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Solvable Model with a Roughening Transition for a Planar Ising Ferromagnet

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An exactly solvable modification of the planar Ising ferromagnet is proposed which has a roughening transition below the Curie temperature. The computation confirms the de Gennes–Fisher scaling theory of correlations with homogeneous surface fields, giving an exponent value $\Delta_1 = \frac{1}{2}$.

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The nature of the interface, or domain wall, between oppositely magnetized phases of a ferromagnet below its Curie temperature T_C has been the subject of considerable recent interest.[1-4] It has been realized that, even though there exists a well-defined specific incremental free energy for a domain wall,[5,6] in many situations the actual structure of such a wall is averaged out by capillary fluctuations unless some external stabilizing force is applied.

A phenomenology which is generally accepted is that the domain wall may undergo large fluctuations on a length scale determined by the area of the interface, but carries with it a local structure which, in the critical region, varies on the scale of the correlation length. It is to this local structure that the successful phenomenological theory developed by van der Waals, by Cahn and Hilliard, and by Fisk and Widom[7] refers.

The following remarks relate to simple-cubic Ising ferromagnets in d dimensions. For $d=2$, the interface between phases with magnetization $\pm m^*$, m^* being the spontaneous magnetization, is always diffuse for $0<T<T_C^{(2)}$; $T_C^{(d)}$ is the d-dimensional critical temperature.[6] For $d=3$, however, it is proven that for $0\leq T<T_C^{(2)}$ the interface is sharp[8]; there is, however, a temperature $T_R \sim T_C^{(2)}$ such that for $T_C^{(3)}>T>T_R$ the interface is diffuse. A *roughening transition* is said to occur at T_R. The evidence for this, which is not beyond dispute, deprives from series expansions[9] and Monte Carlo simulations.[10] A rigorous proof that there exists a $T_R<T_C^{(3)}$ has yet to be given.

In this paper an exactly solvable modification of the planar Ising model will be given which has a mechanism which localizes the interface at low temperatures and which has a roughening transition at a temperature $T_R<T_C^{(2)}$ whose properties can be investigated rigorously in considerable detail.

Consider a lattice $\Lambda(N,M)$ of points (n,m) such that $1\leq n\leq N$, $1\leq m\leq M$. At each such point place a spin $\sigma(n,m)=\pm 1$. A configuration of spins on $\Lambda(N,M)$, denoted by $\{\sigma\}$ has an energy

$$E_\Lambda(\{\sigma\}) = -\sum_{m=1}^{M}\Big[J_1\sum_{n=2}^{N-1}\sigma(n,m)\sigma(n+1,m) + J_0\sigma(1,m)\sigma(2,m) + J_2\sum_{n=1}^{N}\sigma(n,m)\sigma(n,m+1) + h(m)\sigma(1,m) + h'(m)\sigma(N,m)\Big] \quad (1)$$

with normalized canonical probability

$$P_\Lambda(\{\sigma\}) = Z_\Lambda^{-1}\exp[-\beta E_\Lambda(\{\sigma\})], \qquad (2)$$

where $\beta = 1/k_B T$, k_B and T being, respectively, Boltzmann's constant and the absolute temperature. The boundary condition $\sigma(n, M+1) = \sigma(n, 1)$ is imposed in (1). The $J_i \geq 0$ are ferromagnetic coupling constants, and the $h(i)$ and $h'(i)$ are boundary fields. Thus a cylindrical lattice is considered with a seam of misfit J_0 horizontal bonds adjacent to one surface.

In this Letter two types of boundary conditions will be considered:

$\mathcal{A}$: $h(i) = h'(i) = +\infty$ for all i

(this selects the $+m^*$ extremal state in the thermodynamic limit $M \to \infty$, then $N \to \infty$, where m^* is the spontaneous magnetization which vanishes for $T > T_C^{(2)}$); and

$$\mathcal{B}:\ h'(i) = \infty,\ h(i) = \begin{cases} -\infty, & 1 \leq i \leq s \\ \infty, & s < i \leq M. \end{cases}$$

In the contour, or low-temperature-expansion, language we have a long contour γ_0 beginning at $(1, \frac{1}{2})$ and ending at $(1, s+\frac{1}{2})$. Note that when $h(i) \to \infty$ the spin at $(2, i)$ is equivalently subjected to a magnetic field K_0.

