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Influence of Disorder on the Interface Sharpness of an Ising Ferromagnetic System

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We study the thermodynamic behavior of a two-component random ferromagnetic Ising system in the presence of given boundary conditions. The system consists of two species A and B occupying the sites of a Bethe lattice which terminates on a surface layer where the spins are kept fixed. We study the interface of the system when the spins on half of the surface of the lattice are fixed opposite to the spins on the other half. More specifically, we study the influence of disorder on the interface width. We find that disorder clearly increases the interface width at temperatures well below T_c, indicating that the interface roughening of disordered Ising systems in 3D real lattices should occur at temperatures significantly below those of the corresponding ordered ones.

KEY WORDS: Ising; Bethe; interface; disorder.

1. INTRODUCTION

The thermodynamic behavior of a ferromagnetic system under boundary conditions that cause the appearance of two distinct magnetic phases meeting at an interface has been studied for several years.[1–7]

The interface behavior has been studied for ordered Ising systems in 2D (square),[1–3] 3D (cubic),[4,5] and Bethe[7] lattices. 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 $0 \leqslant T \leqslant T_R$,[4–6] where T_R is the roughening temperature. In the disordered system case there is some relatively recent work,[8] studying certain interesting aspects of the interface behavior.

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In the present paper we study the influence of disorder on the interface width of a specific magnetic binary alloy system.

Our system is an Ising ferromagnet on a Bethe lattice and disorder is introduced by assuming two types of species A and B randomly distributed on the lattice sites. In a recent paper[7] the ordered case has been studied by developing a method similar to Eggarter's[9] and here we further extend our method to include disorder.

The starting point for this extension is a system whose bulk behavior is studied in a recent paper.[10] In this system, if we allow species A and B to interchange positions in a way that a certain pair correlation is maintained at a given temperature, we can obtain the exact bulk values of its thermodynamic potentials on the Bethe lattice, and, as shown in ref. 10, these values coincide with the ones obtained by Eggarter's treatment of the corresponding frozen-species (quenched) case. The extension of the interface case is along the lines presented in ref. 7 and the obtained behavior is exact. Proper choice of the parameters defining the ensemble of disordered systems under study can maintain constant the local species concentration and pair correlation and this is a case of a partially annealed system that should resemble closely the quenched one.

Thus, in Section 2 we present the formalism and in Section 3 we present and discuss our results and their relevance to the interface behavior of random Ising systems in 3D real lattices.

2. FORMALISM

We consider an Ising spin system on a Bethe lattice, with spin carrying atoms of two kinds, called species A and B, randomly distributed on the lattice sites.

The Hamiltonian of the system is given by

$$H = -\sum_{\langle ij \rangle} \{J(X_i, X_j)\, \sigma_i \sigma_j + U(X_i, X_j)\} \tag{2.1}$$

where $\sigma_i = \pm 1$ indicates the two possible spin directions on site i, $J(X_i, X_j) > 0$ are the ferromagnetic coupling constants for the neighboring X_i, X_j species ($X = \mathrm{A}$ or B), and $U(X_i, X_j)$ are neighboring species interactions, with $U(\mathrm{A}, \mathrm{A}) > 0$, $U(\mathrm{B}, \mathrm{B}) > 0$ and $U(\mathrm{A}, \mathrm{B}) < 0$.

Our Bethe lattice consists of a Cayley tree, of coordination number z, branching out of a central lattice site 0 in N homocentric layers of sites. The lattice terminates in an external surface layer labeled N. Moving inward, we label $N-1, N-2, \ldots, 1$, the successive layers of the lattice, up to the layer 1 adjacent to the central site 0 (see ref. 7, Fig. 1). Each layer n

contains $N_n = z(z-1)^{n-1}$ lattice sites, and consequently the lattice as a whole contains a total of

$$N_{\text{tot}} = 1 + \frac{z}{z-2}(z-1)^{N+1} - 1$$

sites.

As in the one-species case,[7] we consider here z even ($z=4$ for simplicity) and assume the following phase separating boundary conditions: The spin directions on all sites on one half of the surface layer N are fixed "up" ($\sigma_N = +1$) and those on the other half are fixed "down" ($\sigma_N = -1$), giving rise to magnetic phases 1 and 2, respectively. The species are fixed A throughout the whole surface layer.

