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The Influence of Fixed Spins on the Thermodynamic Behavior of an Ising Ferromagnet

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We study the thermodynamic behavior of a ferromagnetic Ising system on a Bethe lattice in the presence of given boundary conditions. More specifically, we study the interface of the system when the spins on half of the surface are fixed opposite to the spins on the other half. We find an interface width that remains finite in the whole range $(0, T_c)$, a feature due to the special topology of the Bethe lattice. We also study the case where the spin on a certain lattice site belonging to a domain is fixed in a direction opposite to the domain magnetization at all temperatures $T < T_c$. We obtain the influence of that spin on the local magnetization, and we find that the fixed spin nucleates a local domain that extends over a distance of only a few lattice sites from it at all temperatures $T < T_c$.

KEY WORDS: Ising model; Bethe lattice; interface; boundary conditions.

1. INTRODUCTION

The thermodynamic behavior of a magnetic system under given boundary conditions has been studied for several years. Such behavior has been investigated mainly in the case of boundary conditions that cause the appearance of two distinct magnetic phases meeting at a more or less well-defined interface.[1-6]

The interface behavior has been studied both for two-dimensional and three-dimensional magnetic lattices; in the first case basically using a variation of the partition function approach.[2,3] The main conclusion is that in the $d = 2$ case (d is the dimension) the interface remains diffuse at all temperatures T below the critical T_c,[1-3] while in the $d = 3$ case it becomes sharp at low temperatures $0 \leqslant T < T_r$, where T_r is the interface roughening temperature.[4,5]

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In general, one can assume two types of boundary conditions: (1) a "surface" one, where the spins at the surface of the magnetic lattice are properly fixed, and one is interested in the bulk behavior of the two different phases thus induced; (2) a "bulk" one, where a certain spin (or cluster of spins) in the bulk of the system is fixed in the presence of a uniform magnetic phase of opposite magnetization, and one is interested in the behavior of the magnetization around the fixed spin.

The algebraic method used in the literature for treating the interface problem[2,3] consists in calculating rigorously, for a given partition function, the "one-spin" correlation function, or magnetization, along a column of the lattice that divides the interface, using the transfer matrix approach and the matrix element techniques of Abraham.[7] On the other hand, the knowledge of the partition function is not necessary for the calculation of the thermodynamic behavior of an Ising system, according to a method proposed by Eggarter.[8] This method introduces neighboring spin pair probabilities, and is exact for a one-species Ising system on a Bethe lattice and equivalent to the Bethe–Peierls approximation for real lattices. Assuming homogeneous behaviour throughout an infinite system, Eggarter effectively ignores the influence of any specific boundary condition, or rather he considers periodic boundary conditions.

In the present paper we extend Eggarter's method to the case of an Ising system on a Bethe lattice in the presence of given boundary conditions of the "surface" or the "bulk" type mentioned above. One can introduce and calculate site-dependent spin pair probabilities and obtain in this way the thermodynamic behavior of such a system. Our method can easily include an external magnetic field as well and study its influence.

We found that the special topology of the Bethe lattice in the case of "surface" boundary conditions, causing the appearance of two distinct phases, gives results that are qualitatively different from those in real lattices. The main interest of our treatment in this case lies in the fact that the method can be further extended[9] to include substitutional disorder, providing an insight into the influence of the disorder on the interface behavior.

In the case of the "bulk" boundary condition our method gives results that should hold (within the general limitations of the Bethe–Peierls approach) for real lattices, too, because the Bethe lattice imitates quite accurately the local topology of a real lattice.

In Section 2 we present the formalism leading to the behavior of the local magnetization throughout our system. We also present and discuss the results for the case of "surface" as well as "bulk" boundary conditions.

2. DEFINITION OF THE MODEL AND RESULTS

We consider a system of classical spins $\sigma_{z_i} = \pm 1$ with the related magnetic moments $\mu_{z_i} = \sigma_{z_i}\mu_0$, localized on the sites $\{i\}$ of a Bethe lattice, and having the usual Ising interactions:

$$\mathscr{H} = -\sum_{ij} J_{ij}\sigma_{z_i}\sigma_{z_j} - \mu_0 H \sum_i \sigma_{z_i} \tag{1}$$

where $J_{ij} = J > 0$ (ferromagnetic) for i, j nearest neighbors but $J_{ij} = 0$ otherwise, and z denotes the magnetic field direction. For simplicity, from now on we drop the index z from our notation.