Consider the magnetization profile defined by

$$F(x, \tfrac{1}{2}s) = \lim_{N\to\infty}\lim_{M\to\infty}\langle\sigma(x, \tfrac{1}{2}s)\rangle_{\mathcal{B}}. \qquad (3)$$

When $J_0 = J_1$ the following results are known[11]:

$$\lim_{s\to\infty} F(x, \tfrac{1}{2}s) = m_-(x), \qquad (4)$$

where $m_-(x)$ is the magnetization at a distance x from a wall with $h(i) = -\infty$, and $m_-(\infty) = -m^*$. The $+m^*$ state is attained by scaling x with s:

$$\lim_{s\to\infty} F(\alpha s^\delta, \tfrac{1}{2}s) = \begin{cases} -m^*, & \delta < \frac{1}{2} \\ +m^*, & \delta > \frac{1}{2} \end{cases} \qquad (5)$$

$$= m^* g(D\alpha),\quad \delta = \tfrac{1}{2}, \qquad (6)$$

where $D^2 = 2(\cosh 2K_2 - \cosh 2K_1^*)$, $K_i = J_i/k_B T$, $\exp(2K_1^*) = \coth K_1$, and

$$g(x) = 1 - (4/\sqrt{\pi})[x\exp(-x^2) + \int_x^\infty \exp(-u^2)\,du]. \qquad (7)$$

These results show that the long contour γ_0 fluctuates sufficiently to reduce the probability of γ_0 being nearer than $s^{1/2}$ to the boundary to zero as $s \to \infty$.

Suppose now that $J_0 = aJ_1$ with $0 < a < 1$. In this case γ_0 is attracted to the line $x = \frac{1}{2}$ establishing a competition between the entropy of wandering and energetic stabilization. The new result of this Letter is that there is an associated phase transition. Define $K_j = J_j/k_B T$, $j = 0, 1, 2$. Let $T_R(a)$ be the nontrivial solution of the equation

$$\exp(2K_2)[\cosh(2K_1) - \cosh(2aK_1)] = \sinh(2K_1). \qquad (8)$$

Note that $T_R(a)$ decreases from $T_C^{(2)}$ to 0 as a increases from 0 to 1. When $T_C^{(2)} > T > T_R(a)$ results analogous to (4) through (7) obtain except that $m_-(x)$ refers to the case $J_0 \neq J_1$. But when $0 < T < T_R(a)$ we have

$$\lim_{s\to\infty} F(x, \tfrac{1}{2}s) = m_+(x)[1 + h(x, T)], \qquad (9)$$

where $h(\infty, T) = 0$, $h(1, T) = -2$. Near $T_R(a)$, $h(x, T)$ has x scaled by a new length $\xi_s \approx (T_R - T)^{-1}$. The phase diagram is shown in Fig. 1.

The incremental free energy of the domain wall is given by

$$\tau = -\lim_{s\to\infty}\{s^{-1}\ln[Z_{\mathcal{B}}(s)/Z_{\mathcal{A}}]\}, \qquad (10)$$

where the partition functions are the appropriate normalizers of (2). This quantity takes the usual Onsager value for $T_C^{(2)} > T > T_R(a)$,[2,4,12] but the second temperature derivative, or domain-wall specific heat, has a jump discontinuity at $T_R(a)$.

The dual of the partition-function ratio is a correlation function $\rho(s)$ for a pair of spins at a distance s along an edge of a half-planar lattice with *enhanced* bonds along the edge. Associated with the incremental-free-energy singularity there is a change in asymptotic behavior of $\rho(s)$ from an essentially one-dimensional behavior with $T > T_R^*(a)$ to normal $d = 2$ behavior[13] when $T_C^{(2)} < T < T_R^*(a)$. [The temperature $T_R^*(a)$ is related to $T_R(a)$ by the dual transformation.] This observa-

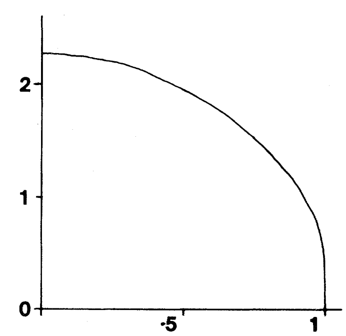

FIG. 1. Phase diagram for roughening transition. Plot of $k_B T_R(a)/J$ against a from solution of (8). The intercept at $a = 0$ is $k_B T_C^{(2)}/J$. $(k_B T/J, a)$ points under curve correspond to a bound domain wall.

tion lends support to the existence of special surface states.[14] Details of the associated crossover phenomenon will be published elsewhere.