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

In a preceding paper,[10] as mentioned in the Introduction, we have shown that the system considered behaves like one with four states per site, where state $1 \equiv (\text{A}, \uparrow)$, state $2 \equiv (\text{A}, \downarrow)$, state $3 \equiv (\text{B}, \uparrow)$, and state $4 \equiv (\text{B}, \downarrow)$. Then the pair and single probabilities introduced above take the simpler form $P_n(k_n, k_{n-1})$, $P_n(k_n)$, where $k_n \equiv (X_n, \sigma_n)$, and obey the relations

$$\sum_{t=1}^{4} \sum_{k=1}^{4} P_n(t, k) = 1 \tag{2.2a}$$

$$\sum_{t=1}^{4} P_{n+1}(t, k) = P_n(k) = \sum_{t=1}^{4} P_n(k, t) \tag{2.2b}$$

The basic thermodynamic relations used originally by Eggarter[9] can be extended as follows:

$$\frac{P(k_n, k_{n+1,1}, k_{n+1,2}, \ldots, k_{n+1,z-1}, k_{n-1,z})}{P(k'_n, k_{n+1,1}, k_{n+1,2}, \ldots, k_{n+1,z-1}, k_{n-1,z})} = \exp\{\beta\, \Delta E(k_0, k'_0, k_1, \ldots, k_z)\} \tag{2.3}$$

where $(n+1, 1)$, $(n+1, 2)$,..., $(n+1, z-1)$ are the $z-1$ nearest neighbors of site n situated on layer $n+1$, $(n-1, z)$ is its zth nearest neighbor situated on layer $n-1$, and the $\{k\}$ ($k = 1, 2, 3, 4$) are the states considered on those sites. This relation is exact in thermodynamic equilibrium due to the Cayley tree topology (ref. 7, Fig. 1).

The imposed boundary conditions imply statistical homogeneity inside each magnetic phase (i.e., on each half of any layer n) and then relations (2.3) can be written in terms of single and pair probabilities:

$$\left(\frac{P_n^i(k)}{P_n^i(1)}\frac{P_{n+1}^i(1,1)}{P_{n+1}^i(1,k)}\right)^{z-1}\frac{P_n^i(1,t)}{P_n^i(k,t)} = e^{\beta\,\Delta E_{k,t}} \tag{2.4}$$

where we consider a transition from state 1 to state k ($k=2, 3, 4$) on a site on layer n, while the state 1 is realized on its $z-1$ neighbors on layer $n+1$ and the state t ($t=1, 2, 3, 4$) on its zth neighbors on layer $n-1$. The $\Delta E_{k,t}$ are given in Table I, and i is a phase index. Omitting from now on the phase index for simplicity, we proceed to derive the equations determining the $P(k, t)$ in each phase.

For given k we divide by parts two of the relations (2.4), one with $t=1$ and the other with $t=t$, and we obtain nine relations of the form

$$\frac{P_n(k,t)}{P_n(1,t)} = x_n(k)\exp\{\beta(\Delta E_{k,1}-\Delta E_{k,t})\} \tag{2.5}$$

where $k=2, 3, 4$; $t=2, 3, 4$; $\Delta E_{k,t}$ are given in Table I, and we define

$$x_n(k) \equiv P_n(k,1)/P_n(1,1) \tag{2.6}$$

Using (2.2b), (2.5), and (2.6) in relations (2.4) for $t=1$, we obtain three relations of the form

$$\left[\frac{1+\sum_{t=2}^{4} x_{n+1}(t)\exp\{\beta(\Delta E_{t,1}-\Delta E_{t,k})\}}{1+\sum_{t=2}^{4} x_{n+1}(t)}\right]^{z-1} = x_n(k)\exp\beta\,\Delta E_{k,1} \tag{2.7}$$

with $k=2, 3, 4$ and $\Delta E_{k,1}$ from Table I, which hold for every site other than the central.

