A New Exact Method for Solving the Two-Dimensional Ising Model

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Received: January 19, 1999; In Final Form: April 28, 1999

We have used the two-dimensional Ising model with a limited number of rows, but with the coordination number of four for each site, to set up the transfer matrix for the model. From the solution of such a matrix, the exact thermodynamic properties have been obtained for the model with a definite number of rows, n. We have solved the matrix for $n \leq 7$ and $n \leq 10$ in the presence and absence of a magnetic field, respectively. On the basis of such solutions, we have proposed an analytical expression for the partition function of the model with any number of rows in the absence of a magnetic field. The proposed expression becomes more accurate when n is larger, in such a way that it becomes very accurate for $n \geq 8$ and is exact for $n \to \infty$. Our results show that the singularity of the specific heat occurs only for the model with infinite number of rows. In the presence of a magnetic field, the solution to the matrixes is too complicated to propose a general analytical expression for the partition function of the model with any number of rows. However, our exact solution for the model with $n = 4$, 5, 6, and 7 reveals an important point that such results are independent of n when the field−spin interaction energy is almost equal to or larger than that of the spin−spin interaction.

Introduction

The equilibrium statistical physics of systems of noninteracting particles or elements with negligible interactions is not essentially a complicated subject, and the treatment of these systems can be reduced essentially to that of a single element. The harmonically vibrating lattices have strong interactions among particles, but they are ideal systems in view of normal modes or phonons. In contrast to these ideal systems, systems that are by no means reducible to ideal systems exist and thus have strong interactions among constituent elements, which can never be ignored. The equilibrium statistical physics of interacting systems presents a vast sea of unsolved problems, based not only in physics and chemistry, but also very much in microbiology, macrobiology, ecology, sociology, economics, and many-people problems in general.

Systems of interacting particles can exhibit correlations, so-called cooperative phenomena, and phase transitions such as condensation, crystallization, spontaneous magnetization (a paramagnetic substance becomes ferromagnetic by cooling below the Curie temperature), order−disorder transition, and ferroelectricity. The Ising model can be adapted to all of these contexts and solved exactly in one and two dimensions as well as approximately in any number of dimensions.

There are several good histories of the Ising model, from the original suggestion by Wilhelm Lenz, based on a paper he published in 1920, to his doctoral student Ernst Ising, who published his eponymic paper in 1925, and on the exact solution in two-dimensional, first by Onsager in 1942, and later by others with easier methods (Brush,[1,2] Domb,[3] Hurst and Green,[4] and McCoy and Wu[5]). Some of the more notable achievements should be mentioned. The mathematician Balthus van der Waerden[6] showed in 1941 that the binary alloy problem of the Bragg−Williams type[7] could be solved exactly, in three dimensions, by counting closed diagrams on a lattice. At about the same time, H. A. Kramers and Wannier[8] located the transition temperature for the two-dimensional Ising lattice and showed that the partition function corresponded to the largest eigenvalue of a characteristic matrix (their method was extended and generalized by others: Ashkin and Lamb,[9] Potts[10]). Lars Onsager's 1942 exact solution of the two-dimensional Ising problem, first published in 1944, was so complicated that few people at the time understood it.[11] His student, Bruria Kaufman,[12,13] improved, extended, and clarified the calculations by use of spinor notation, but they still remained abstruse.

Nowadays, the Ising model has very wide applications in different scientific areas, for example, in adsorption isotherms,[14] phase diagrams for the phase separation transition in ternary system,[15] neural networks,[16−18] molecular biology,[19,20] and even in sociology.[21]

To understand the phenomena associated with the sudden changes in the material properties, which take place during a phase transition, it has proven most useful to work with simplified models that single out the essential aspects of the problem. The Ising model is one of such models.[22] A specific transition, which has been investigated by the Ising model, is spin glass transition. The first example of such transition was found in a dilute alloy system such as $Au_{1-x}Fe_x$ with x very small.[23] Experimentally, one sees a rather sharp maximum in the zero field susceptibility, a broad maximum in the specific heat, and an absence of any long-range order below this spin glass transition temperature, although there is both hysteresis and remanence. Many other materials have since been identified as having a transition of the spin glass type.[24−27]

The techniques, which have been developed in scope and power during the past two decades, are the simulation methods,[27−29] especially the Monte Carlo simulation. In such method, model systems containing a relatively small number of interacting spins (perhaps 1000) are activated kinetically and the equilibrium, or nonequilibrium, property of interest is estimated for the system. By varying the size of the system and

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10.1021/jp9902203 CCC: $18.00
Published on Web 08/12/1999

extrapolating, it is possible to estimate bulk properties. Binder gives a general introduction to the use of Monte Carlo methods for spin systems in a review article;[30] more recent developments are described.[31-34]

Analytic solutions of the Ising model in three dimensions, and for the model in two dimensions in an external magnetic field, B, have remained beyond the abilities of everyone who has tried. Here our goal is to introduce a new approach for solving the two-dimensional square lattice of the Ising model, from which the thermodynamic properties of the model can be obtained analytically.