It may prove possible to investigate the phenomenon described in planar uniaxial ferromagnets by using suitable surface fields. There may also be analogous phenomena in binary mixtures.

With use of the transfer-matrix theory and recently developed techniques[15] it can be shown that, for $T<T_C$,

$$m_+(x)=\sum_{n=0}^{\infty}\frac{1}{(2n)!}\frac{1}{(2\pi)^{2n}}\int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi}d(\omega)_{2n}M_0((\omega)_{2n})M((\omega)_{2n})\exp[-x\sum_1^{2n}\gamma(\omega_j)],\tag{11}$$

where $(\omega)_n$ is an n-uple and $\gamma(\omega)$ is Onsager's function[12] given by

$$\cosh[\gamma(\omega)]=\cosh 2K_1^*\cosh 2K_2-\sinh 2K_1^*\sinh 2K_2\cos\omega\tag{12}$$

with $\exp(2K_1^*)=\coth K_1$. The factors M are defined recursively by

$$M((\omega)_{2n})=\sum_{j=2}^{2n}(-1)^j f(\omega_1\omega_j)M(\Delta_{1j}(\omega)_{2n}),\tag{13}$$

where $\Delta_{1j}(\omega)_{2n}$ is $(\omega)_{2n}$ with ω_1 and ω_j omitted, and

$$f(\omega_1,\omega_2)=\frac{1}{\exp[i(\omega_1+\omega_2)]-1}\left(\frac{g(\omega_1)}{g(-\omega_2)}-\frac{g(\omega_2)}{g(-\omega_1)}\right).\tag{14}$$

In the above

$$g(\omega)=[(e^{i\omega}-A)/(e^{i\omega}-B)]^{1/2}\tag{15}$$

with $A=\coth K_1^*\coth K_2$ and $B=\tanh K_1^*\coth K_2$. The boundary condition on the recurrence is $M(\varphi)=m^*$. $M_0((\omega)_{2n})$ has an analogous definition except that f is replaced by

$$f_0(\omega_1,\omega_2)=i\delta(\omega_1+\omega_2)B(\omega_1)/A(\omega_1),\tag{16}$$

where

$$A(\omega)=(\cosh 2K_0^*-\sinh 2K_0^*\cos\omega)\exp(K_2)\cos\tfrac{1}{2}\delta^*(\omega)+\sinh 2K_0^*\exp(-K_2)\sin\omega\sin\tfrac{1}{2}\delta^*(\omega),\tag{17}$$

$$B(\omega)=(\cosh 2K_0^*-\sinh 2K_0^*\cos\omega)\exp(K_2)\sin\tfrac{1}{2}\delta^*(\omega)-\sinh 2K_0^*\exp(-K_2)\sin\omega\cos\tfrac{1}{2}\delta^*(\omega),\tag{18}$$

$$e^{i\delta^*(\omega)}=[(e^{i\omega}-A)(e^{i\omega}-B^{-1})/(e^{i\omega}-A^{-1})(e^{i\omega}-B)]^{1/2}(B/A)^{1/2},\quad M_0(\varphi)=1.\tag{19}$$

This allows one to confirm an important recent conjecture of de Gennes and Fisher[16]: In the critical region $m_+(x)$ has the scaling form

$$m_+(x)=m^*F(x\gamma(0),\hat{K}_0),\tag{20}$$

where as usual $1/\gamma(0)$ is the correlation length and $\hat{K}_0$ is the scaled magnetic field: $\hat{K}_0=K_0t^{-1/2}$ with $t=(T_C-T)/T_C$. This establishes the prediction $\Delta_1=\frac{1}{2}$. The function F is given explicitly by the calculation.

