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The Combinatorial Factor Method for Investigation of Order-Disorder in Two-Dimensional Binary Alloy

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(Received 17 December 2009, Accepted 7 April 2010)

The aim of this study was to investigate order-disorder in the two-dimensional AB alloy to find out whether the number of components, N_A and N_B , was equal or not. To this end, using the nearest neighbor interactions, first, we applied a two-dimensional lattice which consisted of infinite rows, R and columns, L , so that, $RL = N_A + N_B$. For such a model, using the combinatorial factor method, we derived an exact equation for the partition function. Because, the derived partition function was very complicated, the thermodynamic properties of the lattice could not be calculated; however, but these properties could be estimated for the models with a limited number of rows. Our results show that, for models with finite number of rows, for each mole fraction of A in the specific temperature, a phase transition, like Onsager transition, takes place.

Keywords: Isin model, Spin glasses, Binary alloy, Combinatorial factor, Phase transition

INTRODUCTION

One of the factors which exerts considerable influence on the behavior of some metal systems is ordering. Properties of metals such as elastic modulus, shear strength, electrical resistivity, and hardness can be enormously influenced by order-disorder transformations [1,2]. There are many metal compounds which exhibit ordering or are classified as superlattice alloys. Such systems as copper-gold, copper-zinc, copper-beryllium, copper-lead, silver-mercury, nickel-aluminum, iron-cobalt, gold-nickel, iron-silicon and iron-aluminum are some of the AB type of structures which have such characteristics. If the previously mentioned properties of these alloys are affected by the order-disorder transformation, friction characteristics may also be influenced. The Ising lattice systems with interactions involving three or more sites

[3], whose Hamiltonian comprises interaction terms of the form $-J_{ij\dots k}\sigma_i\sigma_j\dots\sigma_k$, where $i \neq j \neq \dots \neq k$ correspond to different lattice sites, and $J_{ij\dots k}$ is the coupling constant between these sites, have been used to model a variety of physical situations, like, for example, some binary alloys [4], lipid bilayers [5] and gauge-field theory models [6]. In this paper, using the combinatorial factor method, we intend to introduce a new method for solving binary alloy, which can easily be applied to spin glasses compounds. Calculation of the partition function by this method is possible not only for one-dimensional and two-dimensional lattices, but also for three-dimensional cases.

Second-order phase transitions are subtle ones. In the case of a binary alloy, configuration takes place without the release of latent heat. The transition point is marked by a discontinuity which does not exist in the same form at any other temperature. The most important model of a system that exhibits a phase transition is the Ising model. The model was

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proposed by Wilhelm Lenz [7] and was first solved exactly for the one-dimensional case by his student Ernest Ising [8]. However, Ising was very disappointed because the one-dimensional case did not have a phase transition. Kramers and Wannier [9] calculated the Curie temperature using a two-dimensional Ising model, and a complete analytic solution was subsequently offered by Onsager [10]. He showed that there was a phase transition in two-dimensionals. Solving the three-dimensional model remains as one of the basic problems in statistical mechanics, although a lot is now known about it from approximate methods.

Recently, the Ising model for limited number of rows was solved by the transfer matrix [11,12] and combinatorial factor method [13,14]. On each site, there is a variable which can take two different values, spin up or spin down, (in the case of a binary alloy atom A or atom B). Each spin interacts with its nearest neighbors on the lattice through an exchange interaction which favors any given pair of spins pointing in the same direction. In the case of a binary alloy, the internal energy of the crystal can be written as

$$E = N_{AA}\mathcal{E}_{AA} + N_{BB}\mathcal{E}_{BB} + N_{AB}\mathcal{E}_{AB}$$

where \mathcal{E}_{AA} , \mathcal{E}_{BB} and \mathcal{E}_{AB} are the interaction energies of nearest neighbor AA, BB, and AB atom pairs, and N_{AA} , N_{BB} and N_{AB} are the numbers of such pairs.

Studying this study, we investigated order-disorder in a binary alloy lattice by different or identical mole fractions. We considered a two-dimensional binary alloy which is consisted of two interacting particles as A and B. First, the lattice was considered to have an exact combinatorial factor. Then, by considering the precise amount of the internal energy of the system as well as its limitations, using the uncertain Lagrange coefficient, we minimized the Helmholtz free energy and calculated thermodynamic properties of the system such as the heat capacity, entropy and internal energy.

