56$ (∇, $\circ$, $\square$, Δ) and $L=280$ ($\times$). For $L=56$ the corresponding wave vectors are $\frac{1}{4}(\nabla)$, $\frac{15}{56}(\circ)$, $\frac{2}{7}(\square)$, and $\frac{17}{56}(\Delta)$.

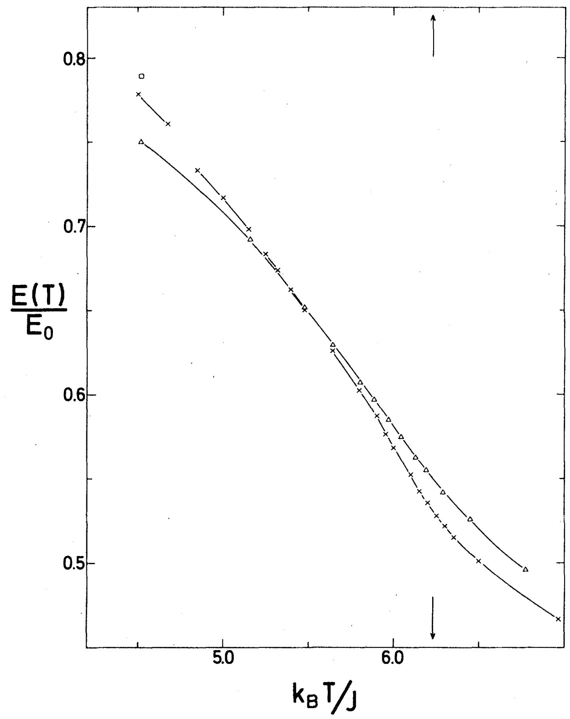

FIG. 4. Temperature dependence of the normalized internal energy, $E(T)/E_0$, for the various observed phases. The arrows indicate the temperature where the high-temperature-series analysis predicts a transition from the paramagnetic phase to a sinusoidal phase. The other symbols are explained in Fig. 3.

phases with wave vectors, $q=\frac{1}{4}, \frac{15}{56}, \frac{2}{7}$, and $\frac{17}{56}$. For $L=280$, there are 16 ordered phases. Among these we find the four phases listed above. The internal energies for the phases with $q=\frac{1}{4}, \frac{15}{56}$, and $\frac{2}{7}$ are on almost linear extrapolations of the energy curves for $L=56$. For $k_BT/J>5.7$ the internal energies for the phase with $q=\frac{17}{56}$ are numerically lower than the corresponding data found for $L=56$. We ascribe this difference to finite-size effects.[16] The remaining 12 phases in the $L=280$ case have internal energies, which in groups of four are placed between the energies of the phases described above. The calculation of consecutive coarse-grained averages suggests that all phase transitions between the ordered phases are of first order, as apparent from Fig. 3. The typical jump in the internal energy between two neighboring phases is $\Delta E/E_0 \approx 0.05$ for $L=56$ and $\Delta E/E_0 \approx 0.01$ for $L=280$, where E_0 is the energy of the ground state. These jumps are well above the uncertainty in the internal energy, $s(E)$, which typically is $s(E)/E_0 \approx 0.001$. The calculations, especially in the $L=280$ case, display extremely long relaxation times due to long-lived metastabilities. For $L=280$ and $3.9<k_BT/J<4.2$ some of the calculations performed at the same temperature but with different initial configurations do not lead to observation of the same stable phase even after 6×10^4 MCS/site. Such situations also arise in experiments, where some phases occasionally may be missed (cf. Refs. 5 and 6).

For all ordered phases there is a sharp peak both in the individual values of the amplitude function, Φ_k as well as in the thermal averages, $\langle\Phi_k\rangle$. This shows, that approximate sinusoidal ordering is present at all times during the MC calculations. Except for the low temperature phase, $q=\frac{1}{4}$ the phase angle, ϕ_k corresponding to the equilibrium wave vector shows a continuous change during an MC calculation indicating, that the sinusoidal ordering is drifting back and forth in the lattice.