Our Bethe lattice consists of a Cayley tree, of coordination number Z, branching out of a central lattice site O in N homocentric layers of sites. The lattice terminates in an external boundary layer labeled N. Moving inwards, we label $N-1$, $N-2$,..., 1 the successive layers of the lattice up to the layer 1 adjacent to the central site O. Each layer n contains $N_n = Z(Z-1)^{n-1}$ lattice sites, and consequently the lattice as a whole contains a total of

$$N_{\text{tot}} = 1 + \frac{Z}{Z-2}\left[(Z-1)^{N+1} - 1\right]$$

sites.

We introduce the following layer-dependent spin pair probabilities $P_n^+(\sigma_n, \sigma_{n+1})$ and $P_n^-(\sigma_n, \sigma_{n-1})$, referring to neighboring sites on two adjacent layers, and the corresponding single-site probabilities $P_n^+(\sigma_{n+1}/\sigma_n)$, $P_n^-(\sigma_{n-1}/\sigma_n)$, and $P_n(\sigma_n)$.

The following relations hold:

$$P_n^+(\sigma_n, \sigma_{n+1}) = P_n^+(\sigma_{n+1}/\sigma_n)\, P_n(\sigma_n) \tag{2}$$

$$P_n^-(\sigma_n, \sigma_{n-1}) = P_n^-(\sigma_{n-1}/\sigma_n)\, P_n(\sigma_n) \tag{3}$$

$$P_n^+(\sigma_n, \sigma_{n+1}) = P_{n+1}^-(\sigma_{n+1}, \sigma_n) \tag{4}$$

$$P_n(\sigma_n) = \sum_{\sigma_{n+1}} P_n(\sigma_n, \sigma_{n+1}) = \sum_{\sigma_{n-1}} P_{n-1}^+(\sigma_{n-1}, \sigma_n) \tag{5}$$

and

$$\sum_{\sigma_n, \sigma_{n+1}} P_n^+(\sigma_n, \sigma_{n+1}) = 1 \tag{6}$$

2.1. Fixed Spins on the Surface

We introduce first the following "surface" boundary conditions: The spins on half of the layer N are fixed "up" ($\sigma_N = +1$) and those on the other half are fixed "down" ($\sigma_N = -1$) (see Fig. 1).

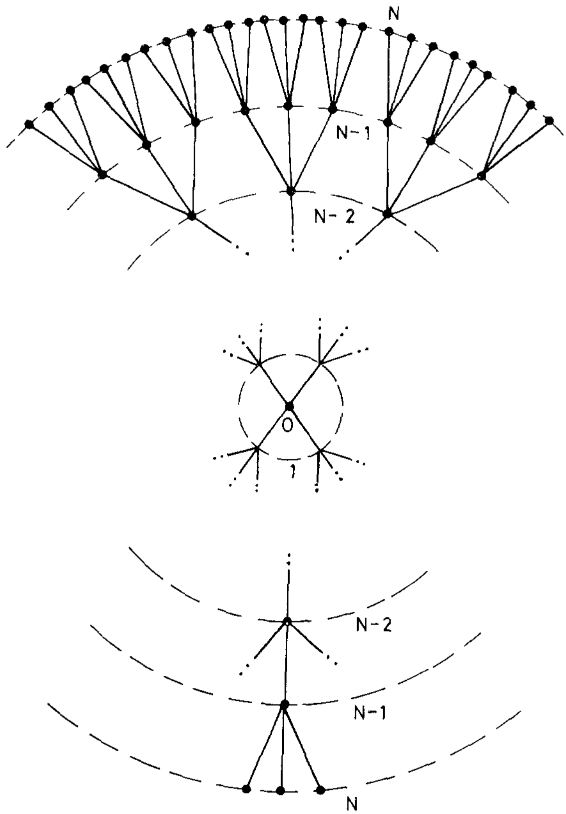

Fig. 1. Bethe lattice with coordination number $Z=4$ and N homocentric layers branching out from a central lattice site O. On the upper half-layer N we fix $\sigma_N = +1$ and on the lower half-layer N we fix $\sigma_N = -1$.

