Phase transitions in Ising ferromagnets with biquadratic exchange interactions

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Phase transitions of Ising ferromagnets with nearest-neighbor ferromagnetic exchange interactions and competing biquadratic exchange interactions on a square lattice are investigated using a Monte Carlo method for spin values $S=1$, $\frac{3}{2}$, 2, and $\frac{5}{2}$. We find that for all the spin values studied in this paper, there always exists a transition line for each spin value in the high-temperature region. However, in the lower-temperature region, different transition behavior may occur for different spin values. In the T-K plane, a line running within the ordered phase, along the nonzero temperature region from $T=0$ and $K/J=-\frac{1}{3}$ to $T=0$ and $K/J=-1.0$ for spin $S=\frac{3}{2}$ and from $T=0$ and $K/J=-\frac{1}{6}$ to $T=0$ and $K/J=-\frac{1}{3}$ for spin $S=2$, separates the region of equal sublattice magnetizations from that of unequal sublattice magnetizations. For spin value $S=\frac{5}{2}$, two low-temperature lines in the T-K plane separate the region of equal sublattice magnetizations from that of unequal sublattice magnetizations with the one line running in the nonzero temperature region from $T=0$ and $K/J=-0.1$ to $T=0$ and $K/J=-\frac{1}{6}$ and the other line running from $T=0$ and $K/J=-\frac{1}{3}$ to $T=0$ and $K/J=-1.0$. A comparison with other approximate techniques is also made.

I. INTRODUCTION

The Ising model has been one of the most actively studied systems. Besides the bilinear exchange interactions in the magnetic insulators, the biquadratic exchange interaction K has been proved both experimentally[1-3] and theoretically[4,5] to play a significant role in the behavior of the Curie temperature, magnetization, and other magnetization properties. In particular, the spin-1 Ising model with a biquadratic exchange interaction has been already investigated by using a variety of methods[6-12,17,18] and found that the introduction of the biquadratic exchange interaction K may have a strong influence on the magnetic behavior of the model. In almost all of these investigations the discussion has been focused mostly on the spin-1 Ising ferromagnet with the biquadratic exchange interaction.[6,10,17,18] An extension of this model is the possibility of inclusion of higher spin values because the effects of the biquadratic exchange interaction on the magnetic properties are expected to be large for the ferromagnetic spin system with large spin as pointed out by Iwashita *et al.*[8,9] This is also an extension of the Blume-Emery-Griffith (BEG) model.[16] Therefore it is worthwhile to investigate the effects of the biquadratic exchange interactions on the magnetic properties of ferromagnets with spins of various values. Higher spin value problems[13,14] have received considerable attention recently; particular interest has been focused on the $S=\frac{3}{2}$ Ising ferromagnet with a crystal-field interaction.[13,14] Recently the phase transitions in the spin-$\frac{3}{2}$ BEG model with nearest-neighbor interactions, both bilinear and biquadratic and with a crystal-field interaction on a cubic lattice, has been studied within the mean-field approximation[11] (MFA) and Monte Carlo simulations.[11] Reference 11 also performed Monte Carlo simulations on a 30×30 square lattice. Besides a transition line occurring at high temperatures, they locate two low-temperature lines. By contrast Bakchich, Bassir, and Berryoussef[12] have used a position-space renormalization-group method based on the Midal-Kadanoff recursion relations to study this model with a very rich phase diagram, which exhibits a wide variety of transition of first and higher order. This paper finds its inspiration in the work of Barreto and Alcantara Bonfim[11] and Bakchich, Bassir, and Berryoussef.[12] In this paper, the effects of the biquadratic exchange interaction K on the Curie temperature of the Ising ferromagnets with the spin $S=1$, $\frac{3}{2}$, 2, and $\frac{5}{2}$, respectively, are investigated with the use of a Monte Carlo (MC) method. The phase diagrams for various spin values are presented, and some new transition lines are found by MC. This magnetic system previously has been studied by the cluster-variation method in pair approximation[7] (CVPA) and by Oguchi pair approximation[8,9] (OPA) and phase diagrams have been obtained on the cubic lattice for spin $S=1$, $\frac{3}{2}$, 2, and $\frac{5}{2}$. The dramatic difference between the phase diagrams obtained by CVPA and OPA and ours is that besides a transition line occurring at high temperatures, the phase diagrams exhibit one or two low-temperature transition lines which have not been predicted by CVPA and OPA. The reasons for us to choose $S=1$, which has been studied by Monte Carlo methods,[6,17,18] is to test our computer program by comparing our results to those of Refs. 6, 17, and 18. Although for $S=\frac{3}{2}$ the model has been studied