The periodic boundary conditions causes the equilibrium wave vector to be commensurate with the lattice length, L, i.e., $q=n/L$, where n is an integer. In order to obtain the trend of the $q(T)$ variation as L goes to infinity we have performed calculations for two different values of L. The choice $L=56$ (and $L=5\times56=280$) is made because it allows the equilibrium wave vector to assume the ground-state value $q=\frac{1}{4}$ and the value $q=\frac{17}{56}$, which is close to the high-temperature-series value $q_0^{\mathrm{HTS}}=0.3026$ derived from series analysis (see Sec. V). From Fig. 4 we see, that the internal energy curves have an inflection point around $k_BT/J=6.05$. At this temperature the amplitude function, $\langle\Phi_k\rangle$ has a maximum at $k=\frac{17}{56}\approx0.3036$ for both the $L=56$ and 280 case. For $k_BT/J>6.05$, there is still a peak in $\langle\Phi_k\rangle$ for $k=\frac{17}{56}$, which we ascribe to finite-size effects.[16] For increasing tempeatures the height of the peak decreases whereas its width increases. We take $k_BT_N^{\mathrm{MC}}/J=6.05\pm0.25$ as the reduced transition temperature to paramagnetism and $q_0^{\mathrm{MC}}=0.3036$ $(+0.0036, -0.0018)$ as the corresponding wave vector. Our MC data near T_N^{MC} are too few to allow a decision of the order of the transition to the paramagnetic phase.

In Fig. 5 we present the determined values of the wave vector for the stable phases. In a similar fashion to the mean-field results (see Fig. 1), $q(T)$ increases very abruptly with T from the ground-state value. In the MC calculations this happens around $k_BT/J\sim4$, which is somewhat lower than the corresponding mean-field temperature. For $L=56$ the phases with $q=n/56$, $n=14$, 15, 16, and 17, are found to be stable. Extending the lattice length to 280 we find, that all phases with $q=n/280$, $70\leq n\leq85$, are stable. This confirms the mean-field results from Sec. III saying that $q(T)$ assumes every rational value in the interval from $\frac{1}{4}$ to q_0. We expect that further extensions of the lattice length will not lead to any new insight. Consequent-

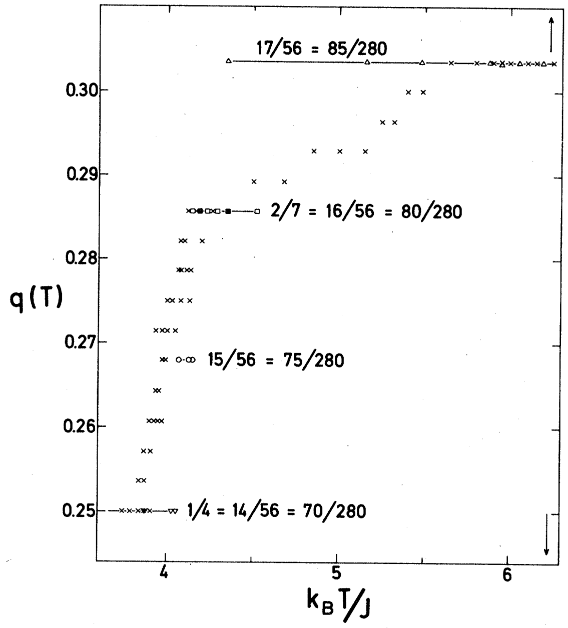

FIG. 5. Temperature variation of the wave vector $q(T)$ of the stable phases determined from Monte Carlo calculations on the model in Eq. (2.1). Periodic boundary conditions are used. The symbols ∇, $\circ$, $\square$, Δ refer to data for lattices of length $L=56$ and $\times$ refers to data for lattices of length $L=280$. The arrows indicate the position where the high-temperature-series analysis predicts a transition from the paramagnetic phase to a sinusoidal phase.

ly, *fluctuations do not change the main feature of the $q(T)$ variation as predicted by the mean-field calculations.*

2. Free surfaces

The use of free surfaces as boundary conditions in the z direction does not allow the wave vector to change freely. The two surface layers and the layers next to them are lacking some of the competing antiferromagnetic interactions given in Eq. (2.1). This results in a tendecy for these layers to be fully magnetized with the following sequence of layer magnetizations: $\pm$ or $\mp$. Assuming sinusoidal ordering, it is easy to see that this effect allows only values of $q \simeq n/2L$. Thus, for a given L, the number of allowed values of the equilibrium wave vector are approximately doubled compared to the case of periodic boundary conditions. Selke and Fisher[10] also discuss the use of different boundary conditions, and these authors especially investigate the different kinetics for systems with periodic boundary conditions and free boundary conditions in the z direction. We have investigated lattices with $L=56$, and we find, for increasing temperature, that $q(T)$ assumes every allowed value between $\frac{1}{4}$ and q_0. This is the same behavior as found in the MC calculations with periodic boundary conditions.

