CURIE TEMPERATURES FOR THREE-DIMENSIONAL BINARY ISING FERROMAGNETS

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Abstract

Using the Swendsen and Wang algorithm, high accuracy Monte Carlo simulations were performed to study the concentration dependence of the Curie temperature in binary, ferromagnetic Ising systems on the simple-cubic lattice. Our results are in good agreement with known mean-field like approaches. Based on former theoretical formulas we propose a new way of estimating the Curie temperature of these systems.

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I. Introduction

Binary Ising systems presented a large interest from both bond and site perspectives [1-6]. In the bond-disordered models the lattice sites are equivalent and the interaction energies between neighbouring sites are randomly assigned from a set of possible values. In the site-disordered model the lattice sites are randomly occupied by two different type of magnetic ions, A and B, with spins \( S_A \) and \( S_B \), and the interaction parameters between two neighbouring spins are completely determined by their species. The randomness in these systems can be considered either quenched or annealed. The annealed systems proved to be handled theoretically much easier by mean-field like methods, and so there are much better understood than the quenched ones. Unfortunately for practical applications the quenched systems are much more appropriate. This is the main reason why we proposed to limit our discussion just for the case of quenched systems.

In the case of only ferromagnetic interactions between the spins, 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]. When antiferromagnetic and ferromagnetic interactions compete, frustration appears, and the system become a Mattis-Luttinger type spin-glass model [8, 9].

For real physical cases the site-disordered models are more realistic, and so we proposed to study the Ising version of this model, considering the simplest case of \( S_A = S_B = \frac{1}{2} \), and all the exchange interactions of ferromagnetic type. The Hamiltonian of our problem will be:

\[
H = - \sum_{<i,j>} [J_{AA} \cdot \delta_{iA} \cdot \delta_{jA} + J_{BB} \cdot \delta_{iB} \cdot \delta_{jB} + J_{AB} \cdot (\delta_{iA} \cdot \delta_{jB} + \delta_{iB} \cdot \delta_{jA})] \cdot S_i^z \cdot S_j^z, \tag{1}
\]

where \( \delta_{ix} = 1 \) if the spin \( i \) is of type \( x \), and 0 otherwise, and the sum is referring to all nearest-neighbours. In this paper we consider the real three-dimensional version of the model, and for results concerning the two-dimensional case we propose [10].

The model considered by us was already investigated by many authors, using different methods. The first molecular-field approximations were due to Vonsovskii
Frustrated systems were studied by Aharony using renormalization-group technics \[13\] and by Tatsumi with Monte Carlo simulations \[9\]. The case of only ferromagnetic interactions 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 \[3\] respective Tahir-Kheli and Kawasaki \[2\]. Ishikawa and Oguchi \[1\] considered a Bethe-Peierls approach and in the work of Honmura, Khater, Fittipaldi and Kaneyoshi \[5\] we find 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 in function of the relative species concentration and the relative interaction energy between unlike ions. Scholten also studied the phase diagram for the three-dimensional problem on cubic lattices for frustrated systems \[17\], and included next-nearest-neighbour interactions too. 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 cataloged in terms of the initial slope \(\frac{\partial \ln T_c}{\partial q}\) of the transition temperature \(T_c\) considered in function of concentration \(q\), at the two points \(q = 0\) and \(q = 1\). With the help 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 effective-field theory with correlations \[18\]. In the book from Vonsovskii \[7\] and in the paper from Luborsky \[6\] one can find promising comparisons between experimental data and mean-field type predictions. Diluted systems, where one of the two components are non-magnetic, also presented a field of interest \[19-21\]. Recently there has been much interest in systems of mixed \(S_A\) and \(S_B\) spins, where \(S_A \neq S_B\) \[22-25\].

In spite of all these earlier works there remained some not completely clarified questions even for the simplest ferromagnetic case. The main problems are concerning the values of the critical exponents and the determination of the critical
temperature of the system in general cases. Our work is intended to study the
dependence of the critical temperature in function of the system composition and
values of the coupling constants. We do this in a review context by comparing
our high-accuracy Monte Carlo simulations with available theoretical formulas. In
this manner we will give a practically useful and easy method of approximating the
Curie temperature of these systems for general composition and general interaction
parameters. We will also check the validity and limitations of different mean-field
type approximations available for the Curie temperature of binary magnetic alloys.

