Curie temperature for three-dimensional binary Ising ferromagnets

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The concentration dependence of the Curie temperature in binary, ferromagnetic Ising systems on the simple-cubic lattice is studied by high-accuracy Monte Carlo simulations using the Swendsen and Wang algorithm. Our results are in good agreement with the known mean-field-like approaches. Based on former theories, a formula for estimating the Curie temperature of these systems is proposed.

I. INTRODUCTION

Binary Ising systems present great interest from both bond and site perspectives.[1-6] In the bond-disordered model the lattice sites are equivalent and the interaction energies between neighboring sites are randomly assigned from a set of possible values. In the site-disordered model the lattice sites are randomly occupied by two different types of magnetic ions (A and B, with spins S_A and S_B) and the interaction parameters between two neighboring spins are completely determined by their species. The randomness in these systems can be considered either quenched or annealed. The annealed systems are much more convenient for theoretical purposes considering mean-field-like approaches, and so they are much better understood than the quenched ones. Unfortunately, for practical applications, the quenched systems are more appropriate, and therefore we shall limit our discussion to the case of quenched systems only.

When all the interactions between the spins are of ferromagnetic type, these models were used with success to describe the magnetic properties of quenched and disordered magnetic alloys of the form A_xB_{1-x}, where A and B are magnetic atoms.[6,7] If antiferromagnetic and ferromagnetic interactions compete, frustration appears, and the system becomes a Mattis-Luttinger-type spin-glass model.[8,9]

The site-disordered models are more realistic, and therefore we propose to study the Ising version of this model, considering the simplest case $S_A=S_B=\frac{1}{2}$, and all the exchange interactions of ferromagnetic type. The Hamiltonian of our problem is:

$$H=-\sum_{\langle i,j\rangle}[J_{AA}\delta_{iA}\delta_{jA}+J_{BB}\delta_{iB}\delta_{jB}+J_{AB}(\delta_{iA}\delta_{jB}+\delta_{iB}\delta_{jA})]S_i^zS_j^z\ , \quad (1)$$

where $\delta_{ix}=1$ if the spin i is of type x, and 0 otherwise, and the sum refers to all nearest neighbors. In this paper we consider the real three-dimensional version of the model; for similar results concerning the two-dimensional case, see Ref. 10.

The considered model (1), was already investigated by many authors, using different methods. Molecular-field approximations were due to Vonsovskii.[11,12] Frustrated systems were studied by Aharony using renormalization-group techniques[13] and by Tatsumi with Monte Carlo simulations.[9] The case of ferromagnetic interactions only was studied using a mean-field-like approach by Kouvel,[14] and with the coherent-potential approximation by Foo and Wu.[15] Mean-field theoretical approaches were also made in the works of Thorpe and McGurn[3] and Tahir-Kheli and Kawasaki.[2] Ishikawa and Oguchi[4] considered a Bethe-Peierls approach, and one can find in the work of Honmura, Khater, Fittipaldi, and Kaneyoshi[5] an effective-field theory for the two-dimensional model. Monte Carlo simulations were performed by Scholten[16] to study the critical temperatures of two-dimensional, binary Ising ferromagnets versus the relative species concentration and relative interaction energy between unlike ions. Scholten also studied the phase diagram for the three-dimensional problem on cubic lattices for frustrated systems including next-nearest-neighbor interactions.[17] The phase diagrams of binary Ising ferromagnets were studied by Thorpe and McGurn[3] both in the site-disorder and bond-disorder cases. They pointed out that the phase diagrams can be usefully classified in terms of the initial slope $\partial \ln T_c/\partial q$ of the transition temperature T_c considered as a function of the concentration q for two points $q=0$ and $q=1$. By means of perturbation theory they also determined the initial slopes for two-dimensional systems. The phase diagrams of binary Ising systems with randomly distributed exchange parameters were investigated by Kaneyoshi and Li, using the effective-field theory with correlations.[18] In Refs. 7 and 6 a good correspondence between experimental data and mean-field-type predictions can be found. Diluted systems, where one of the two components is a nonmagnetic atom present interest also.[19-21] Systems of mixed S_A and S_B spins where $S_A\neq S_B$ have recently been studied by many authors.[22-25]

In spite of so much work there are some not completely clarified questions even for the simplest ferromagnetic case. The main problems concern the values of the critical exponents and the determination of the critical temperature of the system in general cases.