THE MODEL

Consider a two-dimensional binary lattice with chemical formula $A_\theta B_{1-\theta}$, where θ and $1-\theta$ are mole fractions of A and B, respectively ($0 < \theta \leq 1/2$). Suppose this lattice contains $N(N \rightarrow \infty)$ sites, which are arranged in L columns and R rows

($RL = N$) and each of them can be occupied only by one of the two particles A or B. Obviously, the number of sites, which are occupied by A or B, are $N_A = N\theta$ and $N_B = N(1-\theta)$, respectively. The particles interact with each other. However, for the sake of simplicity, we consider the nearest neighbor interactions only, which depend on the type of the pair.

While each site can choose one of the two configurations (A or B), each column must have one of the possible 2^R configurations (for example, with $R = 2$, for each column, there are four configurations as: $\begin{smallmatrix} A \\ A \end{smallmatrix}$, $\begin{smallmatrix} A \\ B \end{smallmatrix}$, $\begin{smallmatrix} B \\ A \end{smallmatrix}$ and $\begin{smallmatrix} B \\ B \end{smallmatrix}$). The state or configuration of the columns and their number may be assigned as A_{rm} and N_{rm} , respectively, where r is the number of B particles in such configurations. It must be said that, for each r ($r = 0, 1, \dots, R$), there are $R!/(R-r)!r!$ configurations which may have different energies; thus, for each r , $m = 1, 2, \dots, R!/(R-r)!r!$. For each value of R ($2 < R \ll N$), to avoid the end effects, we include the periodic boundary conditions, that is, we assume that the first and end sites of each column, such as first and end columns, are the nearest neighbors.

Because of

$$L = \sum_{r=0}^R \sum_{m=1}^{Z(r)} N_{rm} \tag{1}$$

we can impose the following conditions

$$N_A = \sum_{r=0}^R \sum_{m=1}^{Z(r)} (R-r)N_{rm} \tag{2}$$

and

$$N_B = \sum_{r=0}^R \sum_{m=1}^{Z(r)} rN_{rm} \tag{3}$$

where

$$Z(r) \equiv \frac{R!}{r!(R-r)!}$$

After definition $N_{rm} \equiv LP_{rm}$, Eqs. (2) and (3) can be written as

$$R\theta = \sum_{r=0}^R \sum_{m=1}^{Z(r)} (R-r)P_{rm} \tag{4}$$

$$R(1-\theta) = \sum_{r=0}^R \sum_{m=1}^{Z(r)} r P_{rm} \quad (5)$$

Also, if we define $N_{rm}^{sn} \equiv L P_{rm}^{sn}$ as the number of the nearest neighbor columns with A_{rm} , and A_{sn} configurations, then, the following constraints must be considered:

$$\sum_{s=0}^R \sum_{n=1}^{Z(s)} N_{rm}^{sn} = N_{rm}, \quad \begin{cases} r=0, 1, \dots, R \\ m=1, 2, \dots, Z(r) \end{cases}$$

or

$$\sum_{s=0}^R \sum_{n=1}^{Z(s)} P_{rm}^{sn} = P_{rm}, \quad \begin{cases} r=0, 1, \dots, R \\ m=1, 2, \dots, Z(r) \end{cases} \quad (6)$$

The nearest neighbor interaction energies can be considered as ε_{AA} , ε_{BB} and $\varepsilon_{AB} (= \varepsilon_{BA})$, where ε_{ij} s are the interaction energies between the nearest neighbor pair of ij . For simplicity, if we assume that, $-\varepsilon_{AA} = -\varepsilon_{BB} = \varepsilon_{AB} = J$, then the total interaction energy of the lattice can be written as

$$E_j = -NJ \left(\sum_{r=0}^R \sum_{m=1}^{Z(r)} P_{rm} \varepsilon_{rm} + \sum_{r=0}^R \sum_{s=0}^R \sum_{m=1}^{Z(r)} \sum_{n=1}^{Z(s)} P_{rm}^{sn} \varepsilon_{rm}^{sn} \right) \quad (7)$$

where $-J\varepsilon_{rm}$ and $-J\varepsilon_{rm}^{sn}$ are energies within the columns and between the nearest neighbor columns, respectively. The coefficients ε_{rm} and ε_{rm}^{sn} have discrete values and each of them changes from $-R$ to $+R$.