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by MFA and Monte Carlo simulations[11] both on a cubic lattice and a square lattice, the simulational results reported are for a cubic lattice. More importantly, the nontrivial extension of the model for $S=2$ and $S=\frac{5}{2}$ have not been studied previously, to our knowledge.

The outline of the paper is as follows. In Sec. II, we define the model and various quantities we calculated in our Monte Carlo computer simulations. The phase diagrams as well as some temperature dependence of the sublattice magnetization curves are presented in Sec. III. Finally, we summarize our results and draw our conclusion.

II. MODEL AND MONTE CARLO METHODS

The model Hamiltonian is given by[7]

$$H=-J\sum_{\langle i,j\rangle} S_iS_j - K\sum_{\langle i,j\rangle} S_i^2S_j^2 \ .$$

The spins S located at site i on a square lattice can take the values $-S,-S+1\ldots S-1,S$. The first term describes the ferromagnetic coupling ($J>0$) between the spins at sites i and j. The second term describes the biquadratic coupling. Both interactions are restricted to the Z ($Z=4$) nearest-neighbor pairs of spins. The simulations will be confined to the parameter space with $K/J<0$ throughout this paper. Before discussing the various quantities calculated in our simulations, it is necessary to comprehend the ground state for various spin values. By comparing the values of the ground-state energy for each spin S, we find that as spin value S increases, the possible configurations allowed for the ground state increases. Since $K/J<0$ is studied in this paper, we divided the total square lattice into two interpenetrating sublattices. For $S=1$ when $K/J>-1$ both sublattices have $S=1$ (or -1) at every site, when $K/J<-1$ both sublattices have $S=0$ at every site. So for $S=1$ the phase diagram contains two regions with different ground states ($T=0$), namely $(1,1)$ and $(0,0)$. These regions in the phase diagram are separated by a line $K/J=-1.0$. The notation (i,j) (Ref. 11) stands for one sublattice having sites occupied by $S=i$ and the other sublattice having $S=j$. For $S=\frac{3}{2}$, three configurations are allowed for the ground state. The configuration $(\frac{3}{2},\frac{3}{2})$ and $(\frac{3}{2},\frac{1}{2})$ are separated by the value $K/J=-\frac{1}{3}$, the configurations $(\frac{3}{2},\frac{1}{2})$ and $(\frac{1}{2},\frac{1}{2})$ are separated by $K/J=-1.0$. For $S=2$, four configurations are allowed. The configurations $(2,2)$ and $(2,1)$ are separated by $K/J=-\frac{1}{6}$, the configurations $(2,1)$ and $(1,1)$ are separated by $K/J=-\frac{1}{3}$, and the configurations $(1,1)$ and $(0,0)$ are separated by $K/J=-1.0$. For $S=\frac{5}{2}$, five configurations are allowed, the configurations $(\frac{5}{2},\frac{5}{2})$ and $(\frac{5}{2},\frac{3}{2})$ are separated by $K/J=-0.1$, the configurations $(\frac{5}{2},\frac{3}{2})$ and $(\frac{3}{2},\frac{3}{2})$ are separated by $K/J=-\frac{1}{6}$, and the configurations $(\frac{3}{2},\frac{3}{2})$ and $(\frac{3}{2},\frac{1}{2})$ are separated by $K/J=-\frac{1}{3}$, the configurations $(\frac{3}{2},\frac{1}{2})$ and $(\frac{1}{2},\frac{1}{2})$ are separated by $K/J=-1.0$.

The standard Monte Carlo single-spin-flip technique[15] has been used to study the model for the square lattice using periodic boundary conditions in all lattice directions. Each point in the phase diagram we obtained on a 30×30 lattice by analyzing the temperature dependence of the sublattice magnetization, specific heat, and susceptibility curves over sufficient Monte Carlo steps (MCS) after discarding an appropriate number of MCS from the initial perfectly ordered spin configuration. Typical observation times were 3000–5000 MCS/spin with the first 1000–2000 MCS/spin discarded to perform the averages. Our simulations show that increasing the number of MCS's used to perform the averages or discarded does not substantially change the observed values of the thermodynamic quantities.