Our work intends to study the values of the critical temperature depending on the system composition and coupling constants. We do this in a review context by comparing our Monte Carlo simulations with the avail-

able theoretical formulas. In this manner we provide a useful and easy method of approximating the Curie temperature of these systems for general compositions and for general interaction parameters. The validity and the limitations of different mean-field-type approximations for this problem are also discussed.

II. THEORETICAL BACKGROUND

The localized model of ferromagnetism involving nearest-neighbor exchange integrals has an attractive simplicity in the description of many magnetic systems. Although due to the partially itinerant nature of the magnetic electrons this approach is not completely acceptable in metallic systems, the results usually proved to be in good agreement with the experimental data. In the case of binary magnetic alloys we are in a similar situation. The localized model based on the Heisenberg or Ising Hamiltonian (1) with nearest-neighbor exchange, or the molecular-field theories proved to describe well the variation of the critical temperature versus the alloy composition.

A formula based on the molecular-field approximation was derived by Vonsovskii,[11,12] and was used successfully to calculate the transition temperatures of binary magnetic alloys. The proposed formula was

$$T_c(q)=T_c(A,A)-2[T_c(A,A)-T_c(A,B)]q+[T_c(A,A)+T_c(B,B)-2T_c(A,B)]q^2 , \quad (2)$$

where $T_c(A,A)$ and $T_c(B,B)$ are the Curie temperatures of the pure A and B species, $T_c(A,B)$ is the Curie temperature for a pure system characterized by all the exchange interactions being equal to the one between the A and B magnetic ions (J_{AB}), $T_c(q)$ is the Curie temperature of the mixture, and q is the concentration of the B component.

We mention here that in the framework of an Ising model the critical temperature T_c for an Ising system on the simple cubic lattice characterized by J exchange interaction constants (considering just nearest-neighbor interactions) is given by $T_c \approx 4.444\,25J/k_B$,[26] where k_B is the Boltzmann constant. Thus the values of $T_c(A,A)$, $T_c(A,B)$, and $T_c(B,B)$ indicate the J_{AA}, J_{AB}, and J_{BB} interaction parameters, respectively, apart from the given proportionality constant.

By using a phenomenological model based on a suitably modified mean-field theory, allowing the individual atomic moments to vary in magnitude with their local environment, and by considering only nearest-neighbor interactions, Kouvel[14] proposed the formula

$$T_c(q)=\tfrac{1}{2}[T_c(A,A)(1-q)+T_c(B,B)q]+\{\tfrac{1}{4}[T_c(A,A)(1-q)-T_c(B,B)q]^2+T_c(A,B)^2q(1-q)\}^{1/2} . \quad (3)$$

In the work of Foo and Wu,[15] the disordered composition-dependent exchange interaction is treated in a coherent-potential approximation (CPA). In the limit of weak scattering, their method yields mean-field-like results, but in the strong-scattering limit they predict such effects as a critical concentration for the appearance of ferromagnetism in diluted systems,[21] which is not obtained by the mean-field theories. They proposed the following cubic equation for $T_c(q)$:

$$\alpha^2T_c(q)^3+\{\alpha[T_c(A,A)+T_c(B,B)+T_c(A,B)]-\alpha(1+\alpha)\langle T_c\rangle\}T_c(q)^2+\{(1+\alpha)T_c(A,A)T_c(B,B)T_c(A,B)\left\langle\frac{1}{T_c}\right\rangle-\alpha[T_c(A,A)T_c(B,B)+T_c(A,B)T_c(A,A)+T_c(A,B)T_c(B,B)]\}T_c(q)-T_c(A,A)T_c(B,B)T_c(A,B)=0 , \quad (4)$$

where

$$\alpha=\frac{z}{2}-1 , \quad (5)$$

with z the coordination number of the lattice (in our case $z=6$), and

$$\langle T_c\rangle=(1-q)^2T_c(A,A)+2q(1-q)T_c(A,B)+q^2T_c(B,B) , \quad (6)$$

$$\left\langle\frac{1}{T_c}\right\rangle=\frac{(1-q)^2}{T_c(A,A)}+\frac{2q(1-q)}{T_c(A,B)}+\frac{q^2}{T_c(B,B)} . \quad (7)$$