The combinatorial factor for this lattice can be written as [13,14]

$$\Omega = \prod_{r=0}^R \prod_{m=1}^{Z(r)} \frac{(NP_{rm})!}{\prod_{s=0}^R \prod_{n=1}^{Z(s)} (NP_{rm}^{sn})!} \quad (8)$$

Using the Stirling approximation, we find the Helmholtz free energy, $A = E - kT \ln \Omega$, as

$$A = N \left(\sum_{r=0}^R \sum_{m=1}^{Z(r)} P_{rm} (-J\varepsilon_{rm} + kT \ln P_{rm}) + \sum_{r=0}^R \sum_{s=0}^R \sum_{m=1}^{Z(r)} \sum_{n=1}^{Z(s)} P_{rm}^{sn} (-J\varepsilon_{rm}^{sn} + kT \ln P_{rm}^{sn}) \right) \quad (9)$$

or in the reduced form

$$\frac{A}{NkT} = \sum_{r=0}^R \sum_{m=1}^{Z(r)} P_{rm} (-j\varepsilon_{rm} + \ln P_{rm}) + \sum_{r=0}^R \sum_{s=0}^R \sum_{m=1}^{Z(r)} \sum_{n=1}^{Z(s)} P_{rm}^{sn} (-j\varepsilon_{rm}^{sn} + \ln P_{rm}^{sn}), \quad (10)$$

where $j = J/kT$.

To obtain the equilibrium state, Eq. (10) must be maximized. For this task, regarding as our constraints, we use the Lagrange multipliers method. After maximization, we have

$$\Phi = \frac{A}{NkT} - \alpha \sum_{r=0}^R \sum_{m=1}^{Z(r)} (R-r) P_{rm} - \beta \sum_{r=0}^R \sum_{m=1}^{Z(r)} r P_{rm} - \sum_{r=0}^R \sum_{m=1}^{Z(r)} \alpha_{rm} \left[\sum_{s=0}^R \sum_{n=1}^{Z(s)} P_{rm}^{sn} - P_{rm} \right] \quad (11)$$

where α , β and α_{rm} s are the Lagrange multipliers. Because $\varepsilon_{rm}^{sn} = \varepsilon_{rm}^{sm}$, we can use the equal *a priori* probabilities principle [15] and put

$$P_{rm}^{sn} = P_{rm}^{sm} \quad (12)$$

With definition of

$$Y \equiv \frac{P_{01}}{P_{01}^2}, \quad y \equiv \left(Y \frac{P_{R1}^{R1}}{P_{R1}} \right)^{\frac{1}{R}}, \quad q = e^{2Rj} y^{R(\theta-1)} Y$$

from maximization of Φ , we conclude the following expressions

$$A = -NkT \ln q^{1/R} \quad (14)$$

$$P_{rm}^{sn} = \sqrt{P_{sn}^{sn}} \sqrt{P_{rm}^{sm}} \exp(j\varepsilon_{rm}^{sn} - jR), \quad (15)$$

$$P_{sn} = Y P_{sn}^{sn} y^{-s} \exp(jR - j\varepsilon_{sn}), \quad (16)$$

$$\sum_{s=0}^R \sum_{n=1}^{Z(s)} \sqrt{P_{sn}^{sn}} \{ \exp[(\varepsilon_{rm}^{sn} + \varepsilon_{rm} - 2R)j] - y^{-s} Y \delta_{rm,sn} \} = 0, \quad \begin{cases} r=0, 1, \dots, R \\ m=1, 2, \dots, Z(r) \end{cases} \quad (17)$$

$$Y \sum_{s=0}^R \sum_{n=1}^{Z(s)} P_{sn}^{sn} y^{-s} \exp(jR - j\varepsilon_{sn}) = R(1-\theta) \quad (18)$$

$$Y \sum_{s=0}^R \sum_{n=1}^{Z(s)} P_{sn}^{sn} y^{-s} \exp(jR - j\varepsilon_{sn}) = 1 \quad (19)$$

where $\delta_{r,m,sn}$ is Kronecker delta.

Know, from solution nonlinear Eqs. (18) to (19), the exact roots of Y and y can be determined and using them, the thermodynamic properties of lattice such as the Helmholtz free energy, internal energy, entropy and heat capacity can be calculated. In the next section, these calculations will be accomplished for simple models.