To develop the boundary condition $\mathcal{B}$ the procedures of Ref. 6 are used. This gives

$$F(x,\tfrac{1}{2}s)=m_+(x)+[Z_{\mathcal{B}}(s)/Z_{\mathcal{A}}]^{-1}\sum_{n=1}^{\infty}\sum_{j,k=1}^{2n}\theta(j,k)\int_0^{2}\cdots\int_0^{2\pi}d(\omega)_{2n}\exp[\tfrac{1}{2}i(\omega_j+\omega_k)s]$$
$$\times\exp\{\tfrac{1}{2}i[\delta^*(\omega_j)+\delta^*(\omega_k)]\}[A(\omega_j)A(\omega_k)]^{-1}M_0(\Delta_{jk}(\omega)_{2n})M((\omega)_{2n})\exp[-x\sum_1^{2n}\gamma(\omega_j)],\tag{21}$$

where $\theta(j,k)=(1-\delta_{jk})\,\mathrm{sgn}(j-k)$ and with

$$Z_{\mathcal{B}}(s)/Z_{\mathcal{A}}=\delta(s)+\pi^{-1}\int_0^{2\pi}d\omega\, e^{is\omega}C(\omega)/A(\omega),\tag{22}$$

$$iC(\omega)=(\cosh 2K_0^*+\sinh 2K_0^*\cos\omega)\exp(-K_2)\sin\tfrac{1}{2}\delta^*(\omega)+\sinh 2K_0^*\exp(K_2)\sin\omega\cos\tfrac{1}{2}\delta^*(\omega).\tag{23}$$

The limit $s\to\infty$ is taken in (21) and (22) by looking at the singularities in ω_j and ω_k in the complex plane. There are branch points at $e^{\pm i\omega}=B, A$. In addition, $A(\omega)$ has simple poles at $\omega=iv_0+2n\pi$,

$n=0, \pm 1, \ldots,$ where

$$\cosh v_0 = \tfrac{1}{2}(B+1/B)+1-\tfrac{1}{2}(w+1/w), \quad (24)$$

$$w=\exp(2K_2)(\cosh 2K_1 - \cosh 2K_0)/\sinh 2K_1. \quad (25)$$

In addition the poles must satisfy

$$\sinh\gamma(\omega)=\tfrac{1}{2}(w-1/w), \quad (26)$$

so that on the physical branch of $\gamma(\omega)$, for which $\gamma(\omega) \geq 0$ on $[0, 2\pi]$, there are no poles if $w<1$. Consequently, the pole dominates the asymptotics in s when $w>1$, which defines the region $0 \leq T < T_R(a)$, from (8). Note that $\gamma(iv_0)>0$ so that the integral in (21) decays to zero as $x \to \infty$ on a length scale $1/\gamma(iv_0)$, which is a new feature encountered in this problem. For $T_C^{(2)} > T > T_R(a)$ the branch point at $e^{i\omega}=B^{-1}$ dominates giving results (5) to (7). Note also that the domain-wall free energy defined by (10) has the value $\ln B$ for $T_C^{(2)} > T > T_R(a)$ but the value $|v_0|$ from (24) and (25) for $T<T_R(a)$.

We may interpret the phenomenon in terms of the nucleation of a droplet of opposite phase by a modified boundary fugacity in a region length s; for $T<T_R(a)$ the amount of entrained matter is of order s, whereas for $T_C^{(2)} > T_R(a)$ it is of order $s^{3/2}$.

When we take the solid-on-solid, or Onsager-Temperley, limit[17] $J_1 \to \infty$ with $J_0 = J_1 - b$, a phase transition persists whenever $b>0$, but $T_C^{(2)} \to \infty$. The high-temperature phase is dominated by capillary fluctuations which can be understood by applying central-limit-theorem ideas[6] to the usual low-temperature expansion. The mechanism of phase transition is different from the $d=3$ solid-on-solid case; there the interface is bound at its perimeter and a simple Peierls argument[18] enables one to understand fluctuation damping and the finite mean square fluctuation of the sheet at low temperature; in the high-temperature region height conservation around closed loops still damps effectively producing a non-Gaussian result and a phase of Kosterlitz-Thouless type.[19-21] Probably $T=\infty$ is a singular point at which Gaussian fluctuations are recaptured.

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