We mention that other, more involved possibilities of calculating the Curie temperature based on the Ising model (1) of the system exist, such as mean-field-like renormalization-group techniques, series expansion, and perturbation methods. Unfortunately, these very technical approaches do not yield practical formulas.

III. THE COMPUTER SIMULATION METHOD

As was stated earlier, Monte Carlo simulations were performed on the considered model (1) by Scholten[16] in the ferromagnetic case [$T_c(A,A)>0$, $T_c(A,B)>0$, and $T_c(B,B)>0$], and by Tatsumi[9] and Scholten[17] on frustrated systems. Scholten's work for purely ferromagnetic systems refers to the two-dimensional case. He used the classical single-spin-flip Metropolis algorithm,[27] and therefore his calculations were rather time consuming. Thus, only a few choices for the interaction parameters were considered. He compared his Monte Carlo results with the ones obtained in Refs. 2–5.

In this paper, we attempt to complete the earlier works on the three-dimensional case of the simple cubic lattice

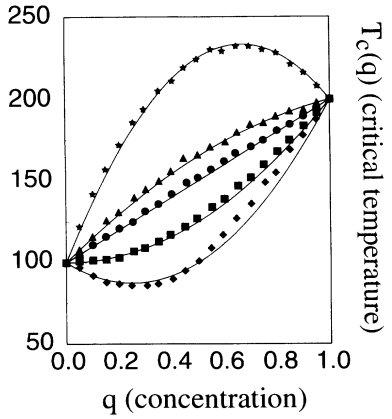

FIG. 1. Monte Carlo results for the Curie temperature versus the B component concentration for five choices of the $T_c(A,B)$ critical temperature, $T_c(A,B)=50$ (♦), 100 (■), 150 (●), 180 (▲), and 300 (★). The values of $T_c(A,A)=100$ and $T_c(B,B)=200$ are fixed. Solid curve is given by Eq. (2).

by a high-accuracy Monte Carlo simulation. We use the performant cluster-flip Swendsen and Wang Monte Carlo method[28] with an original recursion-type algorithm and compare our results with the ones given in Refs. 11, 12, 14, and 15.

The simulations were performed on relatively large $50\times50\times50$ simple cubic lattices. The critical temperature was found by detecting the maximum in the fluctuation of the absolute value of the magnetization. For achieving statistical equilibrium we considered up to 600 cluster flips and then we studied the fluctuation for 1000 more iterations. The sensitivity in the determination of the critical temperature was in general of the order of $0.01T_c(A,A)$. Usually $T_c(A,A)=100$ (units) was considered and we proposed various values for the $T_c(A,B)$ and $T_c(B,B)$ parameters. For every chosen set of interaction parameters we covered the $q\in(0,1)$ concentration interval with 19 equidistant simulation points. The program was written in C and the simulations were performed on a Cray Y-MP4D/464 computer and IBM R-6000 RISC workstations.

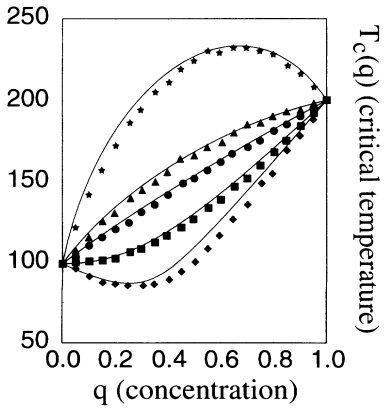

FIG. 2. Monte Carlo results from Fig. 1 in comparison with the curve given by Eq. (3).