The thermodynamic quantities calculated in our simulations are the sublattice magnetization per spin

$$\langle |M_A|\rangle=\frac{2}{N}\left\langle \left|\sum_A S_i\right|\right\rangle ,$$

$$\langle |M_B|\rangle=\frac{2}{N}\left\langle \left|\sum_B S_i\right|\right\rangle ,$$

and the susceptibility χ_Q (Ref. 11) is defined as

$$\chi_Q=\beta N(\langle Q^2\rangle-\langle Q\rangle^2) ,$$

where Q is defined as

$$Q=\frac{2}{N}\left[\sum(S_A)^2-\sum(S_B)^2\right] ,$$

where N is the total number of sites of the lattice and A and B designate the sublattice. The specific heat per spin is determined from the fluctuation dissipation relation:

$$C/K_B=\beta^2(\langle E^2\rangle-\langle E\rangle^2)/N .$$

III. SIMULATION RESULTS

In order to test our computer program, we first choose $S=1$ by fixing the biquadratic exchange interaction to a certain value, we then increase K_BT/J from the low-temperature region to the high-temperature region with an increment temperature of 0.2. By analyzing the temperature dependence of the specific heat we locate the temperature at which a well pronounced peak appears to be a transition temperature. The phase diagram for $S=1$ is presented in Fig. 1. For $S=1$ this model has been extensively studied by various treatments.[17,18] Here we compare our results with one of the two high statistics Monte Carlo studies.[17] Let us first take $K=0$. In this case the model is reduced to the spin-1 Ising model with only the bilinear pair interaction. Our result at $K=0$ for $K_BT_c/J=1.72$ is roughly in agreement with the result of a high statistics Monte Carlo study[17] ($K_BT_c/J=1.69$). As the value of K/J approaches -1, it has been suggested[17] that the critical temperature approaches zero linearly given by

$$T_c=3.8J(1+K/J) .$$

Our result near $K/J=-1$ indicates that this is valid for

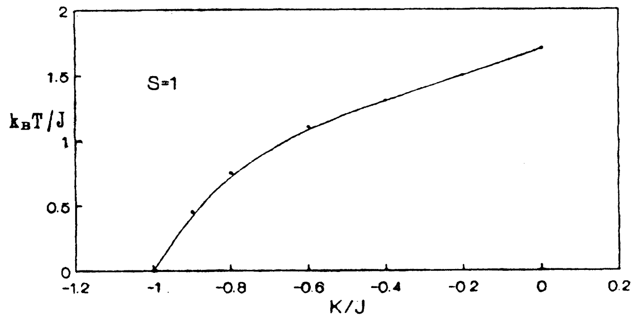

FIG. 1. The phase diagram for $S=1$ obtained by the MC method.

$-1 \leq K/J < -0.85$. Our phase diagram is also in agreement with an early Monte Carlo study[6] and causes us to conclude that our computer program is correct. In the present Monte Carlo simulations, no hysteretic behavior is found for any value of the driving parameters. This indicates that the nature of the phase transition is of second order.

Now we turn our study to $S=\frac{3}{2}$, 2, and $\frac{5}{2}$. The phase diagrams are shown in Figs. 2–4. For $S=\frac{3}{2}$ as $K \rightarrow -\infty$, the model is equivalent to the spin-$\frac{1}{2}$ model and the critical temperature for $K \rightarrow -\infty$ in Fig. 2 is equal to 0.5 which is close to exact result $K_B T_c/J = 2.269/4 = 0.565$. So for $S=\frac{3}{2}$ the transition line can be extended to $K/J \rightarrow -\infty$, while for $S=2$ the transition line will terminate at $K/J = -1.0$ exactly. The phase diagrams for $S=\frac{3}{2}$, 2, and $\frac{5}{2}$ are very different from that of $S=1$. For $S=1$ there is only a second-order transition line which separates the ordered phase from the disordered phase. However for $S=\frac{3}{2}$, 2, and $\frac{5}{2}$, besides a transition line occurring at high temperatures for each spin S, the phase diagrams may exhibit one (for $S=\frac{3}{2}$, 2) or two (for $S=\frac{5}{2}$) low-temperature transition lines. The transition lines in the high-temperature region are obtained by locating the temperature at which the specific heat has a narrow peak. The low-temperature transition lines are obtained by a direct calculation of M_A and M_B or by locating the temperature at which the susceptibility χ_Q has a peak. For $S=\frac{3}{2}$, we show in Figs. 5 and 6 the sublattice magnetiza-

