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Two exactly soluble Ising systems with new boundary conditions

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Two Ising systems are investigated with the two extended-mean-field boundary conditions recently considered by Bolton and Johnson. The systems are N spins on a line with boundary spins on either side and at each end. The exact solutions are obtained by the use of the modified-transfer-matrix method. A general formula for the critical temperature is found for each system. The critical temperature is found to take an asymptotic form similar to that obtained by Ferdinand and Fisher for the two-dimensional planar infinite Ising lattice. The thermodynamic limits of the results are discussed.

I. INTRODUCTION

In recent years there have been many theoretical investigations on the equilibrium and nonequilibrium properties of finite Ising systems. Most of these analyses have been numerical and have used computer-simulation methods.[1-3] Ferdinand and Fisher[4] analytically studied the finite properties of a two-dimensional planar Ising lattice with periodic boundary conditions by using Kaufman's exact expression for the partition function of the whole system. Recently Au-Yang and Fisher[5] investigated the finite properties of the Ising lattice with cylindrical boundary conditions by using finite-size scaling theory.

We are interested here in the physical properties of finite Ising systems, especially the asymptotic behavior of their critical temperatures, with two new boundary conditions introduced by Bolton and Johnson.[6] The asymptotic behavior for $N \to \infty$ is important as an aid to understanding the numerical behavior of small clusters and possible extrapolations to the thermodynamic limit (Bolton and Gruen).[7] The physical quantities depend on the imposed boundary conditions and we seek exact solutions for some finite systems.

The analytical solution for the Ising lattices used periodic boundary conditions, but calculations with other boundary conditions have been recently done; Abraham[8] used cylindrical boundary conditions, and Abraham and Martin-Löf[9] used "pure phase" (±) boundary conditions.

In this paper we use two other boundary conditions discussed by Bolton and Johnson[6] which are called extended-mean-field boundary conditions using the average which we abbreviate to EA, and extended-mean-field boundary conditions using probability which we abbreviate to EP. In EA each boundary spin just outside the system is replaced by the average value of the spin obtained from the system itself. In EP each boundary spin is assumed to take values ± 1 such that its probabilistic average is the same as the average for the system itself.

Unlike the EA method, there is no unique way to treat the boundary spins in EP. We always have to calculate the partition function by averaging over the spins inside the finite system. Then we have to average it over the boundary spins and this "boundary averaging" can be done in two ways. Either we do it immediately after calculating the partition function or we take the free energy and then do the boundary averaging. Though this latter choice would be of more physical interest it is algebraically very complicated. We will merely consider the former choice in detail. Similar types of averaging occur also in the theories of spin systems containing impurities where one has either annealed or quenched systems. In these EA and EP, the average spin is determined self-consistently. Finite Ising systems with these boundary conditions exhibit a sharp transition and have a critical temperature below which the average spin is finite and above which it is zero. For finite systems, the critical exponents are classical and in particular β, the critical exponent for the magnetization or average spin, is $\frac{1}{2}$.

We will discuss here two exactly soluble Ising systems using these boundary conditions. They are chain systems and using both EA and EP we will derive exact expressions for the partition functions, average magnetizations, and critical temperatures. We will also discuss the one-dimensional analog of these systems where these boundary conditions act on the end spins only.

II. DESCRIPTION OF THE TWO SYSTEMS

Consider an Ising chain of N spins labeled $1, 2, \ldots, N$ called "internal" spins with two boundary spins for each internal spin $2, \ldots, N-1$ and three boundary spins for spins 1 and N. The positive interaction energy J acts between each near-

est-neighbor pair of internal spins and between an internal spin and each of its boundary spins. Each internal spin has a spin variable $s_i = \pm 1$, $i = 1, \ldots, N$. Letting s_b denote a boundary spin, then the configuration of the whole system is denoted by $\{s_i, s_b\}$.

Since the models are distinguished by the boundary conditions it seems appropriate to label the two models by A or P. In model A we let all boundary spins take some average value s with $|s| \leq 1$. We will eventually determine s by equating it to the average magnetization of the internal spins. Just as in the familiar mean-field approximation, which is A applied to a single site, the self-consistency allows s to be found as a function of temperature. We can obtain other physical quantities as functions of s.