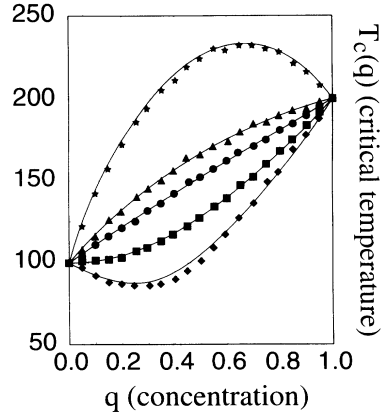

FIG. 3. Monte Carlo results from Fig. 1 in comparison with the Curie temperature calculated from the arithmetic mean of formulas (2) and (3).

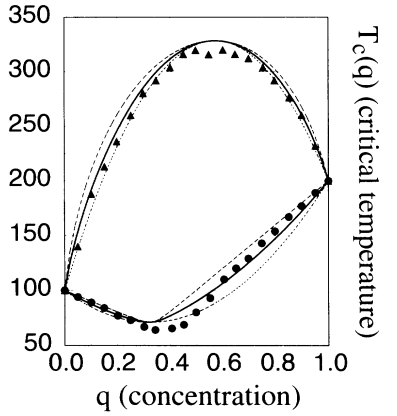

FIG. 4. Dots [$T_c(A,B)=10$] and triangles [$T_c(A,B)=500$] represent Monte Carlo simulations for the given values of the $T_c(A,B)$ critical temperature. The thin dashed lines indicate the results obtained from formulas (2) and (3) [short dashes corresponding to (2)]. The continuous dark line is the Curie temperature obtained from the arithmetic mean of (2) and (3).

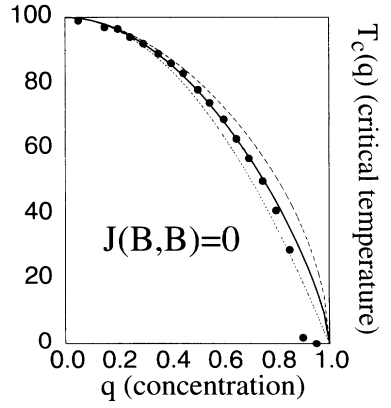

FIG. 5. The case when we have no exchange interactions between the atoms of the B component ($J_{BB}=0$) and $T_c(A,A)=T_c(A,B)=100$. Dots are Monte Carlo results and the curves have the same meaning as in Fig. 4.

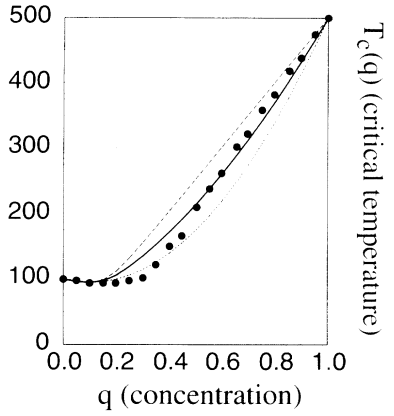

FIG. 6. Monte Carlo results (dots) for $T_c(A,A)=100$, $T_c(B,B)=500$, and $T_c(A,B)=50$. The curves represent the same formulas as in Fig. 4.

IV. RESULTS

Our Monte Carlo results for the variation of the Curie temperature versus the B component concentration are plotted with different symbols in Figs. 1–7. As stated earlier the simulations were made on a simple cubic lattice. The curves indicate theoretical results obtained from Eqs. (2) and (3).

In Fig. 1 we compare our Monte Carlo results with those obtained from Eq. (2), considering four choices of the J_{AB} interaction parameters (J_{BB} and J_{AA} fixed). Figure 2 presents the same results in comparison with theoretical data given by Eq. (3). One can observe that, compared to our results, formula (2) predicts lower values, and by contrast to this Eq. (3) yields higher values for the transition temperatures. We also checked that Eq. (4) gives lower values even than (2), so it is much less appropriate for our model. As a first observation, we conclude that in these cases the real transition temperatures are limited by the two curves given by Eqs. (2) and (3). We are also able to confirm that in these three-dimensional cases the mean-field-like results proved to give quite good estimates for the Curie temperature. In Fig. 3 we illustrate that if we use the arithmetic mean of the values obtained from (2) and (3) almost a perfect fit with the real Curie temperatures can be obtained.

