CURIE TEMPERATURES
FOR BINARY ISING
FERROMAGNETS
ON THE SQUARE LATTICE

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Abstract

High-accuracy Swendsen and Wang Monte Carlo simulations were performed to study the Curie temperature of ferromagnetic, binary Ising systems on the square lattice. Our results are compared with mean-field like approaches. Based on these former theories, we give a new formula to estimate the Curie temperature of the system.

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§1. Introduction

Binary Ising systems were studied from both bond and site perspectives (Katsura and Matsubara 1974; Thorpe and McGurn 1978). In the bond-disordered model the lattice sites are considered to be equivalent and the interaction energies between the neighbouring sites are assigned randomly 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 \( S_B \), the interaction parameters between neighbouring spins being completely determined by their species. In this way there exist three types of exchange interactions \( J_{AA}, J_{AB} \) and \( J_{BB} \), between neighbouring spins in the system. The disorder can be considered either quenched or annealed. The annealed systems are much more easier handled by mean-field like approaches, and so there are better understood than the quenched ones. In spite of this, for practical applications the quenched systems are much more appropriate. This is the main reason why we proposed to limit the discussion only for the case of quenched systems.

In the case of only ferromagnetic interactions between the spins, binary Ising or Heisenberg models were used with success to describe the magnetic properties of magnetic alloys (Vonsovski 1974; Luborsky 1980). When antiferromagnetic and ferromagnetic interactions compete, frustration appears, and the system becomes a Mattis-Luttinger type spin-glass model (Binder and Young 1986; Tatsumi 1977-78).

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

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

where \( \delta_{ix} = 1 \) if the spin \( i \) is of type \( x \), and 0 otherwise. The sum in (1) is referring to all nearest neighbours of the lattice. In this paper we consider the two-dimensional version of the model. For results concerning the three-dimensional, real model we
have just preliminary results (Neda 1994[b]). The first molecular-field approximations for the proposed systems were due to Vonsovskii (1940 and 1948). The frustrated systems were first studied by Aharony (1975) using renormalization-group technics and by Tatsumi (1977-78) with Monte Carlo simulations. The interesting case for us, with all the interactions of ferromagnetic type, was studied using a mean-field like approach by Kouvel (1969), and with the coherent potential approximation by Foo and Wu (1972). Mean-field theoretical approaches were also made in the works of Tahir-Kheli and Kawasaki (1977), respective Thorpe and McGurn (1978). Ishikawa and Oguchi (1978) considered a Bethe-Peierls approach, and in the work of Honmura, Khater, Fittipaldi and Kaneyoshi (1982) we find an effective-field theory for the model. Monte Carlo studies for the critical temperature of binary, ferromagnetic Ising alloys in function of the relative species concentration and relative interaction energy between unlike ions were performed by Scholten (1985) on the square lattice. Scholten (1989) also studied the phase diagram for three-dimensional frustrated systems on simple-cubic lattices, including next-nearest neighbour interactions too. The phase diagrams of binary Ising ferromagnets were studied by Thorpe and McGurn (1978), both in the site-disordered and bond-disordered cases. They realized that these phase diagrams can be usefully cataloged in terms of the initial slope \( \frac{\partial \ln T_c}{\partial q} \) of the transition temperature \( T_c \) plotted in function of concentration \( q \), at the two points \( q = 0 \) and \( q = 1 \). Using the perturbation theory, they also determined the initial slopes for two-dimensional systems. The phase diagrams for binary Ising systems with randomly distributed exchange parameters were studied by Kaneyoshi and Li (1987) using effective-field theory with correlations. In the book from Vonsovskii (1974) and in the paper from Luborsky (1980), one may find promising comparisions between experimental data and mean-field like predictions. Diluted systems \( (J_{AB} = 0 \text{ and } J_{BB} = 0) \) also presented interest for physicists (Wu 1982; Belokon and Semkin 1992; Neda 1994[a]). Recently there has been much interest in systems of mixed \( S_A \) and \( S_B \) spins, where \( S_A \neq S_B \) (Kaneyoshi 1989; Silva and Salinas 1991; Kaneyoshi, Jascur and Tomczak 1992; Zhang and Yang 1993).
Although Monte Carlo simulations were performed by Scholten (1985) on the considered model, there remained some not completely clarified questions even in the simplest two-dimensional and ferromagnetic case. The main problems are concerning the values of the critical exponents and the elaboration of a practically usable and general formula to estimate the critical temperature of the system. Our work is intended to complete Scholtens paper in some sense, studying by a high-accuracy Monte Carlo simulation the Curie temperature of the system. We do this in a review context, comparing our simulation results with available theoretical formulas. In this manner we give a practically usable and easy method of approximating the Curie temperature of the system and illustrate the validity and limitations of different theoretical approaches.