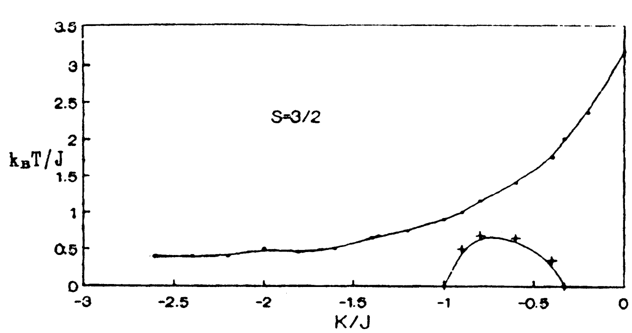

FIG. 2. The phase diagram for $S=\frac{3}{2}$ obtained by the MC method.

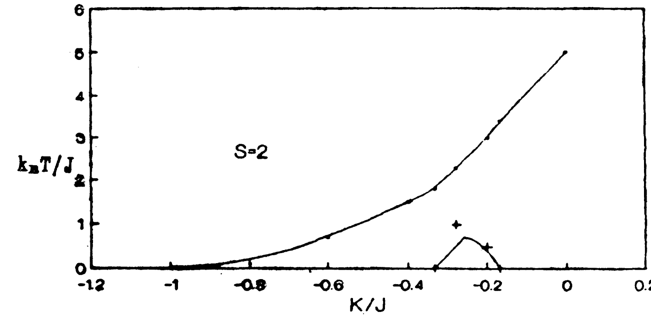

FIG. 3. The phase diagram for $S=2$ obtained by the MC method.

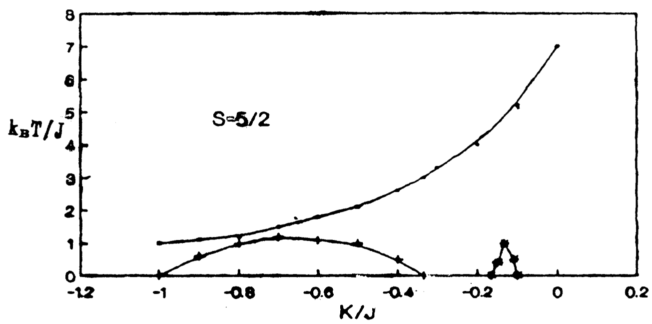

FIG. 4. The phase diagram for $S=\frac{5}{2}$ obtained by the MC method.

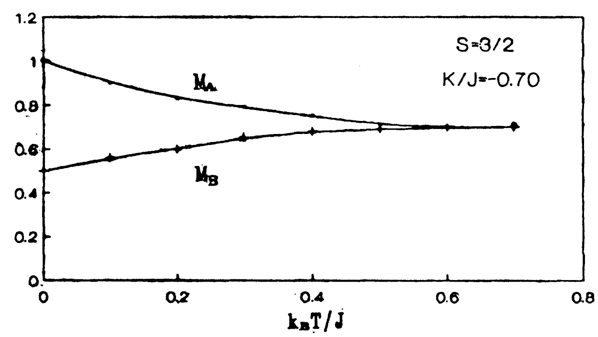

FIG. 5. The sublattice magnetizations M_A and M_B as a function of the temperature for $S=\frac{3}{2}$ and $K/J=-0.70$.