II. Used theoretical formulas

The localized model of ferromagnetism involving nearest-neighbour exchange inte-
grals has an attractive simplicity for describing some magnetic systems. Although
this approach for the magnetism in metallic systems is not completely acceptable due
to the partially itinerant nature of the magnetic electrons, the obtained results are
usually in good agreement with 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-neighbour exchange, or the molecular-field the-
ories proved to be applicable in describing the variation of the critical temperature
in function of the alloys composition.

The first formula based on the molecular-field approximation was derived, as we
stated earlier by Vonsovskii [11, 12], and used with success to describe transition
temperatures of binary magnetic alloys. The proposed formula was:

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

(2)

where $T_c(A, A)$ and $T_c(B, B)$ are the Curie temperatures of the pure $A$ and $B$
systems, $T_c(A, B)$ is the Curie temperature for a pure system characterized with all
exchange interactions equal with the ones 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 the critical temperature $T_c$ for an Ising system on the simple-cubic lattice, characterized with $J$ exchange interaction constants (considering just nearest-neighbour interactions) is given by $T_c \approx 4.44425 \cdot \frac{J}{k_B}$, with $k_B$ the Boltzmann constant.

Using a phenomenological model based on mean-field theory suitably modified, so that the individual atomic moments are allowed to vary in magnitude with their local environment, and considering only nearest-neighbour interactions Kouvel [14] proposed the formula:

$$T_c(q) = \frac{1}{2} \cdot [T_c(A, A) \cdot (1 - q) + T_c(B, B) \cdot q] +$$

$$+ \left\{ \frac{1}{4} \cdot [T_c(A, A) \cdot (1 - q) - T_c(B, B) \cdot q]^2 + T_c(A, B)^2 \cdot q \cdot (1 - q) \right\}^{\frac{1}{2}}. \quad (3)$$

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 give the mean-field like results, but in the strong scattering limit they predict such effects as critical concentration for the appearance of ferromagnetism in the diluted models [21], which is not obtained in mean-field theories. They proposed the following cubic equation for $T_c(q)$

$$\alpha^2 \cdot T_c(q)^3 +$$

$$+ [\alpha \cdot (T_c(A, A) + T_c(B, B) + T_c(A, B)) - \alpha \cdot (1 + \alpha) \cdot <T_c> \cdot T_c(q)] +$$

$$+ \left\{ [(1 + \alpha) \cdot T_c(A, A) \cdot T_c(B, B) \cdot T_c(A, B) \cdot <T_c> -$$

$$- \alpha \cdot (T_c(A, A) \cdot T_c(B, B) + T_c(A, B) \cdot T_c(A, A) + T_c(A, B) \cdot T_c(B, B))] \cdot T_c(q) -$$

$$- T_c(A, A) \cdot T_c(B, B) \cdot T_c(A, B) = 0, \quad (4)$$

where

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

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

$$<T_c> = (1 - q)^2 \cdot T_c(A, A) + 2 \cdot q \cdot (1 - q) \cdot T_c(A, B) + q^2 \cdot T_c(B, B), \quad (6)$$

$$\frac{1}{T_c} \geq \frac{(1-q)^2}{T_c(A, A)} + \frac{2q(1-q)}{T_c(A, B)} + \frac{q^2}{T_c(B, B)}, \quad (7)$$

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We mention that there are also other, more evaluate possibilities of calculating the Curie temperature, based on the Ising model (1) of the system, such as mean-field like renormalization-group technics, series expansion and perturbation methods. Unfortunately these are all very technical ones, and do not give practically usable formulas.

III. The computer simulation method

As stated earlier, Monte Carlo simulations were performed on the considered model (1) in the ferromagnetic case \( T_c(A, A) > 0, T_c(A, B) > 0 \) and \( T_c(B, B) > 0 \) by Scholten [16], and on frustrated systems by Tatsumi [9] and Scholten [17]. Scholten’s work for purely ferromagnetic systems refers to the two-dimensional case. He used the classical single spin-flip Metropolis algorithm [26], and due to this his calculations were rather time-consuming. So, he considered just a few choices for the interaction parameters. He compared his Monte Carlo results with the ones obtained in [2, 3], [4] and [5].

