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Square Lattice Variational Approximations Applied to the Ising Model

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The variational method developed by Baxter is applied to the zero-field Ising model on the square lattice. The problem is simplified to that of solving a relatively small system of nonlinear equations. The estimates to the spontaneous magnetization and the critical temperature from the sequence of variational approximations are obtained. The results converge rapidly to the exact ones. They exhibit a crossover phenomenon and satisfy a scaling relation.

KEY WORDS: Ising model; variational approximation; spinor representatives; crossover phenomena; scaling.

1. INTRODUCTION

We report here an investigation on the convergence of a variational method when applied to the zero-field Ising model.

The technique was applied to the monomer–dimer system in 1968 by Baxter[1] and to the zero-field Potts model in 1976 by Kelland.[2] Recently, Baxter extended the method to a fairly general Ising model on the square lattice.[3] A set of matrix equations was obtained and a rapidly convergent sequence of approximations to the free energy was developed. It is the purpose of this work to test the convergence of this approach. We apply the method to the zero-field, square lattice Ising model. With this system, it is possible for us to compare the results of the various approximations with the exact solution of the model.

The sequence of approximations generated by the method is solved numerically for the spontaneous magnetization below the critical point and

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for the critical temperature of the system. The convergence of the results to the exact values and the critical behavior of the spontaneous magnetization are studied. The variational method is found to give good estimates to the thermodynamic properties of the system.

We will give the set of variational equations for the case of the zero-field, square lattice Ising model in Section 2. In Section 3, the technique of spinor representations is used to simplify the matrix equations. The problem is reduced to one of solving a relatively small system of nonlinear equations. The analytic solution of these equations for the infinite system is given in Section 4. For the finite system, the equations are solved numerically for the spontaneous magnetization and the critical temperature, and the results are presented in Section 5. They support a scaling hypothesis for the spontaneous magnetization.

2. VARIATIONAL EQUATIONS OF THE ISING MODEL

The model considered here is a set of spins, with values $+1$ or -1, on a square lattice with nearest neighbor interaction energy coefficient J in both the vertical and horizontal directions. It is readily seen that the model is a special case of that considered by Baxter and hence we may start our formulation from the set of variational equations given in Eqs. (30) of Ref. 3. The reader is referred to Ref. 3 for the derivation of the equations and the significance of the matrices involved.

The equations may be written as

$$\sum_{\sigma'} F(\sigma, \sigma')A^2(\sigma')F(\sigma', \sigma) = A^2(\sigma) \tag{1a}$$

and

$$\begin{aligned} \sum_{\sigma', \gamma'} W(\sigma, \sigma', \gamma, \gamma')F(\sigma, \sigma')A(\sigma')F(\sigma', \gamma')A(\gamma')F(\gamma', \gamma) \\ = \kappa A(\sigma)F(\sigma, \gamma)A(\gamma) \end{aligned} \tag{1b}$$

where σ, σ', γ, and γ' take the spin values of $+1$ or -1 and

$$\begin{aligned} W(\sigma, \sigma', \gamma, \gamma') = \exp\{[2J(\sigma\sigma' + \gamma\gamma' + \sigma\gamma + \sigma'\gamma') \\ + H(\sigma + \sigma' + \gamma + \gamma')]/4k_{\mathrm{B}}T\} \end{aligned} \tag{2}$$

is the weight function of a face of the square lattice, with T the temperature of the system, k_{B} the Boltzmann constant, and H the magnetic field. Each of $A(+)$, $A(-)$, $F(+, +)$, $F(+, -)$, $F(-, +)$, and $F(-, -)$ is a $2^m \times 2^m$ matrix.

With suitable normalization, one can use a representation in which $A(+)$ and $A(-)$ are diagonal, the maximum diagonal element of $A(+)$ being unity. The matrices $F(\sigma, \sigma')$ satisfy the symmetry properties

$$F(\sigma, \sigma') = F^T(\sigma', \sigma) \tag{3}$$

In the thermodynamic limit, the partition function per site of the system is κ. By taking $m = 0, 1, 2, \ldots$, a sequence of variational approximations may be obtained for κ. The case for $m = 0$ is found to be the same as the Kramers–Wannier approximation.[3,4]

Following a similar procedure to Ref. 3, we define matrices

$$H(\sigma, \sigma'|\gamma) = \sum_{\gamma'} W(\sigma, \gamma', \gamma, \sigma')F^T(\gamma', \sigma)A(\gamma')F(\gamma', \sigma') \tag{4}$$

$$F_2(\sigma) = \begin{pmatrix} A(+)F(+, \sigma)A^{-1}(\sigma) \\ A(-)F(-, \sigma)A^{-1}(\sigma) \end{pmatrix} \tag{5}$$

and

$$U(\sigma) = \begin{pmatrix} H(+, +|\sigma) & H(+, -|\sigma) \\ H(-, +|\sigma) & H(-, -|\sigma) \end{pmatrix} \tag{6}$$

Equation (1b) can be written as

$$U(\sigma)F_2(\sigma) = \kappa F_2(\sigma)A(\sigma) \tag{7}$$

It follows that the elements of $\kappa A(\sigma)$ are contained in the set of eigenvalues of $U(\sigma)$ and all the column vectors of $F_2(\sigma)$ are eigenvectors of $U(\sigma)$. So, with a knowledge of the leading order behavior of the elements of $A(\sigma)$, we are able to select from the set of eigenvalues of $U(\sigma)$ the appropriate elements for the matrices $\kappa A(\sigma)$ and hence obtain the solution for $F(\sigma, \sigma')$ also from the corresponding eigenvectors of $U(\sigma)$.