Relations (2.7) constitute a system of three recurrence relations for the $x_n(k)$, $k=2, 3, 4$. The system has fixed points $\{x_\infty(k)\}$ obtained by putting

Table I. Excitation Energies ΔE_{kt} of Relations (2.4)

t	$k=2$	$k=3$	$k=4$
1	$e^{8\beta(J_{AA})}$	$e^{4\beta(J_{AA}-J_{AB})+4\beta(U_{AA}-U_{AB})}$	$e^{4\beta(J_{AA}+J_{AB})+4\beta(U_{AA}-U_{AB})}$
2	$e^{4\beta J_{AA}}$	$e^{2\beta(J_{AA}-J_{AB})+4\beta(U_{AA}-U_{AB})}$	$e^{2\beta(J_{AA}+J_{AB})+4\beta(U_{AA}-U_{AB})}$
3	$e^{2\beta(3J_{AA}+J_{AB})}$	$e^{\beta(3J_{AA}-J_{BB}-2J_{AB}+3U_{AA}-U_{BB}-2U_{AB})}$	$e^{\beta(3J_{AA}+J_{BB}+4J_{AB}+3U_{AA}-U_{BB}-2U_{AB})}$
4	$e^{2\beta(3J_{AA}-J_{AB})}$	$e^{\beta(3J_{AA}+J_{BB}-4J_{AB}+3U_{AA}-U_{BB}-2U_{AB})}$	$e^{\beta(3J_{AA}-J_{BB}+2J_{AB}+3U_{AA}-U_{BB}-2U_{AB})}$

$x_{n+1}(k) = x_n(k)$ $(k = 2, 3, 4)$ and the iteration of (2.7) converges to attracting $\{x^i_\infty(k)\}$ among those fixed points, depending on the initial values $\{x^i_N(k)\}$, i.e., the boundary conditions.

As discussed above, proper boundary conditions on the surface of the system give rise to magnetic phases $\{i\}$ $(i = 1, 2)$ and the previous analysis shows that the values $\{x^i_\infty(k)\}$ are characteristic of the magnetic phase i and remain such as we approach the central site (interface region) from within the phase i, a behavior similar to the one in ref. 7.

In the presence of the assumed boundary conditions above, around the central site 0, for symmetry reasons, we have

$$P^1_1(X, \sigma; Y, \sigma') = P^2_1(X, -\sigma; Y, -\sigma'), \qquad X, Y = \text{A or B} \tag{2.8}$$

Three more equations similar to (2.7) hold there (when $z = 4$)

$$\frac{P_0(k)}{P_0(1)} \left(\frac{P^1_1(1, 1)}{P^1_1(1, k)} \right)^2 \left(\frac{P^2_1(1, 1)}{P^2_1(1, k)} \right)^2 = e^{\beta \Delta E_{k,1}} \tag{2.9}$$

with $k = 2, 3, 4$ and $\Delta E_{k,1}$ from Table I, which can be written in terms of $P(k, t)$ referring to one of the two phases by using (2.2b) and (2.8). We now have enough equations to determine the 16 $P^i_1(t, k)$ ($i = 1$ or 2) around the central site.

These are the nine relations (2.5), the three relations (2.6) for $x^i_1(k) = x^i_\infty(k)$, $k = 2, 3, 4$ [$x_\infty(k)$ obtained by proper iteration of 2.7], the three relations (2.9), and the normalization condition (2.2a). Having obtained the $P^i_1(t, k)$, we proceed to calculate in successive steps the $P^i_n(t, k)$, $n = 2, 3, \ldots \ll N$, by observing that relations (2.2b) provide three independent equations relating the $P^i(t, k)$ on adjacent layers that replace the (2.9) used for the $P^i_1(t, k)$, the remaining 13 equations holding for every layer n far away from the surface.

The calculation of layer-dependent quantities like magnetization m^i_n,

$$m^i_n = 2[P^i_n(\text{A}\uparrow) + P^i_n(\text{B}\uparrow)] - 1, \qquad i = 1, 2 \tag{2.10}$$

and concentration $c_{\text{A},n}$,

$$c_{\text{A},n} = p^i_n(\text{A}\uparrow) + p^i_n(\text{A}\downarrow), \qquad i = 1, 2 \tag{2.11}$$

is then straightforward by using (2.2b). Under the given boundary conditions they obey $m^1_n + m^2_n = 0$ and $c^1_{\text{A},n} = c^2_{\text{A},n}$.