USE OF COMBINATORIAL FACTOR METHOD FOR SIMPLE MODELS

We start with the simplest model which $R=1$ (the one-dimensional model). When $R=1$ ($r=0, 1$), the coefficients of the interaction energies within and between the columns are $\epsilon_{01} = \epsilon_{11} = 0$, $\epsilon_{01}^{01} = \epsilon_{11}^{11} = 1$ and $\epsilon_{01}^{11} = \epsilon_{11}^{01} = -1$. From Eqs. (17) to (19), we have

$$\sqrt{P_{01}^{01}}(e^{-j} - Y) + \sqrt{P_{11}^{11}}e^{-3j} = 0 \tag{20}$$

$$\sqrt{P_{01}^{01}}e^{-3j} + \sqrt{P_{11}^{11}}(e^{-j} - Y/y) = 0 \tag{21}$$

$$P_{11}^{11} \frac{Y}{y} e^j = 1 - \theta, \tag{22}$$

$$\left(P_{11}^{11} + \frac{P_{11}^{11}}{y} \right) Y e^j = 1, \tag{23}$$

From Eqs. (20) to (23) we can show that

$$y = \frac{\theta}{1-\theta} (Ye^j - 1)^2 e^{4j}, \tag{24}$$

$$Y = \frac{e^{-3j}}{2\theta} \left[2\theta(e^{2j} - e^{-2j}) + e^{-2j} + e^j \sqrt{4\theta(e^{2j} - e^{-2j})(1-\theta) + e^{-2j}} \right], \tag{25}$$

which using them, the Helmholtz free energy Eq. (14), can calculate. For example for $\theta = 1/2$ (the one-dimensional Ising model in the absence of magnetic field), the exact free energy [13] can be obtained as,

$$A = NkT \ln(2 \cosh j). \tag{26}$$

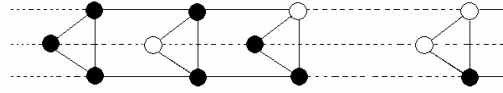


Fig. 1. The two dimensional alloy model using boundary condition.

In addition, Eqs. (25), (26) and Eq. (14), can use to consideration of the one-dimensional spin glasses too (θ is very small).

In the next simplest two-dimensional model we set $R=3$ ($r=0, 1, 2, 3$). Using the periodic boundary conditions, this model is shown in Fig 1. Refereeing to Table 1, Eqs. (17) to (19) and after simplification ($x_{11} = x_{12} = x_{13}$, $x_{21} = x_{22} = x_{23}$), we will find,

$$x_{01}(1-Y) + x_{11}3b + x_{21}3b^2 + x_{31}b^3 = 0 \tag{27}$$

$$x_{01}b^3 + x_{11}(2b^4 + b^2 - y^{-1}Y) + x_{21}(2b^3 + b^5) + x_{31}b^3 = 0 \tag{28}$$

$$x_{01}b^4 + x_{11}(2b^3 + b^5) + x_{21}(2b^4 + b^2 - y^{-2}Y) + x_{31}b^3 = 0 \tag{29}$$

$$x_{01}b^3 + x_{11}3b^2 + x_{21}3b + x_{31}(1 - y^{-3}Y) = 0 \tag{30}$$

$$Y \left(3 \frac{P_{11}^{11}}{yb^2} + 6 \frac{P_{21}^{21}}{y^2b^2} + 3 \frac{P_{31}^{31}}{y^3} \right) = 1 - \theta \tag{31}$$

$$3Y \left(P_{01}^{01} + 3 \frac{P_{11}^{11}}{yb^2} + 3 \frac{P_{21}^{21}}{y^2b^2} + \frac{P_{31}^{31}}{y^3} \right) = 1 \tag{32}$$

where $x_{sn} = \sqrt{P_{sn}^{sn}}$ and $b = e^{-2j}$. Using Eqs. (28) to (32) the partition function for the model with $R=3$, can be obtained numerically.

Finally, the same approach as the above can be used to calculate the partition function for the model with $R > 3$. When R increases, the solution of the nonlinear equations becomes more complicated, so much so that we were only able to solve it for $R(\theta=0.5) \leq 15$ and $R(\theta=0.6, 0.7, 0.8 \text{ and } 0.9) \leq 10$ by numerical methods. The results of such calculations are given in Figs. 2 to 8, for the reduced free energy, internal energy, heat capacity, and entropy.