The Ising Problem

We assume that each lattice point in a crystal has an atom with a spin. Let the spin in the jth lattice point be s_j; then the Hamiltonian of this spin system in a magnetic field B applied in the z-direction is[35]

$$H = -2\sum_{\langle ij\rangle} J_{ij}\mathbf{s}_i\cdot\mathbf{s}_j - g\mu_B B\sum_i s_i^z \qquad (1)$$

where $\sum$ stands for the sum over the pairs of spins. The quantities s^z, g, and μ_B are the z-components of the spin operator s, Lande's factor, and the Bohr magneton, respectively. J_{ij} is the exchange integral, which depends on the distance between the ith and jth spins and can be assumed zero for pairs other than the nearest ones. $J_{ij} > 0$ for ferromagnetic and $J_{ij} < 0$ for antiferromagnetic interactions. The scalar product $\mathbf{s}_i\cdot\mathbf{s}_j$ expressed in terms of their components as

$$\mathbf{s}_i\cdot\mathbf{s}_j = s_i^x s_j^x + s_i^y s_j^y + s_i^z s_j^z \qquad (2)$$

If the magnitude of s equals $^1/_2$, the components are expressed by Pauli matrices as

$$\left.\begin{aligned} s_j^x &= {}^1/_2(\sigma_x)_j = {}^1/_2\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}_j \\ s_j^y &= {}^1/_2(\sigma_y)_j = {}^1/_2\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}_j \\ s_j^z &= {}^1/_2(\sigma_z)_j = 1/2\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}_j \end{aligned}\right\} \qquad (3)$$

This interaction is isotropic with respect to the x,y,z-components of different spins. This is called the Hisenberg model. When the x- and y-components of the interactions are negligible, the Hamiltonian reduces to

$$H = -2\sum_{\langle ij\rangle} J_{ij}s_i^z s_j^z - g\mu_B B\sum_i s_i^z \qquad (4)$$

In this case, s_i^z takes $^1/_2$ or $-^1/_2$ and quantum mechanical effect of the commutation properties of the spin operators have no longer to be taken into consideration. This model is called the Ising model. On the other hand, when z-components can be ignored and x- and y-components have anisotropic contributions to the Hamiltonian, then we have

$$H = -2\sum_{\langle ij\rangle} J_{ij}[(1 + \eta_{ij}s_i^x s_j^x) + (1 - \eta_{ij}s_i^y s_j^y)] - g\mu_B B\sum_i s_i^z \qquad (5)$$

Here η_{ij} is a constant which depends on the distance between the ith and jth spins. This is called the XY model.

No real system has been found which can be approximately represented by an XY model, in contrast to the Ising model, which can be applied to real system having a strong anisotropy in one direction.

Solving the Ising Model for a Linear Chain

A general Ising lattice is a regular array of elements, each of which can interact with other elements of the lattice and also with an external magnetic field, such that the nonkinetic part of the Hamiltonian given by eq 4 can be written as

$$H = -{}^1/_2\sum_{i,j=1}^{N*}\frac{J_{ij}}{2}\sigma_i\sigma_j - cB\sum_{i=1}^{N}\sigma_i \qquad (6)$$

where the cB term represents a magnetic dipole energy in the applied field B, $J_{ij}/2 = J$ if points i and j are the nearest neighbors and zero otherwise, σ_i are spin variables, to which two values of ± 1 can be assigned, the $*$ on the first summation means that terms with $i = j$ are not allowed, and the $^1/_2$ factor is to avoid the overcounting of ij pair.

Since the kinetic and nonkinetic parts of the partition function are separated, and since the interesting behavior is exhibited entirely by the nonkinetic factor, the kinetic factor will not be carried along in the development to follow, and the term *partition function* will be understood to mean the nonkinetic term.

The partition function may be written as

$$Z_N = \sum_{\sigma_1=\pm 1}\sum_{\sigma_2=\pm 1}\cdots\sum_{\sigma_N=\pm 1}\exp[j\sum\sigma_i\sigma_j + b\sum_{i=1}^{N}\sigma_i] \qquad (7)$$

where $j = J/kT$ and $b = cB/kT$. For simplicity, the sums in eq 7 will be denoted as $\sum_{\{\sigma_i=\pm 1\}}$, which is taken over the set of σ_i's, each of which can be ± 1 independently.

The simple Ising problem in one dimension can be solved by several ways. Let us first consider a chain of length N with free ends and in the zero external field. Then for such a model, the Hamiltonian and partition function are given by[36]

$$H = -J\sum_{i=1}^{N-1}\sigma_i\sigma_{i+1} \qquad (8)$$

$$Z_N = 2(2\cosh j)^{N-1} \qquad (9)$$

The free energy in the thermodynamic limit ($N \to \infty$) is then

$$A = -NkT\ln(2\cosh j) \qquad (10)$$

We can also obtain an expression for the free energy in the presence of a magnetic field. To avoid the end effects, we include the periodic boundary conditions, that is, to assume that the Nth spin is connected to the first spin so that the chain forms a ring, in which the elements of i and $N + i$ are the same. Using eq 6, the partition function may be written as

$$Z_N = \sum_{\{\sigma_i\}}\prod_{i=1}^{N}\exp\left[j\sigma_i\sigma_{i+1} + \frac{b}{2}(\sigma_i + \sigma_{i+1})\right] \qquad (11)$$

To solve eq 11 for Z_N, there are a few approaches. We shall give only a brief introduction to the most convenient approach, i.e., the transfer matrix method. It is convenient to introduce a 2×2 *transfer matrix* $\mathbf{M}_1$ as,

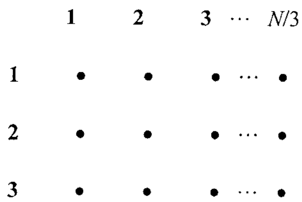

Figure 1. Simplest two-dimensional Ising model with three rows and infinitive columns.