Following Eggarter, we consider a spin σ_n on layer n and its Z neighbors, $Z-1$ of which belong to the layer $n+1$ and the other one to the layer $n-1$. We express the probability of having σ_n surrounded by v_{n+1} spins up and μ_{n+1} down on layer $n+1$ $(v_{n+1}+\mu_{n+1}=Z-1)$ and v_{n-1} up and μ_{n-1} down on layer $n-1$ $(v_{n-1}+\mu_{n-1}=1)$ as

$$\begin{aligned} &P_n(\sigma_n, v_{n+1}, \mu_{n+1}, v_{n-1}, \mu_{n-1}) \\ &\quad = P_n(\sigma_n)\, P_n^+(\uparrow/\sigma_n)^{v_{n+1}}\, P_n^+(\downarrow/\sigma_n)^{\mu_{n+1}}\, P_n^-(\uparrow/\sigma_n)^{v_{n-1}}\, P_n^-(\downarrow/\sigma_n)^{\mu_{n-1}} \qquad (7) \end{aligned}$$

The change in energy when we flip spin σ_n from "up" to "down" is

$$\Delta E = 2\mu_0 H + 2J[(v_{n+1}-\mu_{n+1}) + (v_{n-1}-\mu_{n-1})]$$

and

$$\frac{P_n(\uparrow, \nu_{n+1}, \mu_{n+1}, \nu_{n-1}, \mu_{n-1})}{P_n(\downarrow, \nu_{n+1}, \mu_{n+1}, \nu_{n-1}, \mu_{n-1})}$$
$$= \exp(2\mu_0 \beta H) \exp\{2\beta J[(\nu_{n+1} - \mu_{n+1}) + (\nu_{n-1} - \mu_{n-1})]\} \quad (8)$$

where $\beta = 1/kT$. The relation is satisfied for all values ν_{n+1}, μ_{n+1}, ν_{n-1}, and μ_{n-1} such that $\nu_{n+1} + \mu_{n+1} + \nu_{n-1} + \mu_{n-1} = Z$.

Relation (8) can give two independent equations. The first is obtained by giving any specific values to the (ν, μ). For example, for $\nu_{n+1} = Z - 1$, $\nu_{n-1} = 1$, and $\mu_{n+1} = \mu_{n-1} = 0$ we obtain

$$\left(\frac{P_n^+(\uparrow/\uparrow)}{P_n^+(\uparrow/\downarrow)}\right)^{Z-1} \frac{P_{n-1}^+(\uparrow, \uparrow)}{P_{n-1}^+(\uparrow, \downarrow)} = \exp(2\beta\mu_0 H + 2\beta Z J) \quad (9a)$$

and for $\nu_{n+1} = 0$, $\nu_{n-1} = 1$, $\mu_{n+1} = Z - 1$, and $\mu_{n-1} = 0$

$$\left(\frac{P_n^+(\downarrow/\uparrow)}{P_n^+(\downarrow/\downarrow)}\right)^{Z-1} \frac{P_{n-1}^+(\uparrow, \uparrow)}{P_{n-1}^+(\uparrow, \downarrow)} = \exp[2\beta\mu_0 H + 2\beta(2 - Z)J] \quad (9b)$$

The second relation is obtained when (9a) or (9b) is divided by the equation that is derived from (8) when $\nu'_{n+1} = \nu_{n+1} - 1$, $\mu'_{n+1} = \mu_{n+1} + 1$, $\nu_{n-1} = 1$, and $\mu_{n-1} = 0$:

$$\frac{P_n^+(\uparrow, \uparrow)\, P_n^+(\downarrow, \downarrow)}{P_n^+(\downarrow, \uparrow)\, P_n^+(\uparrow, \downarrow)} = e^{4\beta J} \quad (9c)$$