Moving away from the interface region, we obtain the bulk behavior of the system that obtains in those layers $\{n\}$ for which $1 \ll n \ll N$. There $P^i_n(k, t) = P^i_\infty(k, t)$ and $m^i_n = m^i_\infty$ $(i = 1, 2)$, $c_{\text{A},n} = c_{\text{A},\infty}$, where (∞) denotes the corresponding bulk value.

Those bulk values coincide with the ones obtained by Eggarter's bulk method[9] when the values of concentration $c_{A,\infty}$ and species correlation

$$P_{A/B,\infty} = (1 - c_{A,\infty})^{-1} \sum_{\sigma,\sigma'} P_{\infty}(A\sigma, B\sigma')$$

obtained above are used in his formalism.[9]

3. RESULTS AND DISCUSSION

As discussed in the Introduction, the formalism developed in Section 2 treats exactly the interface behavior of a magnetic binary alloy with given species concentration and pair correlation on a Bethe lattice, i.e., the close equivalent to the frozen-species one.

The thermodynamic behavior obtained through our formalism is thus an approximation (a "Bethe–Peierls type" one according to Eggarter[9]) to the frozen-species case, since only species concentration and pair correlation are really frozen in it. Our formalism therefore constitutes the Eggarter-equivalent approximation for the interface behavior of a frozen-species system and our results have a similar validity, which has so far been successfully tested in the bulk cases.[9,11–13]

Applying the above formalism to our system, one can get the local magnetization and species concentration profile in the interface region. The magnetization profile we get is similar to the one-species case,[7] being sharp throughout the whole temperature range 0 to T_c. Figure 1 shows the magnetization and concentration profile.

The concentration profile is symmetric around the central site and with proper choice of parameters can become constant throughout the whole bulk and interface region of the system.

One such choice is to take $J_{AA} = J_{BB}$ and $c_A = 0.5$. In such a case there remain three independent parameters, namely J_{AA}, J_{AB}, and the species correlation $P_{A/B}$.

The variance of J can serve as a measure of the disorder of such a binary system in analogy with the case of binary electronic disorder.[14] The variance is expressed in terms of the independent parameters as

$$\langle (J - \langle J \rangle)^2 \rangle = 4P_{A/B}(1 - P_{A/B}) \left(\frac{J_{AA} - J_{AB}}{2} \right)^2 \tag{3.1}$$

In what follows we study the behavior of a system in which we vary $P_{A/B}$ while keeping $J_{AA} = J_{BB} = 10J_{AB}$ fixed. In this case the disorder changes proportionally to the parameter $\sigma \equiv 4P_{A/B}(1 - P_{A/B})$ according to (3.1).

Following the one-species case,[7] we study the influence of the dis-

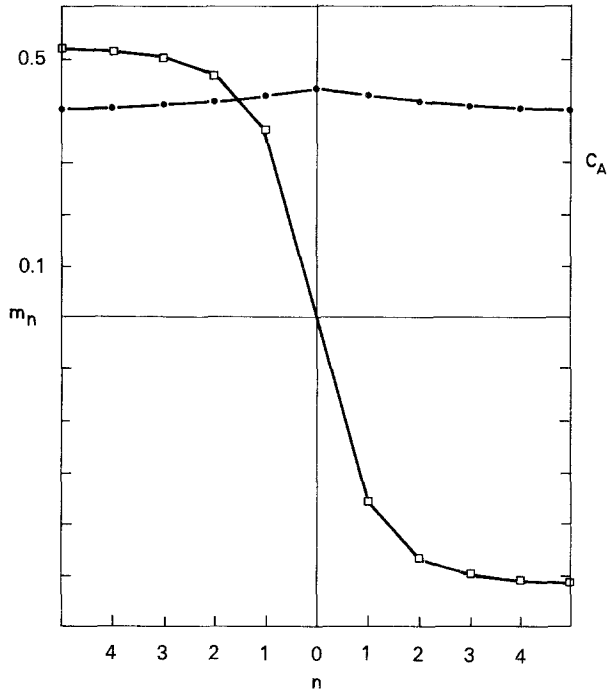

Fig. 1. Magnetization (m_n) and concentration (c_A) behavior on successive layers $n = 1, 2, 3,...$ away from the central site 0 for the case $c_A = 0.4$, $T = 0.9T_c$.