$$\mathbf{M}_1 = \begin{bmatrix} h\sqrt{m} & 1/\sqrt{m} \\ 1/\sqrt{m} & \sqrt{m}/h \end{bmatrix} \qquad (12)$$

where

$$m = e^{2j}, \quad h = e^{b} \qquad (13)$$

Then the partition function in terms of the trace of the transfer matrix, Tr $\mathbf{M}_1^N$, is given as

$$Z_N = \sum_{\{\sigma_i=\pm 1\}} \langle\sigma_1|\mathbf{M}_1|\sigma_2\rangle\langle\sigma_2|\mathbf{M}_1|\sigma_3\rangle...\langle\sigma_N|\mathbf{M}_1|\sigma_1\rangle = \mathrm{Tr}\ \mathbf{M}_1^{\ N} \qquad (14)$$

Since $\mathbf{M}_1$ is a real symmetric matrix, it may be diagonalized by an ortogonal transformation

$$|\mathbf{M}_1 - \lambda\mathbf{I}| = 0 \qquad (15)$$

which preserves its trace. Then Tr $\mathbf{M}_1^N$ can be written as $\sum\lambda_i^N$, and eq 14 becomes

$$Z_N = \lambda_1^N[1 + (\lambda_2/\lambda_1)^N] \cong \lambda_1^N \qquad \text{as } N \to \infty \qquad (16)$$

where λ_1 is the largest eigenvalue. The solution of eq 15 gives

$$\lambda_{\max} = \sqrt{m}\cosh b + \sqrt{m\sinh^2 b + 1/m} \qquad (17)$$

Then the free energy is given by

$$A = -NkT\ln(\sqrt{m}\cosh b + \sqrt{m\sinh^2 b + 1/m}) \qquad (18)$$

Solving the Ising Model for the Square Lattice

Consider a model lattice of N spin ($N \to \infty$) in a plane composed of n rows and n' columns ($N = n \times n'$). Each spin can take either the state +1(a) or −1(b). The mutual spin−spin and spin−external magnetic interactions are the same as those of the one-dimensional model, which was explained before. Furthermore, we assume that the interaction energy of two vertical and horizontal neighboring spins are the same. Our goal is to find the macroscopic properties of the model when n and n' both approach infinity. Since solving such a problem is too complicated, we shall use some simpler models in which the number of rows are finite; then the results of such a simple model will be extended to the case that $n \to \infty$. We start with the simplest model, in which $n = 3$ and $n' = N/3$, as shown in Figure 1. Except for the first and last columns, each spin in the middle row has four neighbors, while those in the first and third rows each have three neighboring spins. Therefore, the coordination number of spins is different and depends on the position of spin. However, in the actual model, in which n and n' are both infinity, the side effects are negligible, and hence all spins are identical; each has four nearest neighbors. In order to eliminate such a difference between the simple model (with $n = 3$) and the actual model (with $n \to \infty$), the former model has to be modified in such a way that each spin has four nearest neighbors. To carry out such a modification, we may treat the spins on the first and third rows of each column as the nearest neighbors. If we denote the interacting nearest neighbor spins by a line connecting two spins to each other, our modified model is that which is shown in Figure 2a. The periodic boundary condition is taken into account by assuming that the states of triangular i and $N/3 + i$ in Figure 2a are the same. Since each spin has two states, a or b, each triangular may have 8 states shown in Table 1.

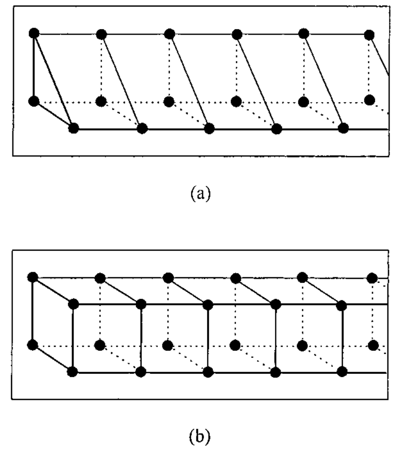

Figure 2. Modified two-dimensional lattice model with (a) three rows and (b) four rows. Each line connecting two spins shows the interacting nearest neighbor spins.

Now, it is possible to treat our model as the one-dimensional Ising model. However, the following two differences have to be taken into account:

(1) In the one-dimensional model each spin has only two states while each triangular has eight states,

(2) Unlike a spin in the one-dimensional model, each triangular has a configurational energy whose value is given in Table 1.

By referring to Table 1, the partition function of our model with $N/3$ triangulars may be written as

$$Z_{N/3} = \sum_{\{\sigma_i=\mathrm{A_1 to A_8}\}} \prod_{i=1}^{N/3} \exp\left[j\sigma_i\sigma_{i+1} + \frac{b}{2}(\sigma_i + \sigma_{i+1})\right]$$
$$= \sum_{\{\sigma_i\}} \langle\sigma_1|\mathbf{M}_{3b}|\sigma_2\rangle...\langle\sigma_{N/3}|\mathbf{M}_{3b}|\sigma_1\rangle = \mathrm{Tr}\ \mathbf{M}_{3b}^{\ N/3} \qquad (19)$$