Define the $2^{m+2} \times 2^{m+2}$ matrix V by

$$V = \begin{pmatrix} U(+) & \\ & U(-) \end{pmatrix} \tag{8}$$

and write $A(\sigma)$ as

$$A(\sigma) \equiv (a_j^\sigma), \qquad j = 1, 2, 3, \ldots, 2^m \tag{9}$$

Let P be an orthogonal matrix which diagonalizes V. Order the column vectors of P in such a way that at low temperatures P is almost diagonal (i.e., $p_{l,l} \simeq 1$ and $p_{l,j} \ll p_{l,l}$ for $l \neq j$), and let the corresponding diagonal matrix containing the eigenvalues of V be

$$C \equiv \begin{bmatrix} d_1^+ & & & & & & & \\ & d_2^+ & & & & & & \\ & & \ddots & & & & & \\ & & & d_\mu^+ & & & & \\ & & & & d_1^- & & & \\ & & & & & d_2^- & & \\ & & & & & & \ddots & \\ & & & & & & & d_\mu^- \end{bmatrix} \qquad (10)$$

where $\mu = 2^{m+1}$. We then find that

$$\kappa = d_1^+ \qquad (11)$$

and

$$a_j^\sigma = d_{2j-1}^\sigma / d_1^+, \qquad j = 1, 2, 3, \ldots, 2^m \qquad (12)$$

$F(\sigma, \sigma')$ can be evaluated from the corresponding eigenvectors of V.

3. THE VARIATIONAL EQUATIONS IN THEIR REPRESENTATIVES

3.1. The Representatives of the Matrices

The argument up to now is still applicable even in the presence of a magnetic field. However, since we are interested in the convergence of the sequence of approximations to the exact solution as m increases, we will focus our attention on the case in which the magnetic field is zero. In this case, we are able to apply Kaufmann's technique of spinor representations.[5]

Given a set of spinor operators Γ_j of dimensions $2^p \times 2^p$ ($j = 1, 2, \ldots, \mu$; $\mu \geqslant 2p$) satisfying the anticommutation rule

$$\Gamma_j \Gamma_l + \Gamma_l \Gamma_j = 2\delta_{j,l}, \qquad j, l = 1, 2, \ldots, \mu \qquad (13)$$

there exists a group of nonsingular $2^p \times 2^p$ matrices such that for all matrices X in the group,

$$X \Gamma_j X^{-1} = \sum_{l=1}^{\mu} \hat{x}_{l,j} \Gamma_l, \qquad j = 1, 2, \ldots, \mu \qquad (14)$$

for some scalar $\hat{x}_{l,j}$. The matrix formed by the elements $(\hat{x}_{l,j})$ is called the representative of X under the set of operators Γ_j and is denoted by $\hat{X}$.

In order to formulate the problem in the spinor representations, we define a set of $(2p + 1)$ spinor operators,

$$\begin{aligned}
\Gamma_1 &= s_1; \qquad \Gamma_2 = (c_1 s_2 + i d_1)/\sqrt{2}; \qquad \Gamma_3 = (c_1 s_2 - i d_1)/\sqrt{2} \\
\Gamma_{2j} &= c_1 \cdots c_{j-1}(c_j s_{j+1} + i d_j)/\sqrt{2} \qquad (15) \\
\Gamma_{2j+1} &= c_1 \cdots c_{j-1}(c_j s_{j+1} - i d_j)/\sqrt{2}; \qquad j = 2, 3, \ldots, p
\end{aligned}$$

where s_j, c_j, and d_j are the Pauli spin operators acting on the jth spin and $i = \sqrt{-1}$

$$s_j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad c_j = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad d_j = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad (16)$$

and

$$s_{p+1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

is the identity matrix. The set of operators is not totally anticommuting with each other, yet the representatives under this set of operators can be obtained by a similarity transformation from the following set of $(2p + 1)$ anticommuting operators:

$$\begin{aligned}
\Gamma_1' &= s_1; \qquad \Gamma_2' = d_1; \qquad \Gamma_3' = c_1 s_2 \\
\Gamma_{2j}' &= c_1 \cdots c_{j-1} d_j; \qquad \Gamma_{2j+1}' = c_1 \cdots c_j s_{j+1}, \qquad j = 2, 3, \ldots, p
\end{aligned} \qquad (17)$$

The representatives $\hat{X}$ under the Γ_j are related to that $(\hat{X}')$ under the Γ_j' by

$$\hat{X} = R^{-1} \hat{X}' R \qquad (18)$$

where

$$R = \begin{bmatrix} 1 & & & & & \\ & i/\sqrt{2} & -i/\sqrt{2} & & & \\ & 1/\sqrt{2} & 1/\sqrt{2} & & & \\ & & & i/\sqrt{2} & -i/\sqrt{2} & \\ & & & 1/\sqrt{2} & 1/\sqrt{2} & \\ & & & & & \ddots \end{bmatrix} \qquad (19)$$

Clearly, the representatives under (15) also form a group G and one can establish the following properties of the representatives:

(i) The inverse of any $\hat{X}$ in G is given by

$$\hat{X}^{-1} = L \hat{X}^T L \qquad (20)$$

where

$$L = \begin{bmatrix} 1 & & & & & \\ & 0 & 1 & & & \\ & 1 & 0 & & & \\ & & & 0 & 1 & \\ & & & 1 & 0 & \\ & & & & & \ddots \end{bmatrix} \tag{21}$$

(ii) If X is diagonal, it must be of the form

$$X = \rho \times \prod_{j=1}^{p} \tfrac{1}{2}[(1 + y_j) + (1 - y_j)s_j s_{j+1}] \tag{22}$$

where ρ is some scalar factor, and $\hat{X}$ is diagonal, with diagonal elements $x_1, x_2, \ldots, x_{2p+1}$ satisfying

$$x_1 = 1, \qquad x_{2j+1} = 1/x_{2j} = y_j, \qquad j = 1, 2, \ldots, p \tag{23}$$

(iii) If X is real and symmetric, then $\hat{X}$ is real and symmetric.