We observe that the set of relations (5), (6), and (8), because of relations (2)–(4), contains the unknown spin-pair probabilities $P_n^+(\sigma_n, \sigma_{n+1})$, $P_{n-1}^+(\sigma_{n-1}, \sigma_n)$, $\sigma = \pm 1$, i.e., four on each layer. These can be calculated only after the boundary conditions of the system have been specified and will be different at different parts of the same layer, depending on the corresponding boundary conditions. Therefore, in the present case the probabilities will be the same on half of each layer, but different from those on the other half, as the assumed boundary conditions require. To obtain such a solution, one has in principle to calculate $8N$ pair probabilities $P^+(\sigma, \sigma')$, $4N$ for every half layer, that are properly matched at the central lattice O, a lengthy but straightforward process. We note, nevertheless, that for the present study of the interface structure a simpler calculational approach can be used.

The boundary conditions on the layer N can be expressed as follows:

$$\begin{aligned} P^+_{N-1}(\uparrow/\uparrow) &= P^+_{N-1}(\uparrow/\downarrow) = 1 \\ P^+_{N-1}(\uparrow, \downarrow) &= P^+_{N-1}(\downarrow, \downarrow) = 0 \end{aligned} \tag{10a}$$

in terms of spin pair probabilities, for the "spin-up" half of the layer. Also,

$$\begin{aligned} P^+_{N-1}(\downarrow/\uparrow) &= P^+_{N-1}(\downarrow/\downarrow) = 1 \\ P^+_{N-1}(\uparrow, \uparrow) &= P^+_{N-1}(\downarrow, \uparrow) = 0 \end{aligned} \tag{10b}$$

for the "spin-down" half of the layer.

These boundary conditions permit the calculation of the quantity

$$X_n \equiv P^+_n(\uparrow, \uparrow)/P^+_n(\uparrow, \downarrow), \qquad n \in [0, N-1] \tag{11}$$

throughout the lattice, by using the following recurrence relations:

$$X^\uparrow_{n-1} = \left(\frac{X^\uparrow_n + 1}{X^\uparrow_n + e^{4\beta J}}\right)^{Z-1} \exp(2\beta ZJ + 2\beta\mu_0 H) \tag{12a}$$

for the "spin-up" part of the layer, and

$$X^\downarrow_{n-1} = \left(\frac{X^\downarrow_n + 1}{X^\downarrow_n e^{-4\beta J} + 1}\right)^{Z-1} \exp[2\beta(2-Z)J + 2\beta\mu_0 H] \tag{12b}$$

for the "spin-down" part.
The recurrence relations follow from (9a) and (9b) by using (2), (5), (9c), and (11).

We observe that at zero magnetic field ($H=0$) relations (12a) and (12b) coincide.

Starting from the surface and using the boundary conditions (10a) and (10b), we obtain the X_{N-2}

$$X^\uparrow_{N-2} = \exp(2\beta ZJ + 2\beta\mu_0 H) \tag{13a}$$

$$X^\downarrow_{N-2} = \exp[2\beta(2-Z)J + 2\beta\mu_0 H] \tag{13b}$$

from Eqs. (9a) and (9b) for $n = N-1$, while the same boundary conditions imply

$$X^\uparrow_{N-1} = \infty, \qquad X^\downarrow_{N-1} = 0$$

from the definition (11) of X_n.

The behavior of the iteration scheme for the X_n [Eqs. (12a) and (12b)], starting from $n = N-2$, is shown in Fig. 2 for the case $Z=4$ and