In the present work we proposed to study by high-accuracy Monte Carlo simulations the three-dimensional case of simple-cubic lattices, completing in some sense the earlier works. We used the more performant cluster-flip Swendsen and Wang Monte Carlo method [27] with an original recursion type algorithm. We proposed to compare our results with the ones given in [11, 12], [14] and [15].

Our simulations were performed on relatively large \( 50 \times 50 \times 50 \) 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 studied the fluctuation for 1000 more iterations. The sensitivity in the determination of the critical temperature was in general of the order of \( 0.01 \cdot T_c(A, A) \). We chose usually \( T_c(A, A) = 100 \) (units) and we proposed to consider 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 uniformly with 19 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.

IV. Results

Our Monte Carlo results for the variation of the Curie temperature in function of the $B$ components concentration, are plotted with different symbols on Fig. 1-7. The simulations, as we stated, earlier were made on a simple-cubic lattice. The curves indicate theoretical results obtained from equations (2) and (3).

In Fig. 1 considering four choices of the $J_{AB}$ interaction parameters ($J_{BB}$ and $J_{AA}$ fixed) we compare our Monte Carlo results with the ones obtained from equation (2). Fig. 2 presents the same results in comparision with theoretical data given by equation (3). One can observ that formula (2) predict in general lower values, and in contrast to this (3) predict higher values for the transition temperature than the real ones. We also checked, that equation (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 with the two curves given by equations (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 almost a perfect fit with the realistic Curie temperatures can be obtained, if we use the arithmetic mean of the values obtained from equations (2) and (3).

In Fig. 4-6 we tried to prove our previous statements considering quite exotic values for the exchange intercation parameters, and thus for the $T_c(A, B)$ and $T_c(B, B)$ critical temperatures. We draw with thin dashed lines the results given by equations (2) and (3) (dense 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 in general the values given by equations (2) and (3) limit nicely our realistic simulation points, and their arithmetic mean give a fairy good estimate for the realistic Curie temperature. In the case when $J_{AB} \notin [J_{AA}, J_{BB}]$, 

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one can also observe, that the strongest difference between the arithmetic mean proposed by us and the simulation results are for concentration values where the critical temperature has an extremum, the real values being lower.

In Fig. 7 we present studies concerning the extrem 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 expected, we get that the simulation curves in the limit of $q = 0$ and $q = 1$ are tending to straight-lines with the slope $\frac{1}{T_c(0)} \cdot \frac{\partial T_c(q)}{\partial q}$, equal with 1.13, characteristic for site-diluted systems [21].

V. Conclusions

From comparison of computer simulation data with results given by formula (2) and (3) we conclude, that in the three-dimensional case, the mean-field like approaches are working satisfactory well. So, in this way it is not surprising the good fit of the mean-field like predictions with experimental data, presented in [6] and [7].

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

The theoretical curve constructed from the arithmetic mean of formula (2) and (3) proved to be a good approximation to obtain easily the Curie temperature for quenched, binary Ising ferromagnets.

In the limit of small couplings between the two components ($J_{AB}$ small), we obtained results in good agreement with the site-diluted model.

Our study is intended to complete the earlier ones by giving a practically useful method of 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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**Figure Captions**

**Fig. 1.** Monte Carlo results for the variation of the Curie temperature as a function of the $B$ components concentration for four choices of the $T_c(A, B)$ critical temperature. The values of $T_c(A, A) = 100$ and $T_c(B, B) = 200$ are fixed. Solid curve is given by equation (2).

**Fig. 2.** The Monte Carlo results from Fig. 1 in comparison with the curve given by equation (3).

**Fig. 3.** The Monte Carlo results from Fig. 1 in comparison with the Curie temperature given by the arithmetic mean of formulas (2) and (3).

**Fig. 4.** The dots and triangles 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) (dense dashes corresponding to (2)). The continuous dark line indicates the Curie temperatures obtained as 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.
Fig. 7. The upper figure shows 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. The figure from below presents Monte Carlo results obtained for the site-diluted system.