§2. Used theoretical formulas

The localized model of ferromagnetism involving nearest-neighbour exchange integrals 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 theories 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 (1940; 1948) and used with success to describe transition temperatures of binary magnetic alloys. The proposed formula was:

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

(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 square lattice, characterized with $J$ exchange interaction constants (considering just nearest-neighbour interactions) is given by $T_c \approx 2.2681 \cdot \frac{J}{k_B}$, 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 (1969) 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 (1972) 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 (Neda 1994[a]), which is not obtained in mean-field theories. They proposed the following cubic equation for $T_c(q)$

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

$$+ [\alpha \cdot (T_c(A, A) + T_c(B, B) + T_c(A, B)) - \alpha \cdot (1 + \alpha) \cdot < T_c >] \cdot T_c(q)^2 +$$

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

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

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

where

$$\alpha = \frac{z}{2} - 1, \quad (5)$$
with \( z \) the coordination number of the lattice (in our case \( z = 4 \)), and

\[
<T_c>(1 - q)^2 \cdot T_c(A, A) + 2 \cdot q \cdot (1 - q) \cdot T_c(A, B) + q^2 \cdot T_c(B, B),
\]

(6)

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

(7)

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.

§3. The computer simulation method

The Monte Carlo simulations performed by Scholten on the proposed model were made by using the classical single spin-flip Metropolis algorithm (Metropolis, Rosenbluth and Teller 1953). Due to this, his simulations were very time-consuming, and he studied just a few choices for the values of the interaction parameters \( J_{AA} = 0, 1, 2, 4 \) and \( J_{BB} = 4 \). He also worked on relatively small \( 40 \times 40 \) square lattices with periodic boundary conditions. For each choice of the interaction parameters value he studied three cases for the concentration of the \( B \) component \( q = 0.25, q = 0.5 \) and \( q = 0.75 \) (the cases \( q = 0 \) and \( q = 1 \) are evident). He compared his results with the ones obtained by (Tahir-Kheli et al. 1977), (Thorpe et al. 1978), (Ishikawa et al. 1978) and (Honmura et al. 1982).

We proposed to continue Scholten’s work by reconsidering the problem with high-accuracy Monte Carlo simulations, using the more powerful cluster-flip Swendsen and Wang method (Swensen, Wang and Ferrenburg 1992) with an original recursion type algorithm. We considered many choices for the values of the \( J_{AB} \) and \( J_{BB} \) interaction parameters, the value of \( J_{AA} \) being fixed. We proposed to compare our results obtained for the Curie temperature with the ones given by equations (2), (3) and (4).
Our simulations were performed on relatively large lattices, up to $200 \times 200$ lattice sites. The critical temperature was obtained by detecting the maximum in the fluctuation of the absolute value of magnetization. To achieve statistical equilibrium we considered up to 1000 cluster-flips and then studied the fluctuation for 2000 more iterations. The sensitivity for the determination of the critical temperature was in general of the order of $0.01 \cdot T_c(A, A)$. For every chosen set of the interaction parameters we covered the $q \in (0, 1)$ concentration interval uniformly with 9 to 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.