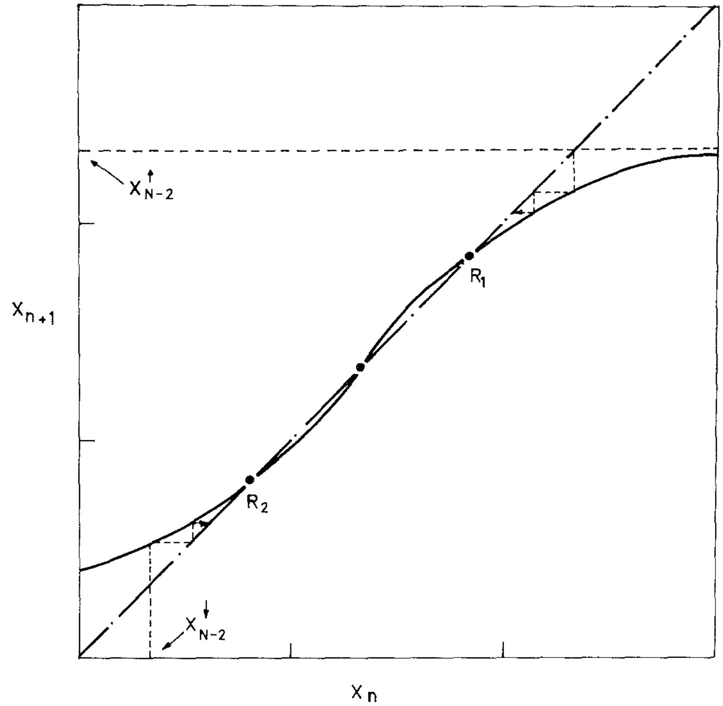

Fig. 2. Iteration scheme for the successive values of X_n, $n = N-2, N-3, \ldots$, for $Z = 4$, $H = 0$, and $kT/J = 2.6$. For any given value of X_n on the X_n axis, the continuous curve determines the subsequent value X_{n+1} and the iteration scheme progresses as indicated by the dashed lines, converging to either one of the fixed points R_i, $i = 1$ or 2, depending on the starting point (phase 1 or phase 2).

$H = 0$. The iteration has two attracting points given by two appropriate roots R_1 and R_2 of the fourth degree (in this case) algebraic equation obtained from (12a) or (12b) when we put $X_{n-1} = X_n = R$ in it. The temperature dependence of R_1 and R_2 is shown in Fig. 3. At $kT/J = 2.8854$ the two roots coincide and we identify this temperature as the critical temperature T_c.

The iteration scheme converges to R_1 or R_2, depending on the boundary value $X^{\uparrow}_{N-2}$ or $X^{\downarrow}_{N-2}$, respectively, and R_1 and R_2 give the bulk (far from the surface) behavior of the corresponding "spin-up" (1) "spin-down" (2) phase. From R_1 and R_2 one can thus calculate the "bulk" spin pair probabilities $P^{\infty}_{1,2}(\sigma, \sigma')$ by putting $P^{\infty}_{1,2}(\uparrow, \downarrow) = P^{\infty}_{1,2}(\downarrow, \uparrow)$ and using (9c) and the normalization condition (6), provided that the system is large enough to consider the bulk region as far from either the surface or the interface region. In this case our solutions coincide with Eggarter's.[8]

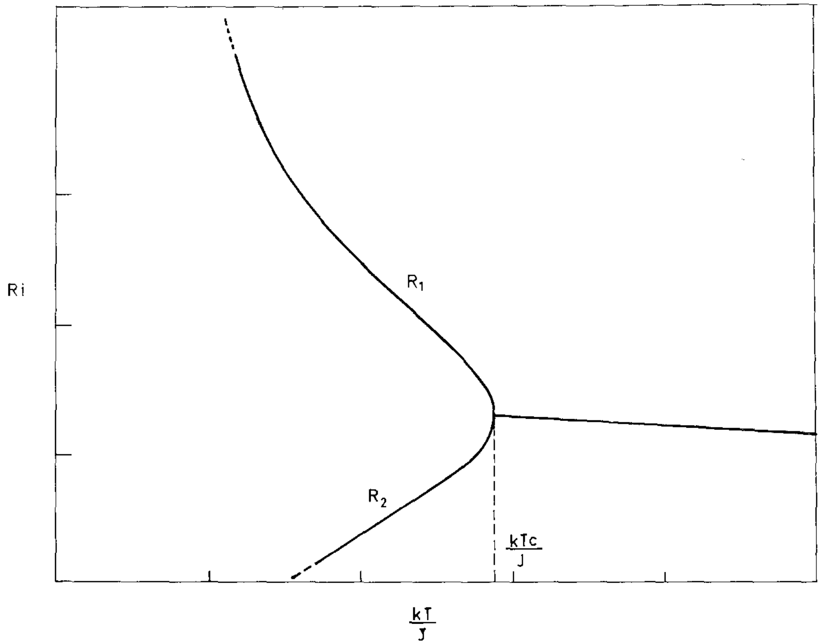

Fig. 3. Temperature dependence of the fixed points R_1 and R_2 of the iteration scheme [Eqs. (12a) and (12b)]. R_1 and R_2 coincide at the critical temperature $kT_c/J = 2.8854$.