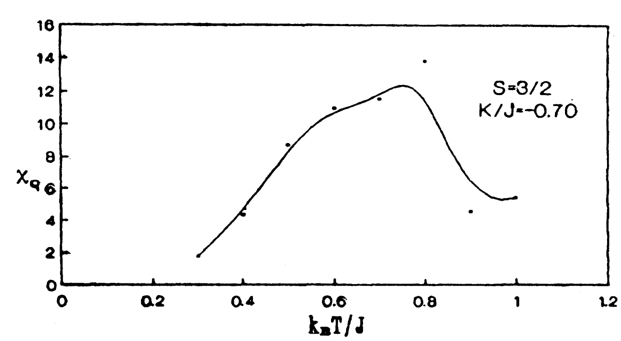

FIG. 6. The susceptibility χ_Q as a function of temperature for $S=\frac{3}{2}$ and $K/J=-0.70$.

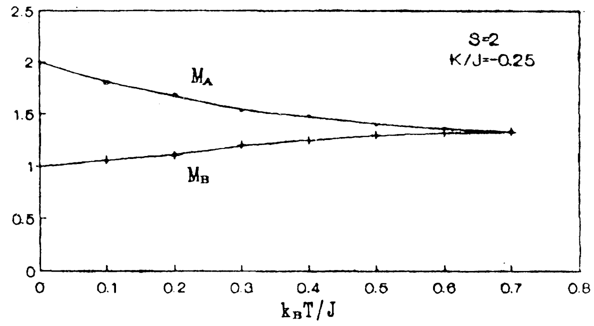

FIG. 7. The sublattice magnetizations M_A and M_B as a function of the temperature for $S=2$ and $K/J=-0.25$.

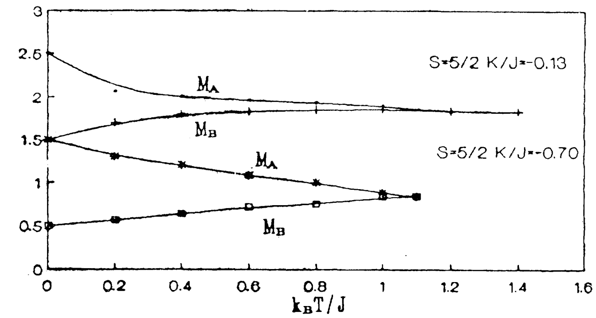

FIG. 9. The sublattice magnetizations M_A and M_B as a function of the temperature for $S=\frac{5}{2}$, $K/J=-0.13$, and $K/J=-0.70$.

tion M_A and M_B and χ_Q as a function of the temperature for $K/J=-0.70$ and T close to the low-temperature phase transition line. The corresponding results for $S=2$ and $S=\frac{5}{2}$ are presented in Figs. 7–10, respectively. We can see the transition when the sublattice magnetizations become equal. We can also see in Fig. 6 there is a maximum susceptibility near the transition temperature. Although the transition temperature read off from Figs. 5 and 6 may differ slightly, we think it is better to choose the temperature at which there is a maximum susceptibility as the effective transition temperature because the susceptibility χ_Q is more sensitive to the phase transition. So the low-temperature transition lines in the phase diagrams were determined by this method. However only one, small lattice size is studied, thus only a rough estimate of transition temperature can be given.

So for $S=\frac{3}{2}$ ($S=2$), the phase diagram presents a disordered phase ($M_A=M_B=0$), an ordered phase with $M_A=M_B\neq 0$, and another ordered phase with $M_A\neq M_B\neq 0$. A transition line separates the disordered phase from the ordered ones. A line running within the ordered phase, along the nonzero temperature region from $T=0$ and $K/J=-\frac{1}{3}$ ($-\frac{1}{6}$) to $T=0$ and $K/J=-1.0$ ($-\frac{1}{3}$), separates the region of the unequal sublattice magnetization from that of equal sublattice magnetization.

The phase diagram for $S=\frac{5}{2}$ is more interesting; some outstanding features are found. In the low-temperature region, the ordered phases are separated by two transition lines which have for start and end points, in the ground state, the exact values $K=-0.1$ and $K=-\frac{1}{6}$ for one line and $K/J=-\frac{1}{3}$ and $K/J=-1.0$ for the other transition line. These results have not been reported previously, to our knowledge.