(iv) If X is orthogonal, $\hat{X}$ is orthogonal and has the following structure:

$$\hat{X} = \begin{bmatrix} a & q & q & r & r & \cdots \\ s & u & v & f & g & \\ s & v & u & g & f & \\ t & y & z & l & h & \\ t & z & y & h & l & \\ \vdots & & & & & \ddots \end{bmatrix} \tag{24}$$

It is more convenient to define matrices

$$\mathscr{A} = \begin{pmatrix} A(+) & \\ & A(-) \end{pmatrix} \tag{25}$$

and

$$\mathscr{F} = \begin{pmatrix} F(+,+) & z^{1/2}F(+,-) \\ z^{1/2}F(-,+) & F(-,-) \end{pmatrix} \tag{26}$$

where

$$z = \exp(-2J/k_B T) \tag{27}$$

It can be verified that the representatives of $\mathscr{A}$ and $\mathscr{F}$ exist under (15) with $p = m + 1$. For matrices V, P, and C, we apply an enlarged set of operators

Γ_j^{en} defined similarly in (15) with $p = m + 2$. From the definitions of the matrices V, P, and C, and the representatives, one can obtain $\hat{V}$ from $\hat{\mathscr{F}}$ and also $\hat{\mathscr{F}}$ from $\hat{P}$. So, in a similar way to Ref. 3, an iterative procedure for solving the equations may be developed.

3.2. Iterative Method of Solution

Given a reasonable initial guess of $\hat{\mathscr{A}}$ and $\hat{\mathscr{F}}$ at a particular value of z and setting $n = m + 2$:

(i) Define $\hat{U}$ by

$$\hat{U} = \hat{\mathscr{F}}^{\mathrm{T}}\hat{\mathscr{A}}\hat{\mathscr{F}} \equiv (u_{l,j}), \qquad l, j = 1, 2, \ldots, 2n - 1 \tag{28}$$

Then $\hat{V}$ is given by

$$\hat{V} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & (u_{1,1} + 1)/2z & \frac{1}{2}(u_{1,1} - 1) & (2z)^{-1/2}u_{1,j-2} & \cdots \\ \vdots & & \frac{1}{2}z(u_{1,1} + 1) & (z/2)^{1/2}u_{1,j-2} & \cdots \\ & & & u_{l-2,j-2} & \\ & & & & \ddots \end{pmatrix},$$

$$l, j = 4, 5, \ldots, 2n + 1 \tag{29}$$

Note that $\hat{V}$ is symmetric.

(ii) Solve the eigenvalue equation

$$\hat{V}\hat{P} = \hat{P}\hat{C} \tag{30}$$

for $\hat{C}$ and $\hat{P}$ such that $\hat{C}$ is diagonal and $\hat{P}$ is orthogonal and almost diagonal.

(iii) With $\hat{C} \equiv (a_j), j = 1, 2, \ldots, 2n + 1$, $\hat{\mathscr{A}}$ is obtained by truncating the last two rows and columns of $\hat{C}$, i.e.,

$$\hat{\mathscr{A}} = (a_j), \qquad j = 1, 2, \ldots, 2n - 1 \tag{31}$$

(iv) Given $\hat{P} \equiv (p_{l,j})$, $l, j = 1, 2, \ldots, 2n + 1$, we define $(h_{l,j})$, $l, j = 1, 2, \ldots, 2n - 1$, by

$$\begin{aligned} h_{1,1} &= (p_{2,2n} + p_{3,2n})/(p_{2,2n} - p_{3,2n}) \\ h_{1,j} &= (a_j/\sqrt{2})[(p_{2,j} + p_{3,j}) - (p_{2,j} - p_{3,j})(p_{2,2n} + p_{3,2n})/(p_{2,2n} - p_{3,2n})] \\ h_{j,1} &= \sqrt{2}\, a_j^{-1}[p_{j+2,2n}/(p_{2,2n} - p_{3,2n})] \\ h_{l,j} &= a_l^{-1}[p_{l+2,j} - p_{l+2,2n}(p_{2,j} - p_{3,j})/(p_{2,2n} - p_{3,2n})]a_j \end{aligned} \tag{32}$$

Then, from (5) and (26) we have

$$\hat{\mathscr{F}} = \left(\begin{array}{c|c} \dfrac{h_{1,1} + v}{1 + vh_{1,1}} & \dfrac{h_{1,j}}{ch(J/k_BT)(1 + vh_{1,1})} \\ \hline & h_{l,j} - \dfrac{vh_{1,j}h_{l,1}}{1 + vh_{1,1}} \end{array}\right), \qquad l, j = 2, 3, \ldots, 2n - 1 \qquad (33)$$

where $v = \tanh(J/k_BT)$.

The whole procedure may be repeated until we arrive at a solution of $\hat{\mathscr{A}}$ and $\hat{\mathscr{F}}$ with satisfactory accuracy.

3.3. Symmetry Properties of $\hat{\mathscr{F}}$

The problem can be further simplified by using the symmetry properties of $\hat{\mathscr{F}}$. Since $\hat{\mathscr{F}}$ is symmetric, it follows from (33) that

$$h_{l,j} = h_{j,l} \qquad \text{for} \quad l, j = 1, 2, \ldots, 2n - 1 \qquad (34)$$

In view of (32) and, at the same time, noting the special structure of $\hat{P}$ from property (iv) of the representatives, we find that $p_{2,j}$ for $j = 2, 3, \ldots, 2n + 1$ and $p_{j+2,j}$ for $j = 2, 3, \ldots, 2n - 1$ are the only independent elements of $\hat{P}$.