while the matrix $\mathbf{M}_{3b}$ is

$$\mathbf{M}_{3b} = \begin{bmatrix} m^3h^3 & mh^2 & mh^2 & mh^2 & h & \mathrm{h} & \mathrm{h} & 1 \\ mh^2 & mh & h/m & h/m & 1 & 1 & 1/m^2 & 1/h \\ mh^2 & h/m & mh & h/m & 1/m^2 & 1 & 1 & 1/h \\ mh^2 & h/m & h/m & mh & 1 & 1/m^2 & 1 & 1/h \\ h & 1 & 1/m^2 & 1 & m/h & 1/mh & 1/mh & m/h^2 \\ h & 1 & 1 & 1/m^2 & 1/mh & m/h & 1/mh & m/h^2 \\ h & 1/m^2 & 1 & 1 & 1/mh & 1/mh & m/h & m/h^2 \\ 1 & 1/h & 1/h & 1/h & m/h^2 & m/h^2 & m/h^2 & m^3/h^2 \end{bmatrix} \qquad (20)$$

Since our aim is to diagonalize the matrix $\mathbf{M}_{3b}$ and to obtain its maximum eigenvalue, we may obtain such a maximum from the following 4×4 matrix

TABLE 1: All Possible Configurations for Each Triangular of Figure 2a along with Its Configurational Energy

group	1	2			3			4
state	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8
configuration	a / a—a	a / b—a	a / a—b	b / a—a	a / b—b	b / b—a	b / a—b	b / b—b
config energy	$-3J - 3cB$		$J - cB$			$J + cB$		$-3J + 3cB$

TABLE 2: Same as Table 1 for a Square

group	1	2	3	4	5	6
configuration	a—a / a—a	a—a / b—a	a—a / b—b	a—b / b—a	a—b / b—b	b—b / b—b
degeneracy	1	4	4	2	4	1
config energy	$-4J - 4cB$	$-2cB$	0	$4J$	$2cB$	$-4J + 4cB$

$$\mathbf{M}_{3a} = \begin{bmatrix} m^3h^3 & mh^2 & h & 1 \\ 3mh^2 & mh + 2h/m & 2 + 1/m^2 & 3/h \\ 3h & 2 + 1/m^2 & m/h + 2/mh & 3m/h^2 \\ 1 & 1/h & m/h^2 & m^3/h^3 \end{bmatrix} \quad (21)$$

In the absence of any magnetic field, the states A_1 and A_8 and also the states A_2 through A_7 given in Table 1 have the same configurational energies. In this case, the maximum eigenvalue of the matrix $\mathbf{M}_{3a}$ can be obtained from diagonalization of the following matrix

$$\mathbf{M}_3 = \begin{bmatrix} 1 + m^3 & 1 + m \\ 3 + 3m & 2 + m + 2/m + 1/m^2 \end{bmatrix} \quad (22)$$

By solving the secular determinant, $|\mathbf{M}_3 - \lambda \mathbf{I}| = 0$, we may obtain the maximum eigenvalue $\lambda_{max} = Z_3^{3/N} = z_3$ as

$$\ln z_3 = \ln 2 \cosh 2j + \frac{1}{3} \ln \frac{1 + 1/m}{1 + 1/m^2} + f_3(p) \quad (23)$$

where

$$f_3(p) = -\ln 2 + \frac{1}{3} \ln(4 - p + \sqrt{(4 + p)(4 - 3p)}) \quad (24)$$

$$p = 2 \tanh 2j/\cosh 2j \quad (25)$$

in which z_3 is the partition function for each spin in the three-row model.

Now, we can add an additional row to the model shown in Figure 1. Again, we face the problem that the number of nearest neighbors of spins in such a four-row model is different, depending on the location of spin. To eliminate such differences, and having a model in which each spin has four nearest neighbors, the model has to be modified. The modified model is shown in Figure 2b, for which each square has 16 states shown in Table 2. For this model, by including the periodic boundary condition, the secular determinant has an order of 16. However, its maximum eigenvalue may be obtained from the following determinant

$$\begin{vmatrix} m^4h^4 - \lambda & m^2h^3 & mh^2 & h^2 & h & 1 \\ 4m^2h^3 & m^2h^2 + 3h^2 - \lambda & 2mh + 2h/m & 2h/m^2 + 2h & 3 + 1/m^2 & 4/h \\ 4mh^2 & 2mh + 2h/m & 2 + m^2 + 1/m^2 - \lambda & 4/m & 2/mh + 2m/h & 4m/h^2 \\ 2h^2 & h + h/m^2 & 2/m & 1 + 1/m^4 - \lambda & 1/m^2h + 1/h & 2/h^2 \\ 4h & 3 + 1/m^2 & 2/mh + 2m/h & 2/m^2h + 2/h & m^2/h^2 + 3/h^2 - \lambda & 4m^2/h^3 \\ 1 & 1/h & m/h^2 & 1/h^2 & m^2/h^3 & m^4/h^4 - \lambda \end{vmatrix} = 0 \quad (26)$$