It should be noted that our Monte Carlo study is not very thorough: only one small lattice size is studied. Thus no finite-size extrapolations are possible. One can claim the order of a transition only after a finite-size analysis. Thus our result is exploratory, not definitive. The small statistics (3000–5000 MCS) can only be used as

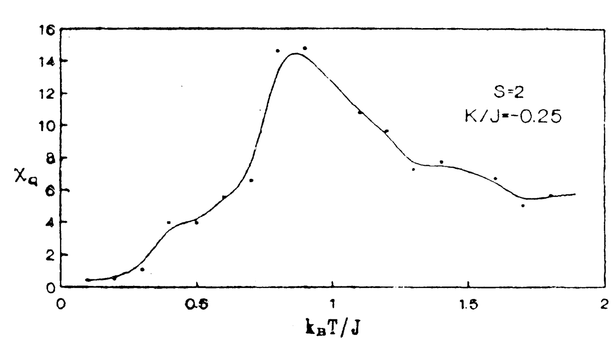

FIG. 8. The susceptibility χ_Q as a function of temperature for $S=2$ and $K/J=-0.25$.

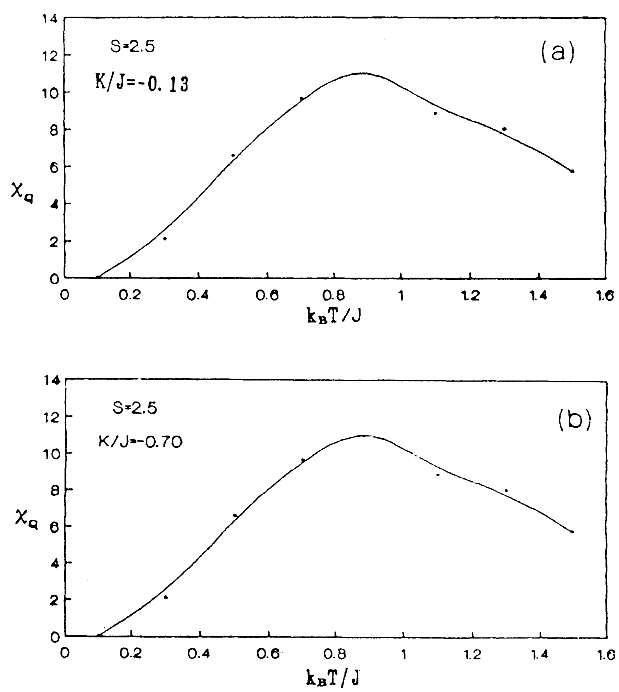

FIG. 10. (a) The susceptibility χ_Q as a function of temperature for $S=\frac{5}{2}$ and $K/J=-0.13$. (b) The susceptibility χ_Q as a function of temperature for $S=\frac{5}{2}$ and $K/J=-0.70$.

an exploratory study. Our study may stimulate further work on this model to give a definitive conclusion.

A comparison with the results from CVPA and OPA obviously leads us to the following conclusions: Both CVPA and OPA cannot predict the low-temperature transition lines, the phase diagram presented in Refs. 7–9 would thus appear to be incomplete at low temperature.

IV. CONCLUSION

In this publication we present an exploratory Monte Carlo study on the spin-1, $\frac{3}{2}$, 2, and $\frac{5}{2}$ Ising model with bilinear interactions (J) and biquadratic interaction (K). We found that for each spin value, there always exists a transition line in the high-temperature region. This transition line has already been studied by CVPA and OPA. However in the low-temperature region, some new transition lines are predicted by our Monte Carlo simulations. In the T-K planes, a line running within the ordered phase, along the nonzero temperature region from $T=0$ and $K/J=-\frac{1}{3}$ to $T=0$ and $K/J=-1.0$ for spin $S=\frac{3}{2}$ and from $T=0$ and $K/J=-\frac{1}{6}$ to $T=0$ and $K/J=-\frac{1}{3}$ for spin $S=2$, separates the region of equal sublattice magnetizations from that of unequal sublattice magnetizations. For spin value $S=\frac{5}{2}$, two low-temperature lines in the T-K plane separate the region of equal sublattice magnetizations from that of unequal sublattice magnetizations with the one line running in the nonzero temperature region from $T=0$ and $K/J=-0.1$ to $T=0$ and $K/J=-\frac{1}{6}$ and the other line running from $T=0$ and $K/J=-\frac{1}{3}$ to $T=0$ and $K/J=-1.0$. Previous studies[7–9] seem to predict an incomplete phase diagram in the low-temperature region.

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