§4. Results

Our Monte Carlo results concerning the variation of the Curie temperature in function of the B components concentration for the proposed two-dimensional model are plotted with various symbols on figures 1 and 3-7. The curves indicate theoretical results given from equations (2) and (4). In Fig. 1 considering four choices for the $J_{AB}$ interaction parameters ($J_{AA}$ and $J_{BB}$ fixed), we compare our Monte Carlo data with results given by equation (2). In Fig. 2 we show some preliminary results for the three-dimensional (simple-cubic) case, obtained with the same interaction parameters as in Fig. 1, in comparision with the curve given by the (2) molecular-field approximation. As one would expect it, we can also observe that in the real, higher dimensional case the considered molecular-field approximation is working better. From Fig. 1 we get, that on the square lattice formula (2) predicts much higher results for the Curie temperature than the real values. We checked that equation (3) predict even higher values than (2). In Fig. 3 we show the same Monte Carlo data as in Fig. 1 in comparision with results obtained from equation (4). From Fig. 1 and 2 we conclude that in the considered cases the real critical temperatures are limited by the two curves obtained from equations (2) and (4). In addition to this, in Fig. 4 we show that almost a perfect fit with the realistic Curie temperatures can be obtained, if we use the arithmetic mean of the $T_c(q)$ values obtained from
In Fig. 5-7 we tried to prove our previous statements. So, we considered other choices for the exchange interaction parameters, and thus for the $T_c(A, A)$, $T_c(B, B)$ and $T_c(A, B)$ critical temperatures. We illustrated with thin dashed lines the results obtained from equation (2) and (4) (dense dashes correspond to the curve calculated from (4)). The continuous darker curve shows the arithmetic mean of the $T_c(q)$ obtained from (2) and (4). We conclude again that in general the values given from equations (2) and (4) limit nicely the realistic simulation data, and their arithmetic mean gives a good estimate for the Curie temperature. This arithmetic mean have stronger differences with our Monte Carlo data in the case when the $J_{AB}$ exchange interaction parameters does not belong to the interval limited by the $J_{AA}$ and $J_{BB}$ values.

§5. Conclusions

Our first conclusion is that the Curie temperatures calculated from equations (2), (3) and (4) are not performant approximations of the real values. However as expected, our simulations on simple-cubic lattices reveal that the same (2) molecular-field approach is giving much better results in the real three-dimensional case (Fig. 2).

For the case of the square lattice, generally the curves obtained for the critical temperature from equations (2) and (4) limit rather nicely the real values. Our Monte Carlo simulations indicate, that a few exceptions could be for the small ($q \to 0$) and big ($q \to 1$) concentration limit, when the $J_{AB}$ interaction parameter is far from the interval limited by the values of $J_{AA}$ and $J_{BB}$.

Our most important conclusion is that, the theoretical curve constructed as the arithmetic mean of the Curie temperatures obtained from equations (2) and (4) proved to be a good approximation for the critical temperature of a binary Ising ferromagnet on the square lattice.

Similar preliminary results for the three-dimensional case are given in a recent preprint (Neda 1994[b]).
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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. Solid curve is given by equation (2).

Fig. 2 The same plot as in Fig. 1 for simulations done on the simple-cubic lattice.

Fig. 3 The Monte Carlo results from Fig.1 in comparison with the Curie temperatures obtained from (4).

Fig. 4 The Monte Carlo results from Fig. 1 in comparison with the arithmetic mean of the Curie temperatures obtained from (2) and (4).

Fig. 5 The dots and triangles represent Monte Carlo simulations for the given $T_c(A, B)$ critical temperatures. The thin dashed lines indicate the results obtained from formulas (2) and (4) (dense dashes correspond to (4)). The dark continuous line indicate the arithmetic mean obtained from (2) and (4).

Fig. 6 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. 7 Monte Carlo results (dots) for $T_c(A, A) = T_c(B, B) = 100$ and $T_c(A, B) = 500$. The curves represent the same as in Fig. 4.