The configuration of model A is $\{s_i, s\}$. The total energy of a configuration for the N spins is

$$E(s) = -J \sum_{i=2}^{N} s_{i-1} s_i - 3Js(s_1 + s_N) - 2Js \sum_{i=2}^{N-1} s_i - mH \sum_{i=1}^{N} s_i , \tag{2.1}$$

where H is the applied magnetic field and m is the magnetic moment of each spin.

In model P we assume that each boundary spin takes the values ± 1 with such probabilities that their average is s, which is assumed to be the average magnetization of the internal spins. We define the probability distribution function Q for each boundary spin $s_{b,j}$ by

$$Q(s_{b,j} = \pm 1) = \tfrac{1}{2}(1 \pm s) , \tag{2.2}$$

We again get a self-consistent equation for s which yields the critical temperature and other physical quantities. Calling s_j', s_j'' the boundary spins of s_j $(j = 2, \ldots, N-1)$ and s_j', s_j'', s_j''' $(j = 1, N)$, the boundary spins of s_1 and s_N, then the total energy of a configuration of model P is

$$E(s) = -J \sum_{i=2}^{N} s_{i-1} s_i - J s_1 s_1''' - J s_N s_N''' - J \sum_{i=1}^{N} s_i (s_i' + s_i'') - mH \sum_{i=1}^{N} s_i \tag{2.3}$$

with J, H, m defined as in (2.1).

It should be noted that because each internal spin in the chain has at least two boundary spins, both models are two dimensional. We will return to this point later.

III. DERIVATION OF RESULTS

We use the modified transfer matrix method as usually given in the discussion of a finite one-dimensional Ising chain with free boundary conditions on the end spins.[10,11] This technique is appropriate because it treats the first and last spins differently from the rest of the internal spins. In the following argument we use the notations $K = \beta J = J/k_B T$ and $h = \beta m H$. We adopt the value $J/k_B = 1$; k_B is Boltzmann's constant.

The partition function of model A with N spins is written

$$Z_N^{(A)} = \sum_{\{s_i\}} \exp\left(K \sum_{i=2}^{N} s_{i-1} s_i + 3Ks(s_1 + s_N) + 2Ks \sum_{i=2}^{N-1} s_i + h \sum_{i=1}^{N} s_i \right) . \tag{3.1}$$

For simplicity, we consider the case when $H = 0$. The transfer matrix method immediately gives

$$Z_N^{(A)} = \langle V_A | P_A^{N-1} | V_A \rangle \tag{3.2}$$

$$= \sum_{j=1}^{2} \lambda_{A_j}^{N-1} |\langle V_A | \phi_{A_j} \rangle|^2 , \tag{3.3}$$

where $|V_A\rangle$ is a ket vector and P_A is the transfer matrix defined as follows:

$$|V_A\rangle = \begin{pmatrix} e^{2Ks} \\ e^{-2Ks} \end{pmatrix} , \tag{3.4}$$

$$P_A = \begin{pmatrix} e^{K(1+2s)} & e^{-K} \\ e^{-K} & e^{K(1-2s)} \end{pmatrix} . \tag{3.5}$$

The eigenvalues λ_{A_1} and λ_{A_2} with $\lambda_{A_1} > \lambda_{A_2}$ of P_A, and their corresponding eigenvectors are given by

$$\left.\begin{matrix} \lambda_{A_1} \\ \lambda_{A_2} \end{matrix}\right\} = e^K \cosh 2Ks \pm a , \tag{3.6}$$

$$|\phi_{A_1}\rangle = \frac{1}{R_A} \begin{pmatrix} 1 \\ e^K (a - b) \end{pmatrix} , \tag{3.7}$$

$$|\phi_{A_2}\rangle = \frac{1}{R_A} \begin{pmatrix} -e^K (a - b) \\ 1 \end{pmatrix} , \tag{3.8}$$

where

$$a = (e^{2K} \cosh^2 2Ks - 2 \sinh 2K)^{1/2} , \tag{3.9}$$

$$b = e^K \sinh 2Ks , \tag{3.10}$$

$$R_A = [1 + e^{2K} (a - b)^2]^{1/2} . \tag{3.11}$$

Note that this N-spin system of model A with $s = 0$ is equivalent to the usual one-dimensional linear chain with free end boundary conditions. In the thermodynamic limit, $N \to \infty$, we have the free energy per spin $f^{(A)}$ as