First, it is trivial that $p_{1,1} = 1$ and $p_{1,j} = p_{j,1} = 0$. If we define

$$\begin{gathered} \alpha_j = a_j^2, \qquad \beta_j = (1 + a_j^4), \qquad j = 2, 3, \ldots, 2n - 1 \\ \beta_{2n} = \infty, \qquad \beta_{2n+1} = 1 \end{gathered} \qquad (35)$$

then

$$\begin{gathered} p_{l+2,j} = \alpha_l\beta_j(p_{3,l}p_{2,j} - p_{2,l}p_{3,j})/(\beta_j - \beta_l) \\ l \neq j, \qquad l = 2, 3, \ldots, 2n - 1, \qquad j = 2, 3, \ldots, 2n + 1 \end{gathered} \qquad (36a)$$

where

$$\begin{aligned} p_{3,2j} &= p_{2,2j+1} \\ p_{3,2j+1} &= p_{2,2j} \qquad \text{for} \quad j = 1, 2, \ldots, n \end{aligned} \qquad (36b)$$

One can substitute (36) into (33) to obtain $\hat{\mathscr{F}}$. If we write

$$\hat{\mathscr{F}} \equiv (f_{l,j}), \qquad l, j = 1, 2, \ldots, 2n - 1 \qquad (37)$$

then

$$\begin{aligned} f_{1,1} &= (p_{2,2n} + zp_{2,2n+1})/g_{2n} \\ f_{1,j} &= f_{j,1} = (2z)^{1/2}a_jr_j/(\beta_jg_{2n}) \\ f_{j,j} &= p_{j+2,j} - \alpha_jg_jr_j/(\beta_jg_{2n}) \\ f_{j,l} &= a_ja_l(g_jr_l - g_lr_j)/(\beta_j - \beta_l)g_{2n} \\ &= f_{l,j}, \qquad j \neq l; \qquad j, l = 2, 3, \ldots, 2n - 1 \end{aligned} \qquad (38)$$

where

$$g_j = p_{2,j} - zp_{3,j}, \qquad r_j = \beta_j(p_{2,2n}p_{3,j} - p_{3,2n}p_{2,j}) \tag{39}$$

The main problem in the iterative procedure is to solve Eq. (30). However, together with the orthogonality properties of $\hat{P}$, i.e.,

$$\hat{P}\hat{P}^T = I \tag{40}$$

relations from (29) and (38), and the fact that

$$a_{2j} = 1/a_{2j+1} \qquad \text{for} \quad j = 1, 2, \ldots, n \tag{41}$$

we observe that

$$p_{2,2j} = p_{2,2j+1}\frac{1 - za_{2j+1}}{z - a_{2j+1}}, \qquad j = 1, 2, \ldots, n \tag{42a}$$

$$p_{j+2,j} = \frac{(1+z^2)^2}{4z(1-z^2)} - \frac{\beta_j(1-z^2)}{4a_j}\left[\frac{p_{2,j}^2}{(z-a_j)^2} + \frac{p_{2,2n}^2\beta_j}{(z-a_{2n})^2a_{2n}a_j^3}\right] \tag{42b}$$

$$j = 2, 3, \ldots, 2n - 1$$

Hence, the matrix equations involve only $2n$ independent variables, namely

$$a_{2j+1} \quad \text{and} \quad p_{2,2j+1} \qquad \text{for} \quad j = 1, 2, \ldots, n$$

After some tedious, yet straightforward calculations, the matrix equations are found to be equivalent to $2n$ independent equations involving these $2n$ variables. To simplify the notation, we define

$$c_j = a_{2j+1}, \qquad c_{1-j} = 1/c_j = a_{2j}, \qquad j = 1, 2, \ldots, n \tag{43a}$$

$$w_j = w_{1-j} = \beta_{2j+1}p_{2,2j+1}^2/(z - a_{2j+1})^2a_{2j+1}, \qquad j = 1, 2, \ldots, n-1 \tag{43b}$$

and

$$w_n = p_{2,2n+1}^2/a_{2n+1}(z - a_{2n+1})^2 \tag{43c}$$

The equations then become

$$\frac{w_j}{4} + \sum_{l=2-n\neq j}^{n-1}\frac{w_lc_lc_j^2(c_l - c_j)}{c_l^4 - c_j^4} + w_n\left(\frac{c_n}{c_j} - \frac{c_n^2}{c_j^2} + c_n^2c_j^2 - c_n^3c_j^3\right)$$
$$= \tfrac{1}{4}\phi(c_j), \qquad j = 1, 2, \ldots, n-1 \tag{44a}$$

$$\frac{w_j}{4} + \sum_{l=2-n\neq j}^{n-1}\frac{w_lc_l^2c_j(c_l - c_j)}{c_l^4 - c_j^4} + w_n\left(c_nc_j - c_n^2c_j^2 + \frac{c_n^2}{c_j^2} - \frac{c_n^3}{c_j^3}\right)$$
$$= \tfrac{1}{4}\phi(c_j), \qquad j = 1, 2, \ldots, n-1 \tag{44b}$$

$$\sum_{l=2-n}^{n-1}\frac{w_lc_l^3}{1 + c_l^4} + w_nc_n(1 + c_n^2) = \frac{1+z^2}{(1-z^2)^2} \tag{44c}$$

$$\sum_{l=2-n}^{n-1}\frac{w_lc_l^2}{1 + c_l^4} + 2w_nc_n^2 = \frac{2z}{(1-z^2)^2} \tag{44d}$$

where

$$\phi(u) = \frac{(1 + z^2)^2}{z(1 - z^2)^2} - w_n c_n^4(u^4 + 2 + u^{-4}) \tag{45}$$

Hence, the iterative procedure for the solution can be replaced by solving the system of equations (44) for the c_j and the w_j.

3.4. Polynomial Form of Equations

Define, for all complex numbers u,

$$G(u) = w_n[c_n(u - u^{-1}) + c_n^2(u^2 - u^{-2}) + c_n^3(u^3 - u^{-3})] + \frac{1}{2}\sum_{j=2-n}^{n-1} \frac{w_j(c_j + u)}{(c_j - u)} \tag{46}$$