The magnetization of the system at any layer n is given by

$$m_n = \mu_0[P_n(\uparrow) - P_n(\downarrow)] = \mu_0[1 - 2P_n(\downarrow)] \tag{14}$$

and away from either the surface or the center of the lattice, is given as

$$\begin{aligned} m_1^\infty &= \mu_0[P_1^\infty(\uparrow) - P_1^\infty(\downarrow)] > 0 \\ m_2^\infty &= \mu_0[P_2^\infty(\uparrow) - P_2^\infty(\downarrow)] < 0 \end{aligned} \tag{15}$$

The two halves of the system that contain phases 1 and 2 correspondingly meet at the central site O, and by symmetry of the construction of the lattice the magnetization should be zero there, $m_0 = 0$. This condition permits the calculation of the magnetization of each phase away from the central site O, according to the following iteration scheme:

Using (5), (9c), and (11), we have

$$\begin{aligned} P_n(\uparrow) &= P_n^+(\uparrow\downarrow)(1 + X_n) \\ P_n(\downarrow) &= P_n^+(\downarrow\downarrow)(1 + X_n e^{-4\beta J}) \end{aligned}$$

and therefore

$$P_{n+1}(\downarrow) = \frac{1 - P_n(\downarrow)}{1 + X_n} + \frac{P_n(\downarrow)}{1 + X_n e^{-4\beta J}} \tag{16}$$

Combining (16) and (14), we obtain for the magnetization the following recurrence relation:

$$\frac{m_{n+1}^i}{\mu_0} = \frac{X_n - 1}{X_n + 1} + \left(1 - \frac{m_n^i}{\mu_0}\right) \frac{X_n}{X_n + 1} \frac{1 - e^{4\beta J}}{X_n + e^{4\beta J}} \tag{17}$$

where $i = 1$ or 2 corresponding to the two phases. This relation determines the magnetization behavior near the surface as well as in the interface or bulk region.

Working in the interface region first, we observe that in the bulk of the lattice, X_n converges to R_i. Since $m_0 = 0$ at the central site, as discussed above, we can obtain the behavior of the magnetization away from the central site O, by substituting $X_n = R_i$ and $m_0 = 0$ in Eq. (17) (where $i = 1, 2$) and iterating relation (17).

Figure 4 shows the behavior of m_n around the central site for three different temperatures. The magnetization changes appreciably over distances

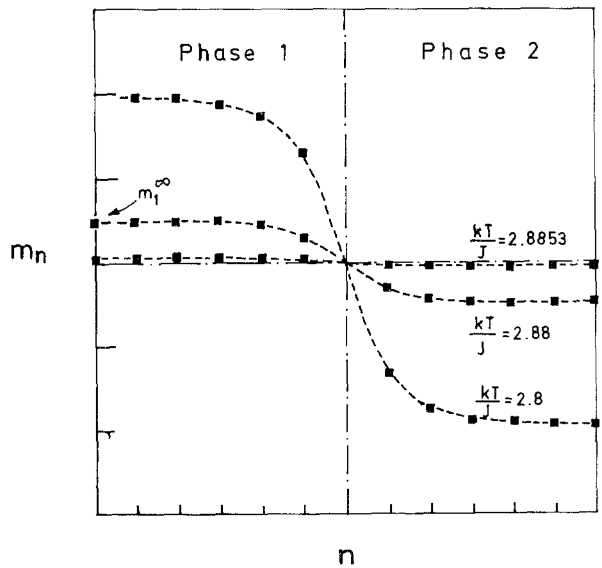

Fig. 4. Magnetization (m_n) behavior on successive layers $n = 1, 2, 3, \ldots$ away from the central site O, where the two phases 1 ("up") and 2 ("down") meet, for the three different temperatures indicated.