$$f^{(A)} = -k_B T \ln\lambda_{A_1} . \tag{3.12}$$

For model P, as we have mentioned in Sec. I, we are considering in detail averaging the partition function over the boundary spins simultaneously with the averaging over the internal spins. This particular choice of treating the boundary spins has been applied to small systems and in the Monte Carlo simulation.[6] The partition function of model P with N spins is then written as

$$Z_N^{(P)} = \sum_{\{s_i, s_b\}} Q(s_1')Q(s_1'')Q(s_1''')\, e^{Ks_1(s_1'+s_1''+s_1''')} e^{Ks_1s_2} e^{Ks_2s_3} \cdots Q(s_N')Q(s_N'')\, Q(s_N''')\, e^{Ks_N(s_N'+s_N''+s_N''')} \exp\left(h \sum_{i=1}^{N} s_i\right) , \tag{3.13}$$

where Q is the probability distribution for a boundary spin given by (2.2). Again, we are only interested in the case when $H=0$. In Eq. (3.13), we sum first over the boundary spin variables and then apply the transfer matrix method as before. Here, we have

$$Z_N^{(P)} = \sum_{j=1}^{2} \lambda_{P_j}^{N-1} |\langle V_P | \phi_{P_j} \rangle|^2 , \tag{3.14}$$

where

$$|V_P\rangle = \begin{pmatrix} (\cosh K + s \sinh K)^2 \\ (\cosh K - s \sinh K)^2 \end{pmatrix} , \tag{3.15}$$

$$P_P = \begin{pmatrix} (\cosh K + s \sinh K)^2 e^{K} & (\cosh^2 K - s^2 \sinh^2 K) e^{-K} \\ (\cosh^2 K - s^2 \sinh^2 K) e^{-K} & (\cosh K - s \sinh K)^2 e^{K} \end{pmatrix} , \tag{3.16}$$

$$\left.\begin{matrix} \lambda_{P_1} \\ \lambda_{P_2} \end{matrix}\right\} = e^{K}(\cosh^2 K + s^2 \sinh^2 K) \pm c , \tag{3.17}$$

$$|\phi_{P_1}\rangle = \frac{1}{R_P} \begin{pmatrix} 1 \\ e^{K}(c-d)/(\cosh^2 K - s^2 \sinh^2 K) \end{pmatrix} , \tag{3.18}$$

$$|\phi_{P_2}\rangle = \frac{1}{R_P} \begin{pmatrix} -e^{K}(c-d)/(\cosh^2 K - s^2 \sinh^2 K) \\ 1 \end{pmatrix} , \tag{3.19}$$

$$c = [e^{-2K}(\cosh^2 K + s^2 \sinh^2 K)^2 + 2s^2 \sinh^3 2K]^{1/2} , \tag{3.20}$$

$$d = s e^{K} \sinh 2K , \tag{3.21}$$

$$R_P = [1 + e^{2K}(c-d)^2/(\cosh^2 K - s^2 \sinh^2 K)^2]^{1/2} . \tag{3.22}$$

Again, in the thermodynamic limit, the free energy per spin is

$$f^{(P)} = -k_B T \ln\lambda_{P_1} . \tag{3.23}$$

IV. EXPRESSIONS FOR THE MAGNETIZATION

We define the ensemble average magnetization s as

$$s = \sum_{i=1}^{N} \langle s_i \rangle / N , \tag{4.1}$$

where $\langle s_i \rangle$ is the ensemble average for the ith spin. The following argument holds for both models and we drop the superscripts and subscripts A, P. Following the standard procedure and the spectral decomposition of the transfer matrix, we can write

$$\langle s_i \rangle = \sum_{j,k=1}^{2} \langle V|\phi_j\rangle\langle\phi_j| \sum_{s_i} |s_i\rangle s_i \langle s_i|\phi_k\rangle\langle\phi_k|V\rangle \lambda_k^{i-1} \lambda_k^{N-i} Z_N^{-1} \tag{4.2}$$