From (43a), $G(u)$ satisfies the relation

$$G(u) + G(u^{-1}) = 0 \tag{47}$$

In terms of this function, Eqs. (44a) and (44b) can be written as

$$2G(-u) - (1 + i)G(iu) - (1 - i)G(-iu) = \phi(u) \tag{48a}$$

$$-2G(-u) + (1 - i)G(iu) + (1 + i)G(-iu) = \phi(u) \tag{48b}$$

for $u = c_{2-n},\ldots, c_{n-1}$, where $\phi(u)$ is defined by (45) and $i = \sqrt{-1}$. An equivalent and simpler form of this pair of equations is

$$2i[G(-u) - G(iu)] = \phi(u) \tag{49a}$$

$$-2i[G(-u) - G(-iu)] = \phi(u) \tag{49b}$$

for $u = c_{2-n},\ldots, c_{n-1}$. We now define $f(u)$ by

$$f(u) = \prod_{j=2-n}^{n-1} (u - c_j) \tag{50}$$

By examining the zeros and poles of (49), one can easily verify the identity, true for all complex numbers u,

$$2i[G(-u) - G(iu)] \equiv \phi(u) - \frac{f(u)f(-iu)}{f(-u)f(iu)}\alpha(u) \tag{51}$$

where $u^4\alpha(u)$ is a polynomial in u of degree eight. Further,

$$\alpha^*(u) = \alpha(iu) = \alpha(1/u) \tag{52}$$

Hence, $\alpha(-\omega u)$ is a polynomial in $(u + u^{-1})$ and

$$\alpha(\omega)\alpha(-\omega) = \alpha(\omega^{-1})\alpha(-\omega^{-1}) \tag{53}$$

where

$$\omega^4 = -1, \qquad \omega = (1 + i)/\sqrt{2} \tag{54}$$

It is clear that $u^8\alpha(u)\alpha(-u)$ is a polynomial in u^4 and so it is possible to factorize $\alpha(u)$ into the form

$$\alpha(u) = \text{const} \times \rho(u)\rho(-iu) \tag{55}$$

For convenience, we define the constant to be $w_n c_n{}^4$.

Three additional equations can be obtained from (51) by replacing u by iu, $-u$, and $-iu$, respectively. The function $G(u)$ can be eliminated between these four forms of (51), giving

$$4\phi(u) = \frac{f(u)[f^2(-iu)\alpha(u) + f^2(iu)\alpha(iu)]}{f(iu)f(-u)f(-iu)} + \frac{f(-u)[f^2(iu)\alpha(-u) + f^2(-iu)\alpha(-iu)]}{f(u)f(iu)f(-iu)} \tag{56}$$

If we consider poles of $f(-u)$ in the equation, it can be easily seen that $f(-u)$ must be a factor of $[f^2(-iu)\alpha(u) + f^2(iu)\alpha(iu)]$ and since $\rho(u)$ is a factor of both $\alpha(u)$ and $\alpha(iu)$ from (55), we obtain

$$f^2(-iu)\rho(-iu) + f^2(iu)\rho(iu) = f(-u)R(u) \tag{57}$$

for some polynomial $R(u)$. The left-hand side of (57) is unaltered by negating u, so $f(u)$ must be a factor of $R(u)$, i.e.,

$$R(u) = f(u)\sigma(u) \tag{58}$$

where $\sigma(u)$ is an even function of u. Substituting (57) and (58) into (56), we find that

$$4w_n c_n{}^4\phi(u) = \sigma(iu)\sigma(u) \tag{59}$$

It follows that

$$\sigma(u) = -2w_n c_n{}^4(u^2 - m_0 + u^{-2}) \tag{60}$$

where

$$m_0 = [(1 + z^2)^2/z(1 - z^2)^2 w_n c_n{}^4]^{1/2} \tag{61}$$

The negative sign of (60) is chosen so as to fit the limit of the left-hand side of (57) as u approaches zero.

We can solve for $\rho(u)$ from Eqs. (44c) and (44d). From these equations,

$$\alpha(\omega^{-1}) = \alpha(-\omega^{-1}) = (1 - 6z^2 + z^4)/z(1 - z^2)^2 \tag{62}$$

and together with the definition of $\alpha(u)$, we find that

$$\rho(u) = (h_1 - u - u^{-1})(h_2 - u - u^{-1}) \tag{63}$$

where

$$h_1^2 = 2 + m_0(1 + 2z - z^2)/(1 + z^2) \tag{64a}$$

$$h_2^2 = 2 + m_0(1 - 2z - z^2)/(1 + z^2) \tag{64b}$$

In summary, the matrix equations are reduced to the following polynomial equation involving c_j ($j = 1, 2, \ldots, n - 1$) and m_0 only:

$$\rho(iu)f^2(iu) + \rho(-iu)f^2(-iu) = -2(u^2 - m_0 + u^{-2})f(u)f(-u) \tag{65}$$

where $f(u)$, $\rho(u)$, and m_0 are given by (50), (63), and (61), respectively.

4. THE INFINITE SOLUTION

It is possible to solve the problem for the infinite system by noting the fact that the matrices $\mathscr{A}$ and $\mathscr{F}$ should tend toward the corresponding "corner transfer matrix" and row (or column) transfer matrix of the infinite lattice as their limit, when n approaches infinity.[3]

Since $\hat{\mathscr{A}}$ is diagonal from property (ii) of the spinor representations, with an appropriate normalization and arrangement of rows and columns, $\mathscr{A}$ can be written as

$$\mathscr{A} = \begin{pmatrix} 1 & 0 \\ 0 & c_1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & c_2 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 & 0 \\ 0 & c_{n-1} \end{pmatrix} \tag{66}$$

for $n = 1, 2, \ldots$.

The corner transfer matrices for the square lattice Ising model were obtained by Baxter in 1977.[7] For the case $n = \infty$, the corresponding corner transfer matrix for $\mathscr{A}$ is similar to that considered by Ref. 7 except that instead of having diagonal interaction energy coefficients J and J', we have interaction energy coefficient J in both the horizontal and vertical directions (Fig. 1). Hence, using a similar argument as Ref. 7, we obtain, within a normalization constant,

$$\mathscr{A} = \begin{pmatrix} 1 & 0 \\ 0 & q^{1/4} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & q^{3/4} \end{pmatrix} \otimes \cdots \tag{67}$$

or

$$c_j = q^{(2j-1)/4}, \qquad j = 1, 2, \ldots \tag{68}$$

for $n = \infty$, where q is the nome of the elliptic function with modulus

$$k = \sinh^{-2}(2J/k_B T) \tag{69}$$

Substituting (68) into (44) with c_n equal to zero and the summation being from negative infinity to positive infinity for $n = \infty$, we obtain

$$w_j = \pi/(2zK), \qquad j = 1, 2, \ldots \tag{70}$$

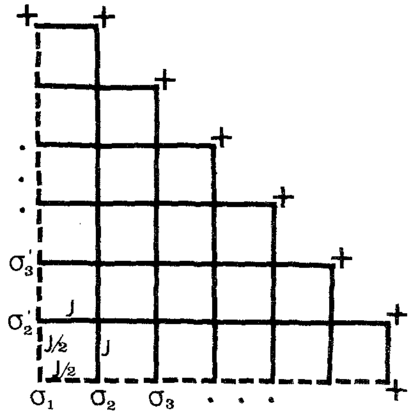

Fig. 1. The upper right corner of the lattice, corresponding to the "corner transfer matrix" $\mathscr{A}$.