Table 1. The Total Energies and Coefficients \mathcal{E}_{rm} within each Row for $R=3$. The Solid and Nonsolid Circles Represent A-Type and B-Type, Respectively

r	0	1			2			3
m	1	1	2	3	1	2	3	1
Configuration	● ● ●	● ● ● ○ ● ●	○ ● ● ● ● ●	● ● ● ● ● ○	○ ● ● ○ ● ●	● ● ● ○ ● ●	○ ● ● ● ● ●	○ ● ● ○ ● ●
A_{rm}	A_{01}	A_{11}	A_{12}	A_{13}	A_{21}	A_{22}	A_{23}	A_{31}
\mathcal{E}_{rm}	3	-1			-1			3
Total energy	$-3J$	J			J			$-3J$

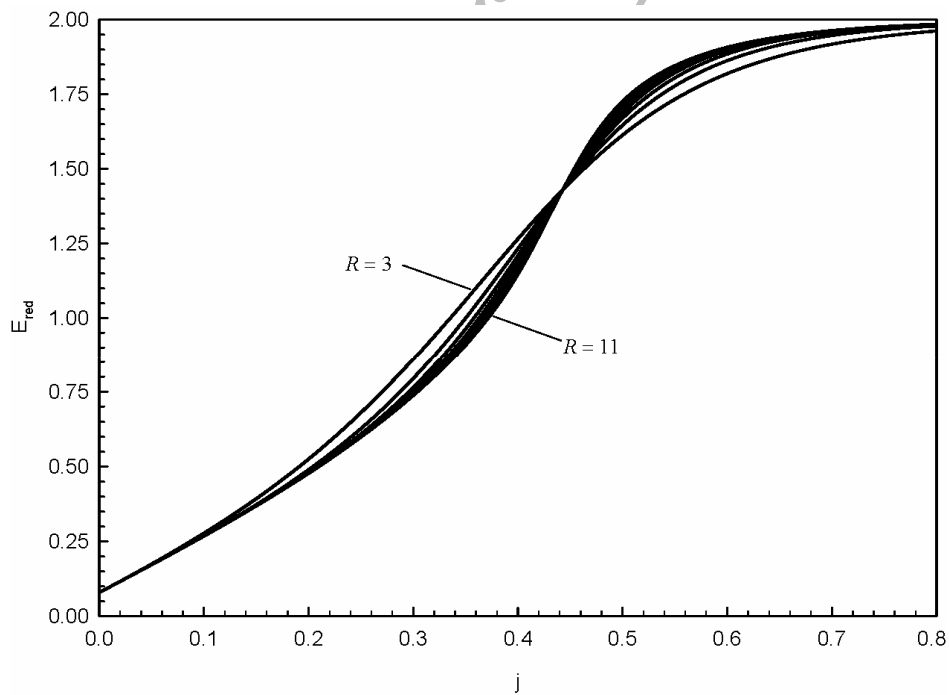


Fig. 2. The reduced internal energy, E_{red} ($-E/NJ$) vs. j for $\theta=0.6$ and $R=3$ to 11.

CONCLUSIONS

In this work, we have used a two-dimensional lattice model with L columns ($L \rightarrow \infty$), and limited number of rows, R , in which the coordination number for each particle was four. We have shown how one can solve the combinatorial

factor for the models with different rows, R . However, due to soft- and hardware limitations, we could only calculate it for $3 \leq R \leq 10$. The results are shown in Figs. 2 to 8. In these figures, there are some interesting points to be made:

1. In Figs. 2 to 7, the behavior of models with the same θ and different rows is similar.

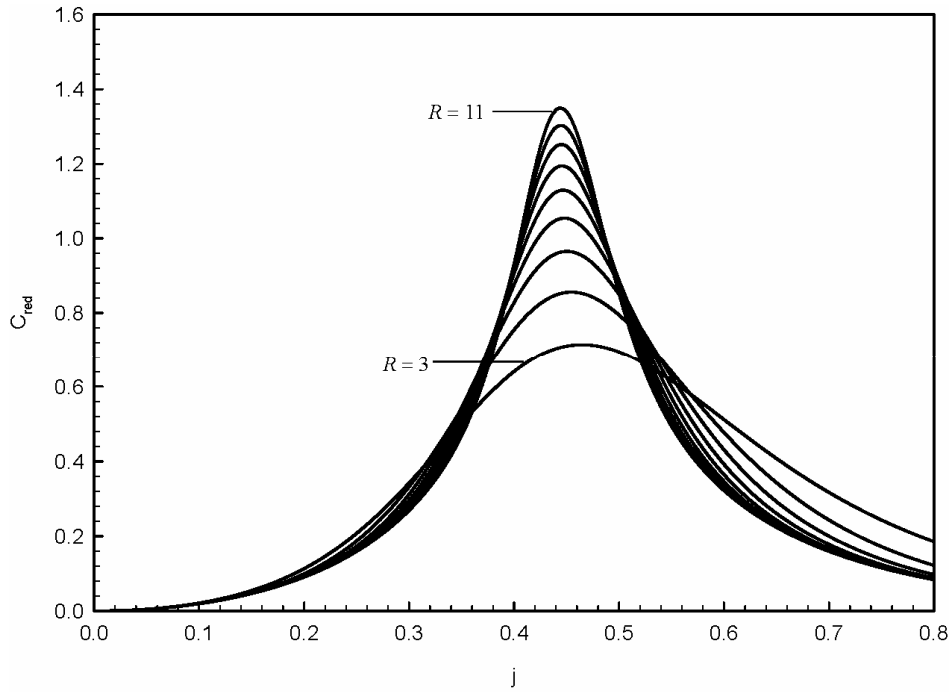


Fig. 3. The same as Fig. 2, for the reduced heat capacity $C_{\text{red}} (C / Nk)$.

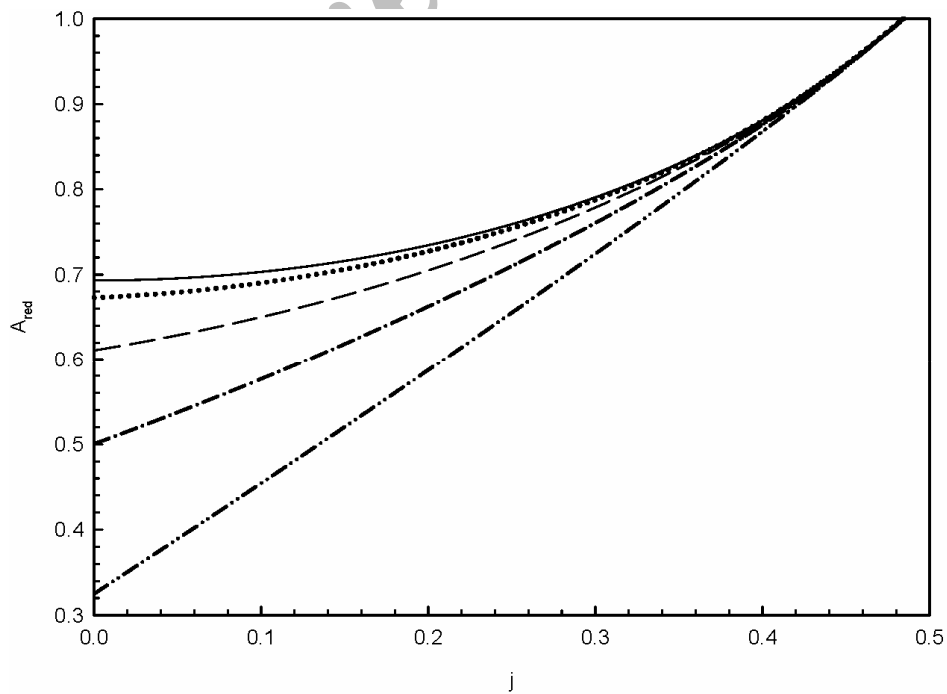


Fig. 4. The reduced Helmholtz free energy, $A_{\text{red}} (-A / NkT)$, vs. j , for the $\theta = 0.5$ (solid line), $\theta = 0.6$ (dot line), $\theta = 0.7$ (dash line), $\theta = 0.8$ (dash-dot line), $\theta = 0.9$ (dash-dot-dot line), and $R = 9$ and 10 .