and

$$s=\Big[\,|\langle V|\phi_1\rangle|^2\langle\phi_1|X|\phi_1\rangle+|\langle V|\phi_2\rangle|^2\langle\phi_2|X|\phi_2\rangle\left(\frac{\lambda_2}{\lambda_1}\right)^{N-1}$$
$$+\frac{2}{N}\langle V|\phi_2\rangle\langle\phi_2|X|\phi_1\rangle\langle\phi_1|V\rangle[1-(\lambda_2/\lambda_1)^N]/[1-(\lambda_2/\lambda_1)]\Big]\;[|\langle V|\phi_1\rangle|^2+(\lambda_2/\lambda_1)^{N-1}|\langle V|\phi_2\rangle|^2]^{-1}\,, \tag{4.3}$$

where

$$X=\sum_{s_i}|s_i\rangle s_i\langle s_i|\,.$$

The right-hand side of Eq. (4.3) is given by (3.4)–(3.11) for model A and (3.15)–(3.22) for model P. This is an exact self-consistent expression for s for the two models. In the expression for X, we use

$$|+\rangle=\begin{pmatrix}1\\0\end{pmatrix}\text{and}\;|-\rangle=\begin{pmatrix}0\\1\end{pmatrix}.$$

In the thermodynamic limit

$$s=\langle\phi_1|X|\phi_1\rangle\,, \tag{4.4}$$

which, written out explicitly for the two models, yields for model A

$$s=(1-C_A)/(1+C_A)\,, \tag{4.5}$$

where

$$C_A=e^{2K}[(e^{2K}\cosh^2 2Ks-2\sinh 2K)^{1/2}-e^K\sinh 2Ks]^2\,;$$

and for model P

$$s=(1-C_p)/(1+C_p)\,, \tag{4.6}$$

where

$$C_p=(e^{2K}\{[e^{-2K}(\cosh^2K+s^2\sinh^2K)^2+2s^2\sinh^3 2K]^{1/2}-se^{2K}\sinh 2K\}^2)/(\cosh^2K-s^2\sinh^2K)\,.$$

Equation (4.5) has an odd function of s on the right-hand side because we can write it as

$$s=[1-e^{2K}(a-b)^2]/[1+e^{2K}(a-b)^2]\,,$$

and using $(a-b)(a+b)=e^{-2K}$ this becomes

$$s=\{1-e^{2K}[e^{-2K}/(a+b)]^2\}/\{1+e^{2K}[e^{-2K}/(a+b)]^2\}\,.$$

Replacing s by $-s$ replaces b by $-b$ [(3.10)], and the function on the right-hand side changes sign as required. Similarly, the function of the right-hand side of (4.6) is an odd function. This is the same behavior as noted by Bolton and Johnson[6]; there is a critical temperature below which there are three solutions $\pm s, 0$ and above which the only solution is $s=0$. The critical exponent β for magnetization is the classical value $\frac{1}{2}$.

V. CRITICAL PHENOMENA

The critical temperature is given by expanding the function on the right-hand side of (4.3) and retaining only the term of order s. For $N=\infty$, the explicit functions in (4.5) and (4.6) yield the following results:

$$\text{model } A:\;\; 2K_ce^{2K_c}=1;\;\; K_c^{-1}=T_c=3.526\ldots; \tag{5.1}$$

$$\text{model } P:\;\; 2e^{4K_c}-3e^{2K_c}=1;\;\; T_c=3.465\ldots\,. \tag{5.2}$$

Note that model P has a lower critical temperature than model A and is slightly closer to the Onsager value 2.269....

The asymptotic behavior of finite systems can be explored by using the full expression (4.3). Calling the critical temperature of the system with N spins by T_N and using $K_N=T_N^{-1}$, we get the following results:

model A:

$$2K_Ne^{2K_N}+\frac{2K_N(2-e^{2K_N})}{N}\left(\frac{1-\tanh^N K_N}{1-\tanh K_N}\right)=1\,; \tag{5.3}$$

model P:

$$2e^{2K_N}\tanh K_N+\frac{2(2-e^{2K_N})\tanh K_N}{N}\left(\frac{1-\tanh^N K_N}{1-\tanh K_N}\right)=1\,. \tag{5.4}$$