where K is the complete elliptic integral of the first kind of modulus k. Hence, from (37) and (38), $\hat{\mathscr{F}}$ is given by

$$\begin{aligned}
f_{1,1} &= (1 + z^2)/(1 - z^2) \\
f_{1,j} &= f_{j,1} = (2z)^{1/2} y_j \\
f_{j,l} &= (1 - z^2) y_j y_l (\beta_j a_l - \beta_l a_j)/(\beta_j - \beta_l), \qquad j \neq l \\
f_{j,j} &= \frac{(1 + z^2)^2}{4z(1 - z^2)} + \frac{(1 - z^2) y_j^2 (3a_j^4 - 1)}{4a_j^3}, \qquad j, l \geqslant 2
\end{aligned} \tag{71}$$

where a_j is related to c_j through (43a) and is given by

$$a_{2j+1} = 1/a_j = q^{(2j-1)/4}, \qquad j = 1, 2, 3, \ldots \tag{72a}$$

$$\beta_j = 1 + a_j^4 \tag{72b}$$

and

$$y_j = \operatorname{sgn}(j)[\pi a_j^3/(2zK\beta_j)]^{1/2} \tag{72c}$$

with

$$\operatorname{sgn}(j) = \begin{cases} +1 & \text{if } j = 1 \text{ or } 2 \text{ (modulo 4)} \\ -1 & \text{if } j = 0 \text{ or } 3 \text{ (modulo 4)} \end{cases} \tag{73}$$

For finite n, we are able to solve the equations numerically only. However, the $n = \infty$ solution for a given matrix element is approximately correct for finite n at low temperature, at least to leading order. Hence, they serve as a good initial guess to the solution for numerical calculations.

5. NUMERICAL SOLUTION

For finite n, the problem reduces to evaluating the c_j and m_0 from the polynomial equation (65). Numerically, we find that m_0 is always greater than 2, so we can define a real parameter c_n by

$$m_0 = c_n^2 + c_n^{-2}, \qquad 0 < c_n < 1 \tag{74}$$

(The c_n defined here is different from that used previously.) The zeros of the right-hand side of Eq. (65) occur at $c_1, c_2, \ldots, c_n$, so

$$\rho(ic_j)f^2(ic_j)/\rho(-ic_j)f^2(-ic_j) = -1, \qquad j = 1, 2, \ldots, n \tag{75}$$

Taking logarithms of both sides, and using considerations from the low-temperature expansions of the equation (75) for the appropriate branch cut in the complex plane, we may write the equation as

$$\begin{aligned} 2\sum_{l=1}^{n-1} \tan^{-1}\frac{c_l^{-1} + c_l}{c_j^{-1} - c_j} + \tan^{-1}\frac{h_1}{c_j^{-1} - c_j} + \tan^{-1}\frac{h_2}{c_j^{-1} - c_j} \\ = (n - j + 1/2)\pi, \qquad j = 1, 2, \ldots, n \end{aligned} \tag{76}$$

where h_1 and h_2 are given by (64).

Equation (76) has been solved numerically for a range of values of z below the critical point, using the Newton–Raphson method. The computation was done on a UNIVAC 1100/42 computer, using double-precision floating point arithmetic with 18 significant digits. A solution was assumed to have converged only when the relative change of each variable, through one iteration, was less than 10^{-14}. As a measure of the degree to which an equation was satisfied, we also calculated the difference between the right- and left-hand sides divided by the absolute sum of all the additive terms in the equation. This was never greater than 10^{-16}.

Solutions were obtained for $n = 2$–20. Since the $n = 2$ case can be solved analytically, it serves as a guide to the degree of accuracy of the solution. Another plausible guide to the accuracy is provided by the fact that some quantities tend very rapidly to their known $n = \infty$ values, differing from them only in the last few digits (see, for example, column 2 in Table I). Combining both, we are able to conclude that the numerical results we obtained are accurate at least to 11 significant figures.

5.1. Spontaneous Magnetization

The spontaneous magnetization of the system can be easily obtained through (66) and is given by[6]

$$M = \frac{\text{Trace } S\mathscr{A}^4}{\text{Trace } \mathscr{A}^4} = \prod_{j=1}^{n-1} \frac{1 - c_j^4}{1 + c_j^4} \tag{77}$$

where $S = s_1 s_2 \cdots s_{n-1}$.

Table I. Approximations to the Spontaneous Magnetization for Various Values of z with n = 2–20[a]

	$M_n - M_\infty$			
n	$z = 0.4$	$z = 0.414$	$z = 0.4142$	$z = 0.414213$
2	0.02392802714	0.27069383063	0.40964931899	0.52166267553
3	0.00114718221	0.13961159480	0.27329853612	0.38495721146
4	0.00003110890	0.06200532571	0.18216108501	0.29280635216
5	0.00000064786	0.02135243598	0.11642461140	0.22459790868
6	0.00000001171	0.00548872105	0.06856599103	0.17146657416
7	0.00000000193	0.00110682362	0.03561995801	0.12882150103
8	0.0	0.00018921799	0.01572474294	0.09408287799
9	·	0.00002906023	0.00583086002	0.06581275992
10	·	0.00000415274	0.00185340100	0.04330353924
11	·	0.00000056384	0.00052339043	0.02626341718
12		0.00000007370	0.00013571881	0.01441855726
13		0.00000000935	0.00003310139	0.00709879411
14		0.00000000116	0.00000771716	0.00314589825
15		0.00000000014	0.00000173848	0.00127286235
16		0.00000000002	0.00000038124	0.00047878871
17		0.0	0.00000008182	0.00017022932
18		·	0.00000001725	0.00005796032
19		·	0.00000000358	0.00001908212
20	0.0	0.0	0.00000000073	0.00000611736
M_∞	0.80554134201	0.48198594815	0.34155136722	0.22944135750

[a] The rate of convergence to the exact value is at least geometric.
$z_{c,\infty}$ = 0.414213562373.