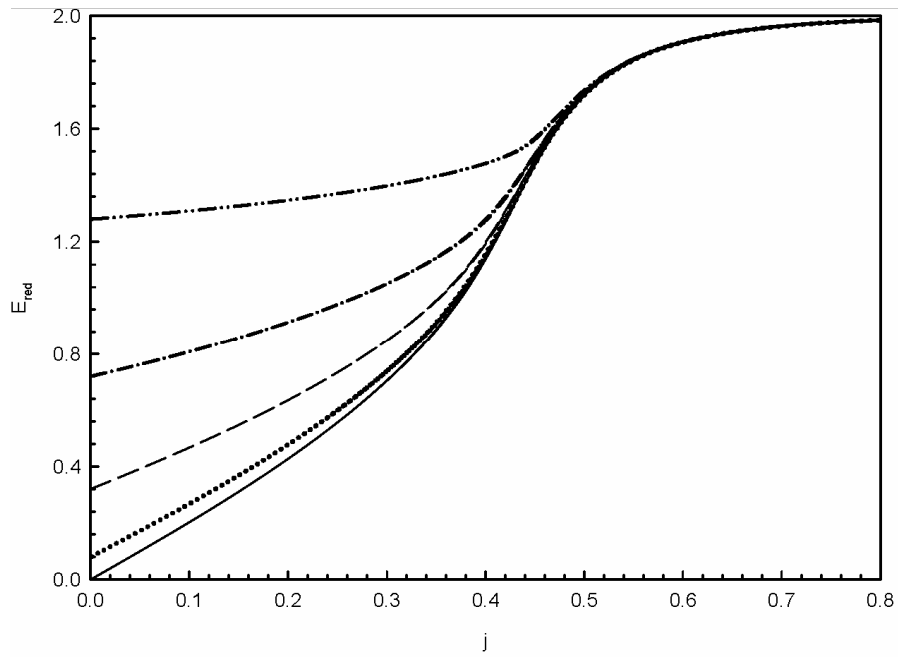


Fig. 5. The same as Fig. 4, for the reduced internal energy.

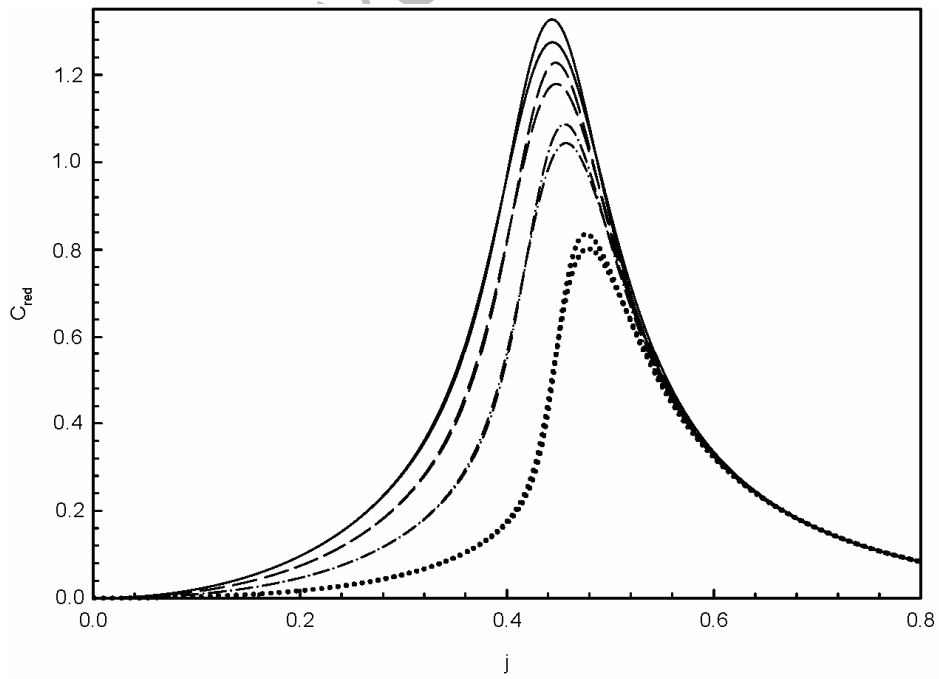


Fig. 6. The same as Fig. 4, for the reduced heat capacity.