In the absence of any magnetic field, the maximum eigenvalue, z_4, can be obtained as

$$\ln z_4 = \ln 2 \cosh 2j + f_4(p) \quad (27)$$

where

$$f_4(p) = -{}^5/_4 \ln 2 + {}^1/_4 \ln(8 - p^2 + \alpha + 2^{1/2} \sqrt{\alpha^2 + (8 - p^2)(2p^2 + \alpha)}) \quad (28)$$

$$\alpha = \sqrt{(8 - p^2)^2 - 32p^2}$$

Adding another row to the former model and considering a similar modification, the partition function per each spin, z_5, can be obtained as

$$\ln z_5 = \ln 2 \cosh 2j + \frac{1}{5} \ln \frac{1 + 1/m}{1 + 1/m^2} + f_5(p) \quad (29)$$

where

$$f_5(p) = -{}^6/_5 \ln 2 + {}^1/_5 \ln(\Theta_1 + \Theta_2 + 2^{1/2} \sqrt{\Theta_2^2 + \Theta_1\Theta_2 + 64p^2 - 16p^3 - 6p^4}) \quad (30)$$

$$\Theta_1 = 16 - p^2 - 4p$$

$$\Theta_2 = \sqrt{256 - 128p - 144p^2 + 40p^3 + 5p^4}$$

The same approach can be used to calculate the partition function for the model with $n > 5$. However, for $n = 6$, 7, and 8 the secular determinant in the absence of any magnetic field gives a polynomial with the order of 8, 9, and 18, respectively. Such polynomials cannot be solved analytically. For this reason, we have not been able to obtain a mathematical expression for the partition function. However, the polynomials can be solved numerically to obtain the partition functions and hence the free energies ($-A/NkT = \ln z$). Also, we may use the polynomials to find the first and second derivatives of the partition function, from which the internal energies ($-E/NJ = \partial \ln z/\partial j$) and heat capacities ($C/Nk = j^2\partial^2 \ln z/\partial j^2$) can be obtained.

All calculations were carried out by a personal computer, using well-known software called "maple". Unfortunately, we were not able to solve analytically the secular determinant for $n > 8$, mainly due to a very long computational time. However, the determinant was solved numerically only for $n = 9$ and 10, from which we have calculated the exact free energy. The results of such calculations are given in Figures 3−5 for the reduced free energy, internal energy, and heat capacity, respectively. The

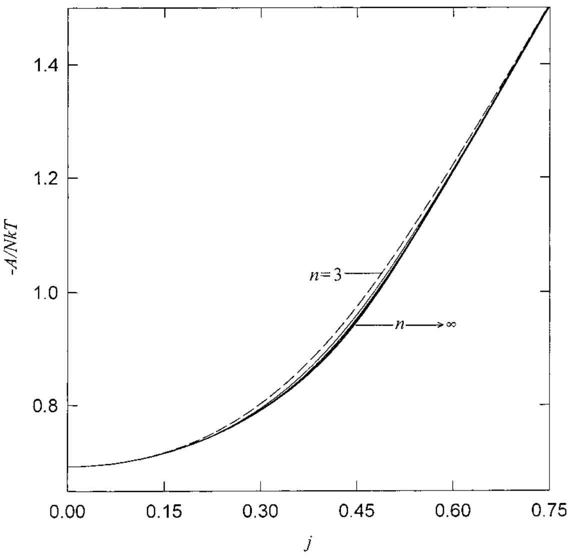

Figure 3. Exact reduced free energy, $-A/NkT$, for the models with $n = 3-10$ compared to that for the square lattice ($n \rightarrow \infty$). The top curve (dashed) is for $n = 3$, the bottom curve is for $n \rightarrow \infty$, and the other curves are for $n = 4-10$ from top to the bottom, respectively.

thermodynamic properties for the square lattice ($n \rightarrow \infty$) are also shown in these figures.

Extension of the Results to the Square Lattice

By increasing one row to our model, the order of the transfer matrix increases by a factor of 2. Therefore, when n increases, the solution of the secular determinant becomes more complicated in such a way that we were able to solve it only for $n \leq 10$. It means that the model cannot be solved for the square lattice ($n \rightarrow \infty$), because of computer restrictions.

However, we may refer to the results of the model for which the analytical expression for the free energy of the model is obtained. The $\ln z_n$ is given in eqs 23, 27, and 29 for $n = 3$, 4, and 5, respectively. These equations have a common term as $\ln(2 \cosh 2j)$, from which we may expect that $\ln z_n$ includes such a term regardless of the value of n. The $\ln z_n$ includes a term as $\ln[(1 + 1/m)/(1 + 1/m^2)]/n$ only for the cases that n is odd, otherwise it is zero. Because of the fact that this term vanishes when $n \rightarrow \infty$, we may ignore such a term. Therefore, we may propose the following expression for the free energy of the model

$$\ln z_n = \ln 2 \cosh 2j + f(n,p) \qquad (31)$$

Note that eq 31 is in accordance with the common intersection point observed in Figure 4 for the internal energy, because of the fact that

$$\frac{\partial f(p)}{\partial j} = \frac{\partial p}{\partial j}\frac{\partial f}{\partial p} = \frac{4}{\cosh 2j}(1 - 2\tanh^2 2j)\frac{\partial f}{\partial p}$$

which is zero at $j_c = J/kT_c = \ln(1 + \sqrt{2})2$, the critical temperature of the square lattice. At such a common point, eq 31 gives $-E/NJ = \sqrt{2}$, which is exactly the same as that shown in Figure 4.