In Figs. 4–6 we tried to prove our previous statements by considering quite exotic values for the exchange interaction parameters, i.e., for the $T_c(A,B)$ and $T_c(B,B)$ critical temperatures. We drew with thin dashed lines the results given by Eqs. (2) and (3) [short dashes correspond to the curve obtained from (2)]. The continuous darker line represents the arithmetic mean of formulas (2) and (3). We conclude again that the values given by Eqs. (2) and (3) limit our simulation points quite nicely, and their arithmetic mean gives a fairly good estimate for the real Curie temperature. In the case when $J_{AB} \notin [J_{AA}, J_{BB}]$, one can also observe that the strongest discrepancy between the arithmetic mean proposed by us and the simulation results appears for concentration values where the critical temperature has an extremum, the real values being lower.

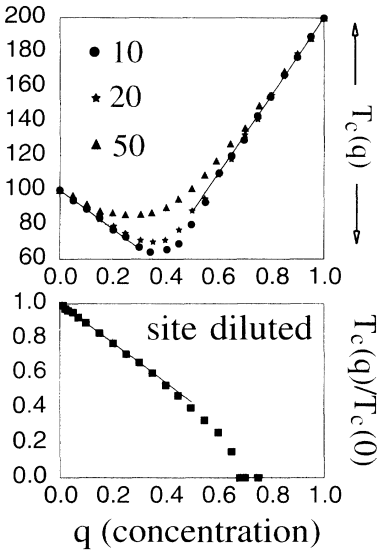

FIG. 7. Upper figure presents Monte Carlo results for three small choices of the $T_c(A,B)$ critical temperature. Solid curves indicate the characteristic straight lines for site-diluted systems in the small-dilution limit. On the lower figure we have Monte Carlo results for the site-diluted system.

In Fig. 7 we present studies concerning the extreme case when the J_{AB} interaction parameter, and thus the $T_c(A,B)$ critical temperature, is getting smaller (weak coupling between the two components). In this case, as was expected, we obtain the result that the simulation curves in the limit of $q=0$ and $q=1$ tend to straight lines with the slope $[1/T_c(0)][\partial T_c(q)/\partial q]$ equal to 1.13, characteristic for site-diluted systems.[21] In the limit of the site-diluted systems $[T_c(A,B)=T_c(B,B)=0]$ we get the well-known result,[21] that for dilutions larger than a critical value, $q_c \approx 0.67$, no spontaneous ordering will appear for temperatures $T>0$ (results presented on the bottom in Fig. 7). In Ref. 21 we also claimed that for the simple cubic lattice this critical concentration is approximately equal to the site-percolation limit.

V. CONCLUSIONS

By comparison of our computer simulation data with the results given by formulas (2) and (3), we conclude that in the three-dimensional case the mean-field-like approaches work satisfactorily. Therefore the good fit of the mean-field-like predictions with the experimental data in Refs. 6 and 7 is not surprising.

Generally, the curves obtained for the critical temperature from Eqs. (2) and (3) limit the real values rather nicely. Exceptions are the cases where the J_{AB} interaction parameter is not in the interval limited by J_{AA} and J_{BB}. In these situations, our previous statement might not be true in the vicinity of the extremum for the Curie temperature.

The theoretical curve drawn from the arithmetic mean of the T_c's obtained with formulas (2) and (3) proved to

be a good approximation for the Curie temperature of quenched, binary Ising ferromagnets. In the limit of small couplings between the two components (J_{AB} small), results in good agreement with the site-diluted model were obtained.

Our study was intended to complete the earlier ones by giving a practically useful approach for estimating the Curie temperature of the proposed system. We also illustrated the validity of our method, and tried to study many possible choices for the interaction parameters.

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