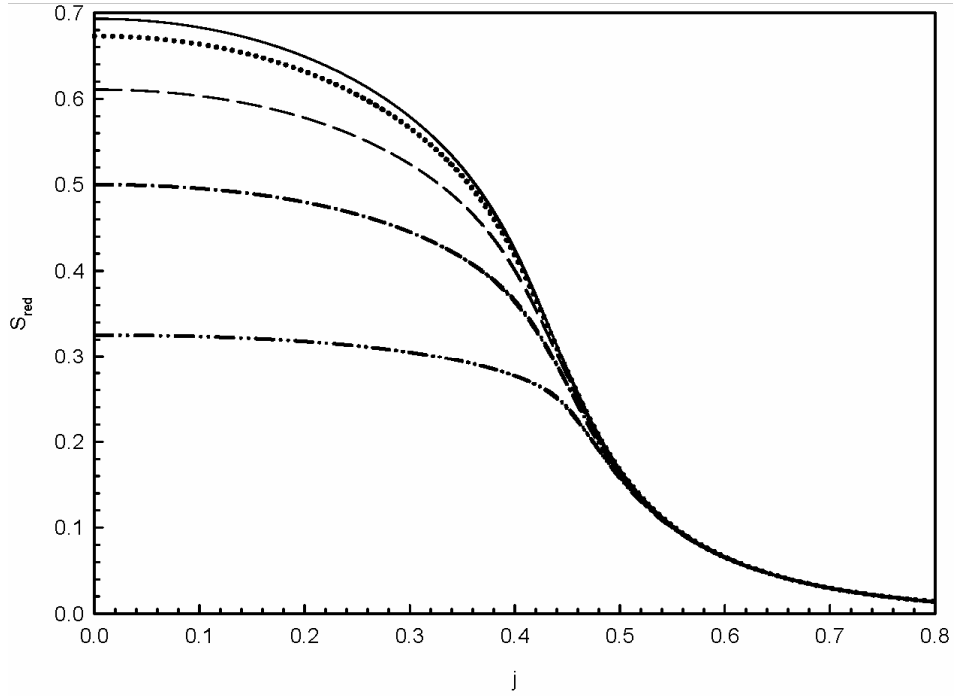


Fig. 7. The same as Fig. 4, for the reduced entropy S_{red} (S / Nk).

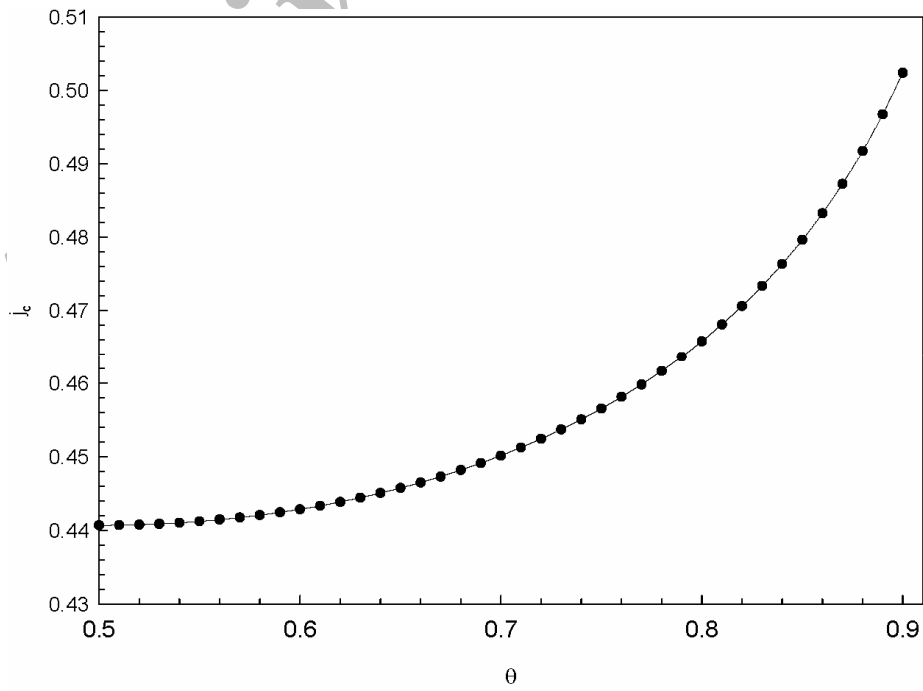


Fig. 8. The inverse of critical temperature *vs.* θ .

2. In Figs. 2 and 5, we see that for each θ , all the internal energy curves pass through specific temperature. This can be considered as a critical point [14]. Thus, the phase transition can be predicted by our method.

3. In Figs. 3 and 6, we see that, around specific j (critical temperature), the heat capacities have maximum values, and when R goes to infinity (actual model), they can also go to infinity (in fact, in this condition, the Onsager phase transition can occur [16]). However, our model can only show diffuse phase transition.

4. For each θ , using the internal energy curves (such as Figs. 2 or 5), we can assign critical temperatures and using them, we can plot the inverse of critical temperature versus θ (see Fig. 8). In these figures, we can see that when θ increases, the critical temperature, T_c , decreases and goes to zero when $\theta \rightarrow 1$.

Finally, it is obvious that the approach suggested in this work can be used for a three-dimensional lattice. However, it must be added that, for these conditions, the calculation of combinatorial factor is a difficult task at present which could be taken up in future.

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