We tabulate in Table I the difference of the spontaneous magnetization calculated at a given n from the exact value, at some particular values of z. The convergence of the approximations for the spontaneous magnetization per site to the exact value is extremely rapid away from the critical temperature of the infinite system (denoted by $T_{c,\infty}$), and even for temperatures very close to $T_{c,\infty}$ (e.g., column 5 of Table I), the convergence is still at least geometric.

5.2. The Critical Temperature

Another quantity of interest is the estimation of the critical temperature of the system and the way it converges toward the exact result.

In the thermodynamic limit, the critical point can be defined to be the point at which the spontaneous magnetization of the system vanishes as the temperature increases. A similar definition may be used for the case when n is finite. From (77), the spontaneous magnetization will vanish if any of the c_j is unity. Since, both from the infinite solution (i.e., when $n = \infty$) and the low-temperature expansions from the equations, all the c_j are less than unity and decrease as j increases for all temperatures below the critical temperature, one can equivalently define the critical point for a system with finite n to be the point at which $c_1 = 1$. As seen from (66), it is also the point at which the maximum eigenvalue of the matrix $\mathscr{A}$ degenerates.

A more convenient temperature parameter to use is

$$t = \operatorname{cosech}^4(2J/k_BT) - 1 \tag{78}$$

(for T near $T_{c,\infty}$, this is proportional to $T - T_{c,\infty}$). From (64b), we have

$$t = (2 - h_2{}^2)(1 + 2z - z^2)(1 + z^2)^3/(c_n{}^2 + c_n^{-2})(1 - z^2)^4 \tag{79}$$

Also, at the critical point of the infinite system ($n = \infty$),

$$t = t_{c,\infty} = 0 \tag{80}$$

Let $t_{c,n}$ be the critical value of t for finite n. At $t = t_{c,n}$, we have $c_1 = 1$, so from (50), $f(1) = 0$. Since $f(u) \propto f(1/u)$ and $\rho(i) = \rho(-i)$, if we set $u = 1$ in (65), we have

$$\rho(i)f^2(i) = 0 \tag{81}$$

Table II. The Values of $t_{c,n}$ and c_n at the Critical Point for n = 2–20

n	$t_{c,n}$	c_n
2	0.38883618289	0.17034166992
3	0.055708351974	0.069221620115
4	0.013533606104	0.034470127987
5	0.0041397721372	0.019108958190
6	0.0014589742584	0.011351755016
7	0.00056804454817	0.0070847910329
8	0.00023846971442	0.0045907985350
9	0.00010626511883	0.0030646532019
10	0.000049720759649	0.0020963364563
11	0.000024234867745	0.0014635757443
12	0.000012232230534	0.0010397980729
13	0.0000063637896075	0.00074998870553
14	0.0000033998957695	0.00054818852449
15	0.0000018597394040	0.00040543697430
16	0.0000010389642033	0.00030303841587
17	0.00000059157832392	0.00022866703980
18	0.00000034270961999	0.00017404462601
19	0.00000020169352724	0.00013351912150
20	0.00000012043354466	0.00010317422824

which implies that

$$\rho(i) = 0 \qquad \text{or} \qquad h_1 h_2 = 0 \tag{82}$$

at $t_{c,n}$. Numerically, we find that both h_1 and h_2 are nonnegative, and from (64), $h_1 > h_2$, so h_2 must vanish at $t = t_{c,n}$ for all finite values of n. Also, for n large, z is then close to the limiting critical value $\sqrt{2} - 1$, so from (79),

$$t_{c,n} \simeq 8\sqrt{2}\, c_n{}^2 \tag{83}$$

In Table II, the critical value of t calculated at the nth level ($t_{c,n}$) is given. We also give the value of c_n at the critical point of the system. We find numerically that we are able to fit the c_n extremely accurately to the formula

$$c_n = 1.6817928304 \exp[-(4.9348022005n - 4.6263770635)^{1/2}] \tag{84}$$

For $n \geqslant 5$, this fits to our numerical accuracy of 11 significant figures. (Even for $n = 2$ it is accurate to seven figures.) It is almost certainly the large-n asymptotic form of c_n. The corresponding asymptotic form for $t_{c,n}$ follows immediately from (83).

5.3. Crossover Phenomenon

It is interesting to study the critical behavior of the spontaneous magnetization per site below the critical point of the system. In terms of the t defined in (78), the exact $n = \infty$ result is[8]

$$M = (-t)^{\beta} \tag{85}$$

where β is the critical exponent and is equal to 1/8. However, for finite n, and t very close to $t_{c,n}$, M vanishes according to the classical law

$$M \propto (t_{c,n} - t)^{1/2} \tag{86}$$

For large, but fixed, n, the crossover from (85) to (86) is easily seen in Fig. 2, where $\log M$ is plotted against $\log \tau$ for various values of n, where

$$\tau = (t_{c,n} - t)/t_{c,n} \tag{87}$$

For t sufficiently less than $t_{c,n}$, this plot is almost a straight line, with slope 1/8, while for t very close to $t_{c,n}$ it changes to one with slope $\frac{1}{2}$. The crossover occurs when $(t_{c,n} - t) \sim t_{c,n}$.