Now, we have to propose a mathematical expression, for $f(n,p)$. Because of the fact that the extra term in $f(3,p)$ and $f(5,p)$ vanishes for the case we are interested in ($n \rightarrow \infty$), we may assume that such a proposition is similar to $f(4,p)$. The expression for f_4 given in eq 28 may be expanded as a power series as

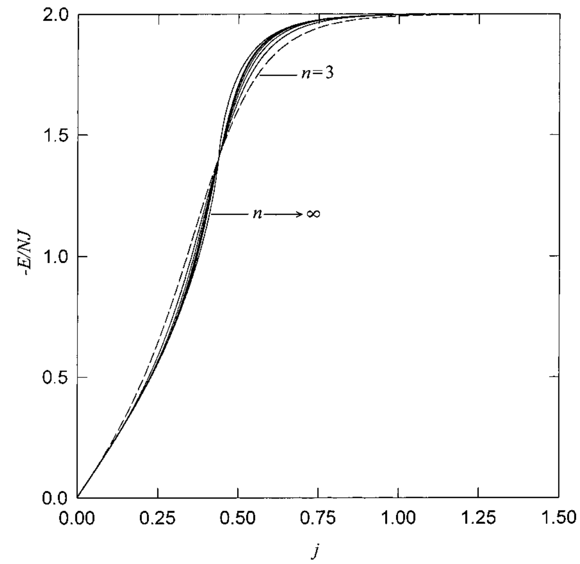

Figure 4. Same as Figure 3, for the reduced internal energy (the results for the model with $n = 9$ and 10 are not included).

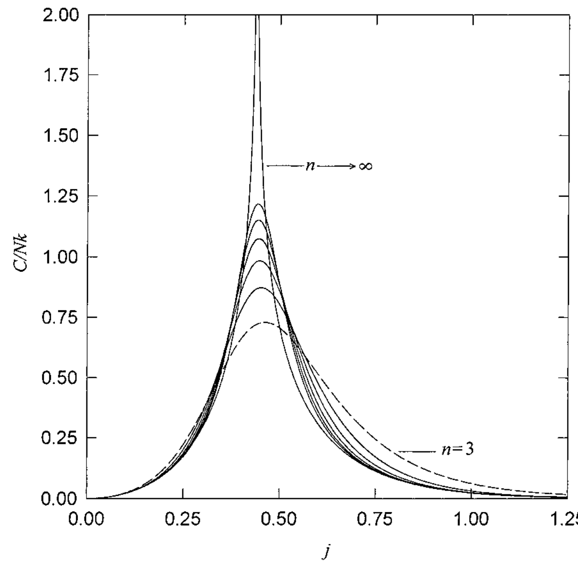

Figure 5. Same as Figure 4, for the reduced heat capacity.

$$f_4 = -0.0625p^2 - 0.0166p^4 - 0.0067p^6 - 0.0032p^8 - 0.0017p^{10} + O(p^{12}) \qquad (32)$$

For the square lattice the exact free energy was obtained from

$$\ln z = \ln 2 \cosh 2j - \frac{1}{\pi}\int_0^{\pi/2} \ln \frac{1 + \sqrt{1 - p^2 \sin^2 \theta}}{2}\, d\theta = \ln 2 \cosh 2j - \frac{1}{4}\sum_{t=1}^{\infty} \frac{1}{t}\left[\frac{(2t)!}{(t!)^2}\right]^2 (p/4)^{2t} \qquad (33)$$

The results given in eqs 31 and 32 are in accordance with eq 33; more specifically, the first term of eq 31 is the same as that of eq 33, and eqs 32 and 33 both have only the even powers of p. From such results, it is possible to propose a polynomial for the free energy of the model and assume that its degree depends on n.

Taking into account such points, along with the exact calculated free energy for the model with $n \leq 10$, we have found that the following expression is appropriate for the partition function

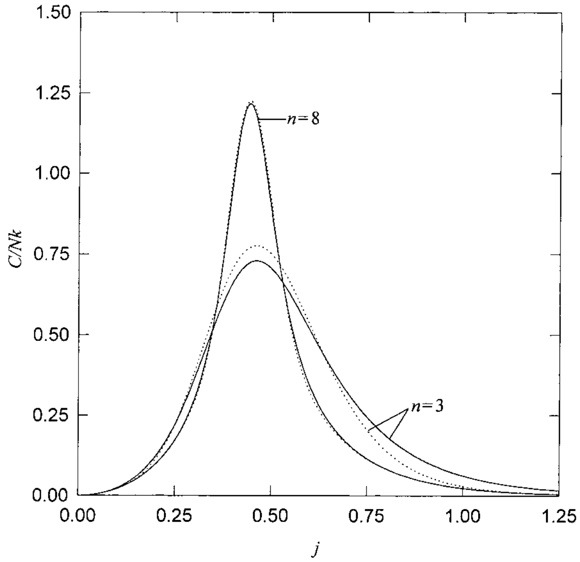

Figure 6. Comparison of the heat capacity calculated from eq 37, dotted curve, with the exact value, solid curve, for the model with $n = 3$ and 8.