V. ESTIMATES OF q_0 AND T_N FROM HIGH-TEMPERATURE SERIES ANALYSIS

For a general choice of coupling constants, J, J_1, and J_2 [see Eq. (2.1)] Redner and Stanley[13] have developed a high-temperature series for the wave-vector-dependent susceptibility, $\chi(q,T)$. Redner and Stanley analyzed the series for $J=J_1$.

We analyze the series with our choice of parameters in order to obtain an independent estimate of T_N and q_0. The method of analysis follows the one used by Stanley and Redner. The series is transformed using an Euler transformation and a singularity replacement.[17] The analysis of the transformed series are done by means of ratio plots and Padé approximations.[18] The results of the analysis are

$$k_B T_N^{\mathrm{HTS}}/J = 6.232 \pm 0.007 \tag{5.1}$$

and

$$q_0^{\mathrm{HTS}} = 0.3026(+0.0032,\ -0.0016)\ . \tag{5.2}$$

These results agree with the estimates from the MC calculations described in Sec. IV.

VI. SUMMARY AND DISCUSSION

We have studied the temperature variation of the wave vector of the sinusoidal phase for a simple model with competing interactions. The study was performed using mean-field (MF) theory, Monte Carlo (MC) calculations, and high-temperature series (HTS) analysis.

The mean-field calculations show, for increasing temperature, that the wave vector increases from $\frac{1}{4}$ to q_0 picking up every value commensurate with the values adopted for the lattice length, L. Here q_0 is the value of the wave vector for the ordered state in the immediate vicinity of the paramagnetic phase; i.e., $T \to T_{N^-}$. MC calculations with $L=56$ and 280 agree with the pattern obtained from the MF calculations. The values of q_0 derived from both MF calculations and HTS analysis are consistent with the MC value. The MC and HTS results for T_N are concordant.

Our MF results differ from the MF results obtained by von Boehm and Bak[11] using the same MF approach for the similar spin-$\frac{5}{2}$ model. They find that certain rational values, $\frac{6}{23}$ and $\frac{4}{15}$ in the interval from $\frac{1}{4}$ to q_0, are not assumed by $q(T)$. These missing values are essential for their argument, that $q(T)$ is nonanalytic. The origin of this discrepancy is not clear, but we note, that the stability of the phases are determined by extremely small differences in the free energy per spin. For $q=\frac{6}{23}$ the stability in our case is determined by differences of the order of $\Delta F/F_0 \approx 10^{-11}$, where F_0 is the ground-state value.

Selke and Fisher[10] (SF) have performed an MC study for the same model but with the interaction parameters $J_1=1$ and J_2 assuming various negative values. Villain and Gordon[19] have shown that a simple transformation maps the model with $J_1<0$ onto the same model with $J_1>0$ (and the same values for J_0, $|J_1|$, J_2). The transformation changes the wave vector from q to $\frac{1}{2}-q$. We can then qualitatively compare our result for $q(T)$ $(J_2/J_1 \approx 0.7)$ and the results for $q(T)$ obtained by SF for $J_2/J_1=-0.6$ and -0.8. In our case the change of $q(T)$ from $\frac{1}{4}$ to q_0 sets in at higher temperature and continues over a larger temperature interval than in the corresponding cases studied by SF. We ascribe the differences to the use of different values for $|J_1|$ and L in the two studies. For $J_2=-0.6$ SF found that for one lattice size $[(L,M)=(56,10)]$ $q(T)$ only assumes three of the four possible values between $\frac{1}{4}$ and q_0, but for three other lattice sizes $[(L,M)=(40,6),\ (40,10),$ and $(56,6)]$ all commensurate values in the interval are adopted. We suggest that the absence of that particular phase may be due to long relaxation times.

Our $q(T)$ results are consistent with a wave-vector variation, which, in the $L\rightarrow\infty$ limit, is continuous assuming every rational value between $\frac{1}{4}$ and q_0. If $q(T)$ also adopts irrational values, then $q(T)$ may be freely changing withour any lock-in at the rational values. If $q(T)$ only adopts rational values, then $q(T)$ is a devil's staircase and thus nonanalytic. In favor of the latter possibility is the long relaxation times due to long-lived metastabilities, as they are described in Sec. IV. These metastabilities give rise to a pronounced hysteresis over a large temperature interval, and this is the physical significance of a devil's staircase.[12]

ACKNOWLEDGMENTS

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