We note that $\tanh^N K_N \to 0$ as $N \to \infty$ and K_N is finite. The asymptotic behavior of T_N for large N can readily be deduced from (5.3) and (5.4):

model A:

$$1/N \approx (2K_N e^{2K_N} - 1)/K_N(e^{2K_N} - 2)(e^{2K_N}+1); \quad (5.5)$$

model P:

$$1/N \approx (2e^{4K_N} - 3e^{2K_N} - 1)/(e^{2K_N} - 2)(e^{2K_N}+1). \quad (5.6)$$

Since the right-hand side of Eq. (5.5) or (5.6) is single valued and all the derivatives exist at $K_N = K_c$ (or $T_N = T_c$), we can therefore express it in a Taylor's expansion. It yields the asymptotic form for T_N namely

$$T_N \sim T_c + \frac{a}{N} + \frac{b}{N^2} + \cdots, \quad (5.7)$$

where for model A

$$a^{(A)} = +0.4174\ldots,$$
$$b^{(A)} = +0.2138\ldots,$$

and for model P

$$a^{(P)} = +0.3893\ldots,$$
$$b^{(P)} = +0.2094\ldots.$$

This has the same asymptotic behavior as was found by Ferdinand and Fisher[4] for the temperature of the maximum on the specific heat of a two-dimensional $N \times N$ lattice with periodic boundary conditions.

We plot in Fig. 1 the values of T_N for the two models against $1/N$. This strengthens the argument used by Bolton and Gruen[7] in their studies on the asymptotic critical behavior of $N \times N$ systems.

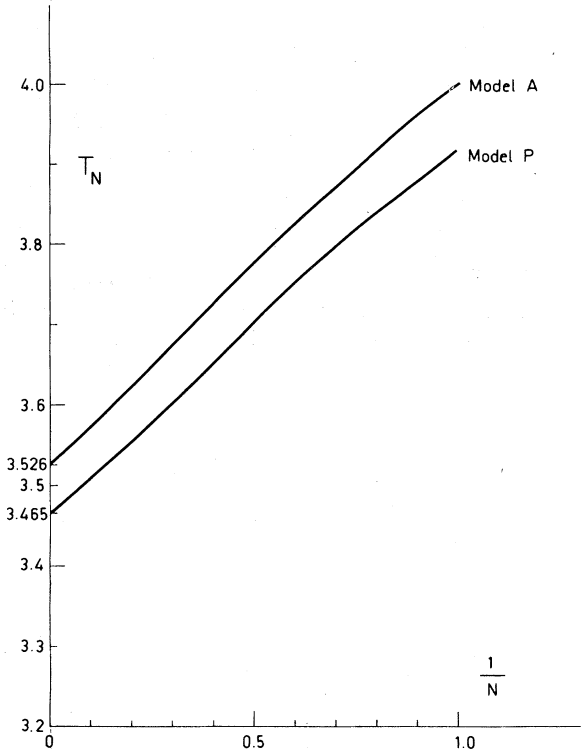

FIG. 1. Plot of critical temperature T_N for the two-dimensional finite Ising models vs $1/N$.

The critical behavior can also be examined through the two-spin correlation function $\langle s_k s_l \rangle$ for the two internal spins on the sites k and l. Using again the general notations we have

$$\langle s_k s_l \rangle = \sum_{p,q,r=1}^{2} \langle V|\phi_p\rangle\langle\phi_p|X|\phi_q\rangle\langle\phi_q|X|\phi_r\rangle\langle\phi_r|V\rangle \left(\frac{\lambda_p}{\lambda_1}\right)^{k-1}\left(\frac{\lambda_q}{\lambda_1}\right)^{l-k}\left(\frac{\lambda_r}{\lambda_1}\right)^{N-l}\left[|\langle V|\phi_1\rangle|^2 + \left(\frac{\lambda_2}{\lambda_1}\right)^{N-1}|\langle V|\phi_2\rangle|^2\right]^{-1}. \quad (5.8)$$