We give in Table III rough estimates of the slope of the curve at various values of τ for $n = 3$ and 6. It is readily seen that even for quite small values of n, the crossover is already predominant, and it is possible to get very good estimates of β provided that we work in the low-temperature region away

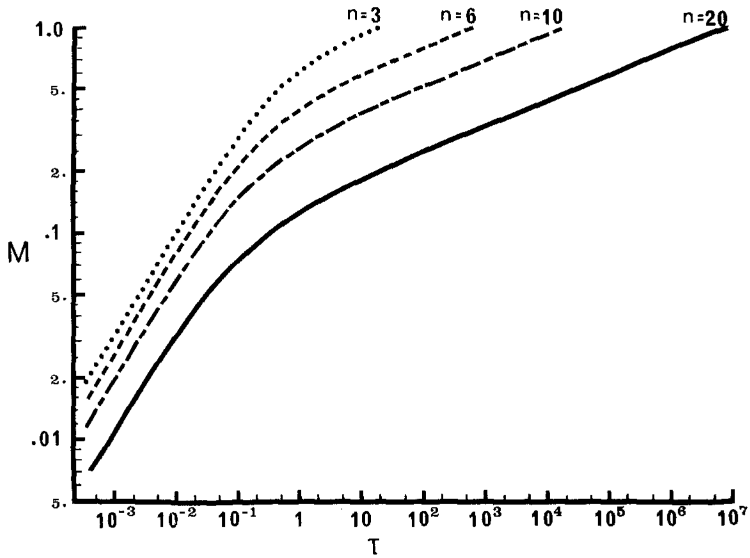

Fig. 2. Log–log plot of spontaneous magnetization vs. the temperature parameter τ for $n = 3$, 6, 10, 20. The crossover can be seen easily even for quite small values of n.

Table III. Estimates of β from Slope of Log–Log Plot of Log M vs. log τ for $n = 3$ and 6

$n = 3$		$n = 6$	
τ	β	τ	β
18.936	0.13197	685.87	0.12518
15.943	0.13338	406.01	0.12531
11.607	0.13687	120.07	0.12612
6.3175	0.14795	59.493	0.12740
2.4218	0.18212	23.767	0.13151
0.70898	0.26037	7.3456	0.14618
0.17427	0.37496	1.8116	0.18763
0.075442	0.43114	0.43840	0.26202
0.025400	0.47476	0.12021	0.35373
0.0075640	0.49062	0.031410	0.44075
0.0023273	0.49715	0.0048358	0.48612
0.00088441	0.49901	0.00092492	0.49752

from the critical point. This is not surprising, since we have chosen the temperature parameter t such that M is exactly equal to $(t_{c,n} - t)^{1/8}$ at all temperatures below the critical point for $n = \infty$.

To describe the crossover phenomenon, we propose a scaling hypothesis similar to that used by Hankey and Stanley for describing the crossover of a system from two dimensions to three.[9]

We assume that the spontaneous magnetization per site as a function of n and the temperature parameter t $(=t - t_{c,\infty})$ satisfies the scaling hypothesis, i.e., for temperature near the critical point and for n large, the spontaneous magnetization per site is asymptotically a generalized homogeneous function,

$$M(t, n) = |t|^{\beta} g(1, \lambda_n t) \tag{88}$$

where $\beta = 1/8$ and λ_n is a monotonic increasing function of n.

At $t_{c,n}$, the left-hand side of (88) vanishes for all values of n. Since t is nonzero at $t = t_{c,n}$, the scaling function $g(1, x)$ must have a zero for some fixed value of x called x_0, and at x_0

$$\lambda_n = x_0/t_{c,n} \tag{89}$$

Equation (88) now becomes

$$M(t, n) = |t|^{\beta} g(1, x_0 t/t_{c,n}) = |t|^{\beta} g(1, x_0(1 - \tau)) \tag{90}$$

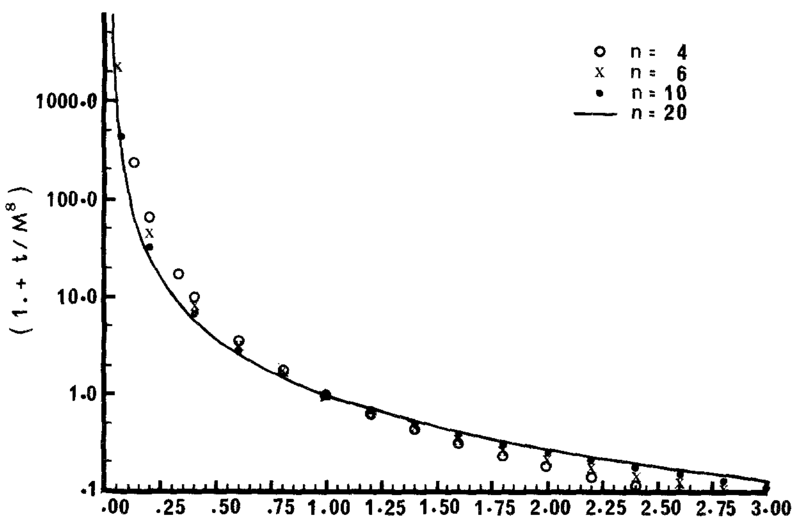

Fig. 3. Plot of $\log(1 + t/M^8)$ vs. τ for $n = 4, 6, 10$, and 20.

where τ is defined by (87). Hence, we have

$$M(t, n)/|t|^{\beta} = \text{a function of } \tau \text{ only} \tag{91}$$

If the left-hand side of (91) is plotted against τ, scaling predicts that all the data points near the critical point should collapse asymptotically into a single curve. In Fig. 3, $\log(1 + t/M^{8})$ is plotted against τ for $n = 4, 6, 10$ and 20. The data support the scaling hypothesis very well.

6. CONCLUSION

For the zero-field Ising model, the variational method converges rapidly to the exact results and gives quite good estimates with only a moderate amount of computational effort. The approximations for M at a given n appear to agree with exact series expansions up to and including terms of the order z^{8n-6}.

It has been shown that the system with finite n exhibits a crossover phenomenon, and good estimates for the exponent β can be obtained.

Finally, the free energy and internal energy per site of the system can be written in terms of determinants involving $\hat{\mathscr{A}}$ and $\hat{\mathscr{F}}$, so their behavior can also be studied.

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