$$\ln z_n = \ln 2 \cosh 2j - \frac{1}{4}\sum_{t=1}^{l}\frac{1}{t}\left(\frac{(2t)!}{(t!)^2}\right)^2 (p/4)^{2t} \tag{34}$$

where the upper bound of the summation, l, is given by

$$l = n + \frac{(n-2)(n-3)}{2} \tag{35}$$

Equation 34 can be used to find the internal energy and heat capacity of the model as

$$-\frac{E}{NJ} = 2 \tanh 2j - 2\frac{p'}{p}\sum_{t=1}^{l}\left(\frac{(2t)!}{(t!)^2}\right)^2 (p/4)^{2t} \tag{36}$$

$$\frac{C}{Nk} = 2j^2\left\{2(1-\tanh^2 2j) + \sum_{t=1}^{l}\left(\frac{(2t)!}{(t!)^2}\right)^2 (p/4)^{2t}\left(\frac{p'^2}{p^2}(1-8t) - \frac{p''}{p}\right)\right\} \tag{37}$$

where

$$p' = \frac{4}{\cosh 2j}(1 - 2\tanh^2 2j) \tag{38}$$

$$p'' = \frac{4p}{\cosh^2 2j}(\cosh^2 2j - 6) \tag{39}$$

In order to investigate the accuracy of the proposed free energy given by eq 34, we have compared the heat capacity given by eq 37 with the exact value in Figure 6 for the lowest and highest values of n for which we had calculated the exact specific heat, i.e., $n = 3$ and 8, respectively. As shown in this figure, we may conclude that the heat capacity, and hence the proposed free energy given by eq 34 becomes more accurate when n becomes larger, the case which we are more interested in. In fact, for the square lattice model with $n \to \infty$, the proposed free energy is exact (compare eq 33 with eq 34 for the case that $l \to \infty$).

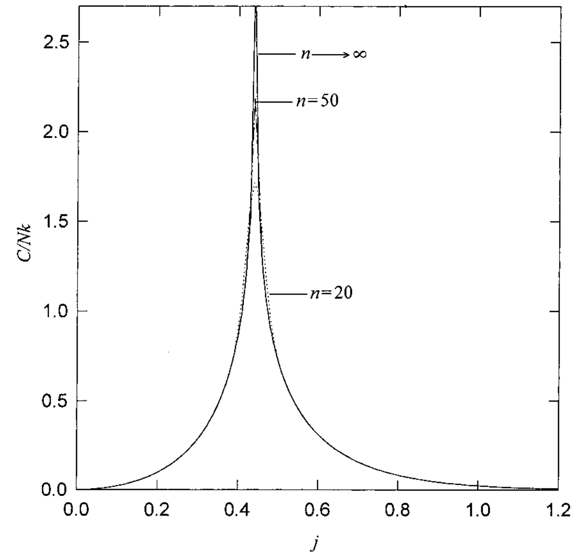

Figure 7. Reduced heat capacity versus the inverse of the reduced temperature, j/kT, calculated from eq 37 for $n = 20$, 50, and ∞ at $B = 0$.

Equation 37 can be used to calculate the heat capacity, the result of which is shown in Figure 7 for $n = 20$, 50, and $n \to \infty$. As shown in this figure, the singularity of heat capacity is observed only for $n \to \infty$ (Onsager transition[37]). Such a conclusion is expected from eq 37, because of the fact that at such point ($j_c = \ln(1 + \sqrt{2})/2$, $p = 1$, $p' = 0$, $p'' = -8$)

$$\frac{C}{Nk} = \left\{{}^1/_2 + 4\sum_{t=1}^{l}\left(\frac{(2t)!}{(t!)^2}\right)^2 (1/4)^{2t}\right\}(\ln(1+\sqrt{2})^2 \tag{40}$$

is infinite only when $l \to \infty$. In other words, for the model with a limited number of rows, we may expect to observe only a diffuse transition[37] or continuous transition.[38]

Solving the Model in Nonzero Magnetic Field

The exact approach given in the previous sections for solving the model in the absence of any external magnetic field can be used to obtain the exact thermodynamic properties of the model in presence of a magnetic field. For example, eqs 21 and 26 can be used to obtain the exact partition function for the models with $n = 3$ and 4, respectively. As explained before for the case that $B = 0$, we can set up a transfer matrix for the model with larger values of n as well. We have set up the matrix for the model with $n = 3$, 4, 5, 6, and 7 and found its maximum eigenvalue. The calculated partition function is used to obtain the thermodynamic properties of the model. For instance, the results for the heat capacities are shown in Figure 8 for a given number of rows of the model at specified magnetic field strengths, $b = cB/kT$. We have also used the exact partition function of the model to calculate the magnetization per spin, I

$$I = \left(\frac{\partial \ln z}{\partial b}\right)_T$$

The results of such calculations are shown in Figure 9 for some given number of rows at specified magnetic field strengths.

Conclusion

In order to solve 2-D Ising model, we have used a two-dimensional model with a limited number of rows, n, in which

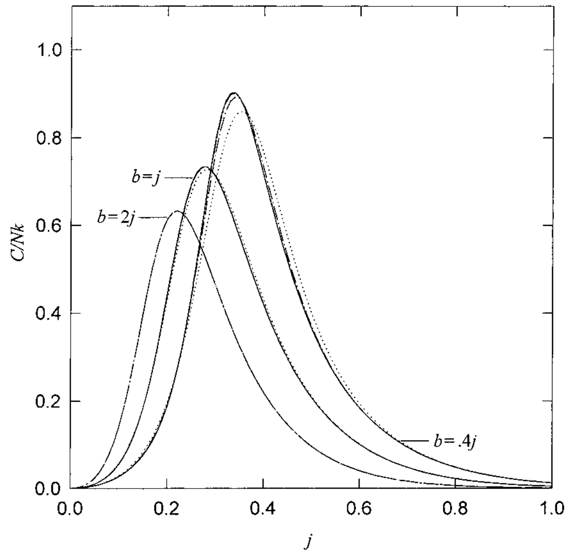

Figure 8. Exact reduced heat capacity versus the inverse of the reduced temperature for given magnetic field for $n = 3$ (···), 4 (- · -), 5 (- ·· -), 6 (—).