In the limit, not only $N \to \infty$ but also $k, l, N-l, N-k \to \infty$. Then the only nonvanishing terms are $p = q = r = 1, q = 2$ and $p = r = 1$, and

$$\langle s_k s_l \rangle = [|\langle V|\phi_1\rangle|^2 |\langle\phi_1|X|\phi_1\rangle|^2 + \text{const}(\lambda_2/\lambda_1)^{l-k}](|\langle V|\phi_1\rangle|^2)^{-1}. \quad (5.9)$$

Taking the limit $|k-l| \to \infty$, we see from (5.9) that

$$\lim_{|k-l|\to\infty} \lim_{N\to\infty} \langle s_k s_l \rangle = |\langle\phi_1|X|\phi_1\rangle|^2 = s^2,$$

since from (4.4) $s = \langle\phi_1|X|\phi_1\rangle$ for $N \to \infty$.

This proves the existence of the long-range order, and brings us back to the question of the dimensionality of the models. They are two dimensional because the boundary spins are treated in some self-consistent way and they simulate the rest of the two-dimensional plane square lattice. This is the spirit of the familiar mean-field approximation and indeed our solution (5.3) in this paper yields for $N = 1$ the familiar mean-field approximation value $K_1 = \frac{1}{4}$. Model A with $N = 2$ and 3 are the Oguchi[12] two-spin and three-spin approximations. We note in passing that our solutions also yield the pure phase boundary conditions ($\pm$). When we replace s by either $+1$ or -1 on the right-hand side of (4.5) we get

$$s = f(K), \quad (5.10)$$

where $f(K)$ is a continuous function of K and we do not have a sharp critical temperature. The critical exponent β is now not defined.

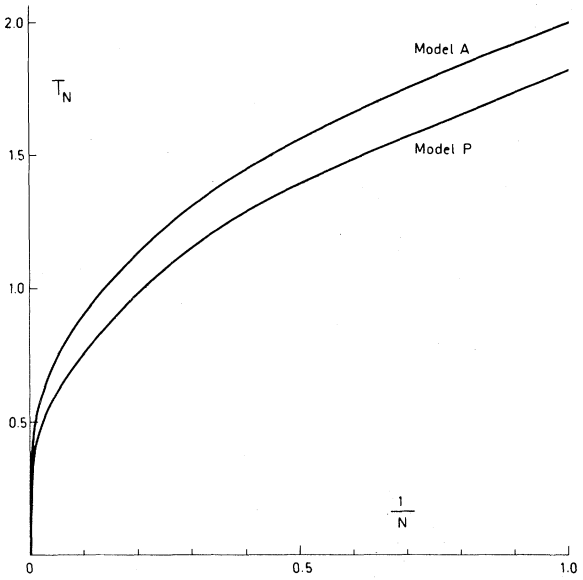

FIG. 2. Plot of critical temperature T_N for the one-dimensional finite Ising models vs $1/N$.

We can now consider the one-dimensional analog of the N-spin systems described above where EA and EP act on the end spins only. We then have the following results:

model A:

$$\frac{2K_N}{N}\left(\frac{\tanh^N K_N - 1}{\tanh K_N - 1}\right) = 1 ; \tag{5.11}$$

model P:

$$\frac{2\tanh K_N}{N}\left(\frac{\tanh^N K_N - 1}{\tanh K_N - 1}\right) = 1 . \tag{5.12}$$

In the thermodynamic limit, these systems are just the usual one-dimensional infinite linear chain. As expected, $T_N \to 0$ as $N \to \infty$. In these cases, no relationship of T_N against N as in Eq. (5.7) exists. The values of T_N vs $1/N$ are plotted in Fig. 2 for these two systems.

Finally, we discuss briefly the second choice of treating the boundary spins in EP, i.e., the free energy of the whole system is given by averaging the logarithm of the partition function over the boundary spins. As mentioned earlier, the calculations of systems under this boundary condition get very involved. Only a few simple examples have been investigated analytically. For a one-dimensional N-spin system having this boundary condition acting only on the end spins, it is found that T_N is always zero for any finite N. Moreover, for one spin with this boundary condition in two dimensions, one gets $T_1 = 3.089...$ compared with the corresponding results 4 for EA and 3.915... for EP (the first choice). This result is considerably closer to the Onsager value 2.269... than those of the other methods. A finite system with this boundary condition is hence a better approximation to the infinite system.

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