order σ on the magnetic interface by introducing a parameter W, indicating the degree of interface sharpness, as $W = (m_\infty - m_1)/m_1$, where m_n ($n = 1,..., \infty$) is the local magnetization at a site n layers away from the central site 0, where m_0 is zero for symmetry reasons. Note that in this definition $W = 0$ means the perfectly sharp interface and $W = \infty$ means the diffuse interface. The study of W with varying temperature is presented in Fig. 2 for three cases of σ ($\sigma = 1$, full disorder; $\sigma = 0.5$, intermediate disorder; and $\sigma = 0$, ordered case, where the W vs. T/T_c curve coincides with the one-species case).

Our results show a clear increase of interface width with respect to the ordered ($\sigma = 0$) case over the whole temperature range and especially around $T_R = 0.5T_c$,[5] where the interface width $W(\sigma)$ increases beyond the $W(\sigma = 0)$ value in a way roughly proportional to the disorder parameter σ. Such behavior indicates a significant influence of the disorder on the interface of our system. Disorder should have a similar influence on the interface of 3D real lattices as well, since in the ordered case there exists a qualitative similarity in the behavior of the interface between these lattices

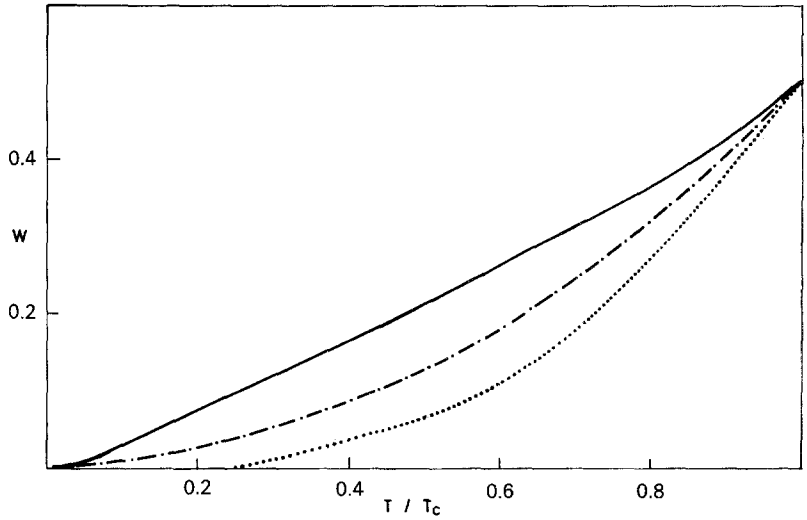

Fig. 2. Interface sharpness parameter W vs. T/T_c for three cases of the disorder parameter σ: (a) $\sigma = 1$ (solid line), (b) $\sigma = 0.75$ (dash-dotted line), and (c) $\sigma = 0$ (dotted line).

and the Bethe lattice, as can be shown through the following line of argument: Although our system depicts a sharp interface throughout the whole temperature range 0 to T_c due to the Bethe lattice topology, our system passes from almost perfect interface sharpness ($W \simeq 0$; see Fig. 2, $\sigma = 0$ case) for temperatures up to $T/T_c \simeq 0.3$, through an intermediate range onto a relatively fast-increasing interface width beyond $T/T_c \simeq 0.7$. We understand this behavior as the Bethe lattice analogy to 3D real lattices, reported as having an interface roughening transition[5] at $T_R/T_c = 0.5$ as discussed above.

In view of this analogy, our results for W (Fig. 2) clearly indicate that the disorder should push the reported[5] roughening transition T_R in 3D real lattices to significantly lower values, depending on the degree of disorder in the system. This qualitative conclusion about T_R is complementary to the results of ref. 8 concerning the influence of weak impurities on the domain wall roughness.

We believe that further study of the interface behavior throughout the whole parameter space of our system would not enhance the qualitative understanding of the role of disorder in real systems beyond the conclusions presented above, although these conclusions all but exhaust the subject.

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