of only a few lattice sites, approaching the corresponding value m_i^∞ $(i=1, 2)$ asymptotically, and therefore the interface region remains sharp (nondiffuse) at all $T<T_c$. Introducing $W=(m_\infty - m_1)/m_1$ as a measure of the interface width, we find that with increasing temperature in the range $(0, T_c)$, W remains almost zero at low T and then, increasing slowly for T around $T_c/2$, W passes to a relatively fast linear increase with T approaching T_c, in qualitative similarity with the cubic lattice case,[5] where the interface becomes diffuse for $T>T_r=T_c/2$.

For the magnetization near the surface of either of the two phases, on the other hand, we cannot proceed by iterating Eq. (17) because (1) starting from the surface where $m_N = \pm\mu_0$, we canot use Eq. (17) for m_{N-1}, since X_{N-1} is zero or infinity, as discussed above, and (2) starting from the bulk where $m_n = m_i^\infty$ and $X_n = R_i$, we cannot iterate (12a) or (12b) toward the surface, since R_i is a fixed point of the iteration. Instead, we develop the following scheme starting from the observation that, according to Eq. (17), m_{n+1} will be larger than m_n only if $m_n < m_n^\rho$, where m_n^ρ is the root of Eq. (17), i.e., the value of m_n that gives $m_{n+1} = m_n$, because [see Eq. (17)]

$$m_{n+1} = m_n^\rho + c_n(m_n + m_n^\rho), \qquad c_n = \frac{e^{4\beta J} - 1}{e^{4\beta J} + X_n} \frac{X_n}{X_n + 1}, \qquad 0 \leqslant c_n < 1 \tag{18}$$

Therefore, the value of m_{N-1} that will produce a sequence of m_n $(n=N-2,\ N-3, \ldots)$ that decreases monotonically away from the surface, converging to m_i^∞ $(i=1$ or $2)$, should be

$$\begin{aligned} m_{N-1} = m_{N-2}^\rho - c_{N-2}\, \Delta m_{N-2}^\rho \\ - c_{N-2} c_{N-3}\, \Delta m_{N-3}^\rho - c_{N-2} c_{N-3} c_{N-4}\, \Delta m_{N-4}^\rho - \cdots \end{aligned} \tag{19}$$

where $\Delta m_n^\rho = m_n^\rho - m_{n-1}^\rho$.

The series converges uniformly in the limit $N \to \infty$, being bounded by a geometric series, because $c_n > c_{n-1}$, $\forall_n$, implying

$$\prod_{i=2}^{k} c_{N-i} < c_{N-2}^{k-1}$$

and $\Delta m_n^\rho \to 0$ as we move away from the surface, since $X_n \to R_i$ there. The convergence is so fast for all finite T that we get adequate accuracy when we keep only the first two terms of the series expansion for m_n, Eq. (19). Figure 5 shows the behavior of m_n away from the surface in phase 1, at $kT/J = 2.6$. The phase 2 case is symmetrically opposite to phase 1.

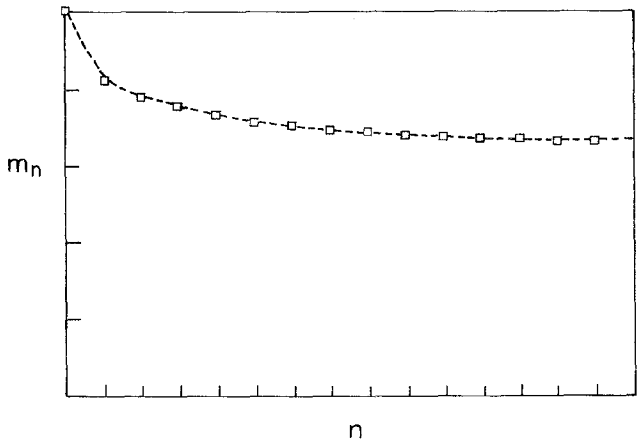

Fig. 5. Magnetization (m_n) behavior on successive layers $n = N-1$, $N-2$,... away from the surface layer N, where we fix $m_N = +\mu_0$, for $kT/J = 2.6$. The $m_N = -\mu_0$ case is symmetrically opposite.