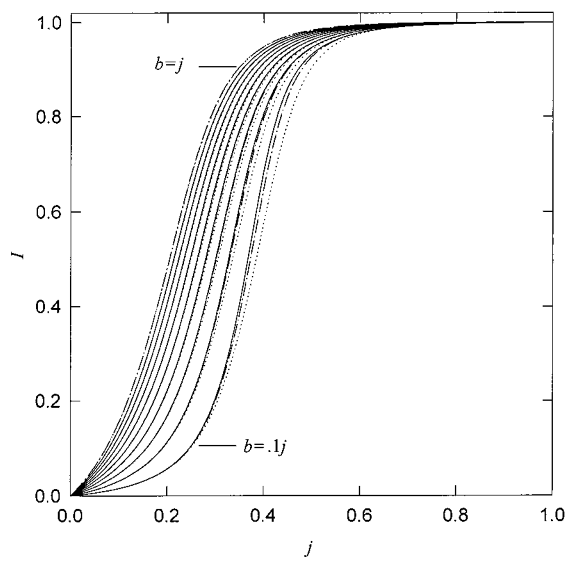

Figure 9. Same as Figure 8, for the magnetization for $n = 4$ (···), 5 (- · -), 6 (—).

the coordination number for each site is equal to four, regardless of the value of *n*. We have shown how one can set up the transfer matrix for the model. The approach introduced in this work can be used to write down the matrix for the model with any number of rows. However, due to soft- and hardware limitations, the matrix can only be solved for the model with a limited number of rows, in our case for $n \leq 7$ and $n \leq 10$ in the presence and absence of an external magnetic field, respectively. Fortunately, the exact analytical expressions for the model with a limited number of rows (given in this work) along with that for the actual 2-D model, given in literature, for $B = 0$ guided us to propose an analytical expression for the partition function of the model with any number of rows, eq 34. As a severe test, the second derivative of the proposed partition function, namely the specific heat capacity, has been compared with the exact value; as an example see Figure 6. The difference in heat capacity becomes smaller when *n* is larger, in such a way that it becomes insignificant for $n \geq 8$ and is exact for $n \rightarrow \infty$. Therefore, we may conclude that eqs 34−36 give very accurate results for the model with $n \geq 8$ and becomes exact for the actual two-dimensional model, the square lattice model, in the absence of any external magnetic field.

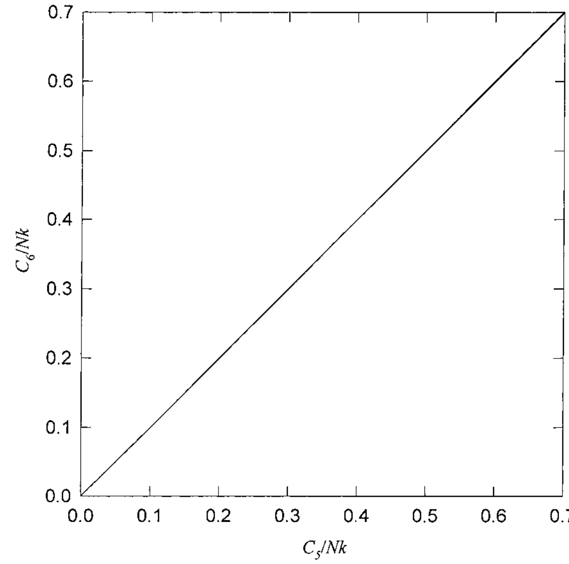

Figure 10. Exact reduced heat capacity for the model with $n = 5$ versus that for $n = 6$ when $b = j$.

According to eq 40, a singular point for the heat capacity is expected to be observed only for the model with an unlimited number of rows ($n \rightarrow \infty$).

We have shown how to set up the transfer matrix in the presence of an external magnetic field; see eqs 21 and 26 for $n = 3$ and 4. Solution to such matrix gives the exact solution for the partition function of the model. Again, the matrix can be written for the model with any number of rows. However, due to the mentioned limitations, it can be solved only for the model with a limited number of rows. In fact, the expression obtained in this case is more complicated than that for the case in which $B = 0$, for any value of *n*. For this reason, unlike the previous case, we have not been able to give a general analytical expression for the partition function when $B \neq 0$. However, the exact heat capacity and magnetization given in Figures 8 and 9 reveal an important conclusion, according to which the calculated results for $n = 3$, 4, 5, and 6 are almost the same when $b \cong j$ or $b > j$. To disclose this point more clearly, we have plotted the exact values of heat capacity for $n = 6$ against that for $n = 5$ in Figure 10 when $b = j$. From such results, we conclude that our exact calculated values for the model with $n = 4$, 5, 6, or 7 are almost the same as those for the actual 2-D model ($n \rightarrow \infty$), when $b \cong j$ or $b > j$. For the case that $B = 0$, the main difference between the thermodynamic properties of the model with different values of *n* appears around the singular point of the heat capacity; see Figure 7. For the case of $B \neq 0$, for which there is no singularity, we may expect that such differences become insignificant, specially for the stronger magnetic fields. This is in accordance with our above conclusion.

Finally, it is obvious that the approach given in this work can even be used for the 3-D Ising model. However, in order to get any significant result, we leave this task for the future, when more sophisticated hard- and software is available.

Acknowledgment. We acknowledge the Isfahan University of Technology for the financial support, and also Dr. B. Najafi for his useful comments.

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