2.2. Fixed Spin in the Bulk

We consider now the case where a spin at a certain site in the bulk of the system is fixed "down" while the system is kept at a uniform phase "up" by properly adjusting the boundary conditions at infinity. For simplicity we take site O as hosting the fixed spin and thus we have $m_0 = -\mu_0$.

According to the analysis presented in Section 2.1, the behavior of the magnetization m_n, $n = 1, 2, 3,\ldots$, around the fixed spin can be obtained iteratively from (17) by putting $X_n = R_1$ (since we are in the bulk of a phase "up") and starting with $m_0 = -\mu_0$.

Figure 6 shows such behavior of m_n for several successive layers around O and for three different T.

2.3. Concluding Remarks

The influence of specific boundary conditions on the thermodynamic behavior of an Ising system has been treated explicitly, and is the main feature of the present work.

In the present study we derive the thermodynamic behavior in all parts of the system and especially in the vicinity of the fixed spins, as well as in the interface region. Although our results have a general validity corresponding only to the Bethe–Peierls approximation for real lattices, some interesting features are brought about in two respects.

First, as mentioned above, is the behavior of the system in the vicinity of the bounds, a characteristic that is apparently retained in the finite

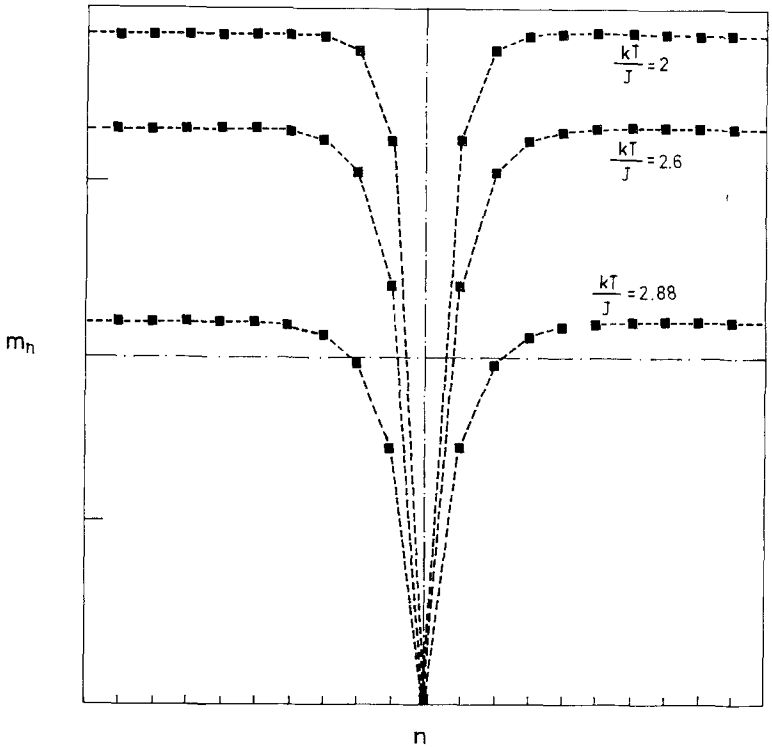

Fig. 6. Magnetization (m_n) behavior on successive layers $n = 1, 2, 3,...$ away from a site O with a fixed spin $\sigma_0 = -1$, in the bulk of an "up" phase, for the three different temperatures indicated.

system, and may be of central importance there. Our analysis not only holds for a finite system, but also shows how the behavior of successively larger systems evolves toward the thermodynamic limit.

A second feature of our analysis is the possibility of its extention[9] to incorporate substitutional disorder, and thus study its influence on the interface region. One thus can reveal qualitative characteristics of such influence that also should be present in real lattices.

In closing, we believe that this last feature opens a way for studying in a more quantitative fashion the role of a factor of importance in many cases (alloys, etc.).

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