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LETTER TO THE EDITOR

Phase separation at the surface of an Ising ferromagnet

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Abstract. The incremental free energy and magnetisation profile are obtained for a domain wall pinned in the surface of an Ising ferromagnetic half-plane.

1. Unpinned edge

In this Letter the results of a derivation of the magnetisation near a domain wall with ends pinned in the surface of a ferromagnetic Ising half-plane will be described. Consider a lattice Λ with spins $\sigma_i = \pm 1$ at points $i = (n, m)$ of Λ where $1 \leq n \leq N$ and $1 \leq m \leq M$. A spin configuration $\{\sigma\}$ has an energy

$$E_\Lambda(\{\sigma\}) = -\sum_{n=1}^{N-1}\sum_{m=1}^{M}(J_1\sigma_{nm}\sigma_{n+1\,m} + J_2\sigma_{nm}\sigma_{n\,m+1}) - H\sum\sigma_{nm} \tag{1}$$

where the $J_i > 0$ are ferromagnetic couplings. Notice that the boundary conditions are cyclic in the $(0, 1)$ direction, but free in the $(1, 0)$ direction. On the faces of the cylindrical Λ thus obtained we impose boundary conditions on the spins as follows:

$$\sigma_{Nm} = +1$$

$$\sigma_{1m} = \begin{cases} -1 & \text{if } 1 \leq m \leq s \\ +1 & \text{if } s+1 \leq m \leq M. \end{cases} \tag{2}$$

Thus we model a domain wall pinned at $(1, \frac{1}{2})$ and $(1, s+\frac{1}{2})$. Henceforth in (1) we shall take $H = 0$ to permit the coexistence of the external states of opposite magnetisation below the critical temperature.

The quantities of interest are the magnetisation profile defined by

$$F(x, y|s) = \lim_{N\to\infty}\lim_{M\to\infty}\langle\sigma_{xy}\rangle \tag{3}$$

where $\langle . \rangle$ denotes the canonical average, and the incremental free energy

$$\tau = \lim_{s\to\infty}\frac{1}{s}\lim_{N\to\infty}\lim_{M\to\infty}\log\frac{Z^{+-}(s)}{Z^{+}} \tag{4}$$

where $Z^{+-}(s)$ is the canonical partition function associated with (1) and boundary condition (2), and Z^+ has boundary conditions $\sigma_{Nm} = \sigma_{1m} = 1$ for all m. $Z^{+-}(s)/Z^+$ is mapped by duality into the surface spin–spin correlation function, and is therefore

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obtainable directly from the work of McCoy and Wu (1967), giving

$$\tau = \sinh(K_2{}^* - K_1), \qquad \exp(2K_2{}^*) = \coth K_2 \tag{5}$$

where $K_i = J_i/kT$, k being the Boltzmann constant and T the absolute temperature in the canonical distribution. This is Onsager's (1944) result for the antiferromagnetic misfit seam. There are other definitions of the bulk surface tension (Gallavotti and Martin-Lof 1972, Abraham *et al* 1973), all of which give Onsager's value. Thus the restricted geometry appears to have no influence on τ.

Our results for (3) are

$$\lim_{s\to\infty} F(p, s/2|s) = -m_+(p) \tag{6}$$

where $m_+(p)$ is the magnetisation at a distance p from an edge with all spins plus. On the length scale of the lattice spacing in the (1, 0) direction the domain wall to the $+m^*$ phase is at infinite distance. This type of result is reminiscent of Gallavotti's (1972) and the calculations of Abraham and Reed (1976); in the low-temperature expansion, we have a 'long contour' with ends in the boundary, separated by a distance s. With probability one we may expect this contour to be at a distance of roughly $\sqrt{s}$ from any point in the plane. The distribution of small contour is, however, non-trivially modified by the restricted geometry, giving (6). The interface between the $(-m^*)$ phase at the wall and the $(+m^*)$ phase in the bulk will now be found by introducing in the scale $p = \alpha s^\delta$, $\alpha \geqslant 0$, $\delta > 0$. Then we have

$$\lim_{s\to\infty} F(\alpha s^\delta, s/2|s) = \begin{cases} -m^* & \text{if } \delta > \frac{1}{2} \\ m^* & \text{if } \delta < \frac{1}{2} \end{cases} \tag{7}$$

but

$$\lim_{s\to\infty} F(\alpha s^{1/2}, s/2|s) = m^* F(D\alpha) \tag{8}$$

where

$$F(x) = 1 - \frac{4}{\sqrt{\pi}}\left(x\,\mathrm{e}^{-x^2} + \int_x^\infty \mathrm{e}^{-t^2}\,\mathrm{d}t\right) \tag{9}$$

and

$$D^2 = 2\sinh 2(K_1 - K_2{}^*)/\sinh 2K_1 \sinh 2K_2{}^*. \tag{10}$$

2. Remarks

(1) The solid-on-solid limit is obtained in the limit K_1, giving the same form of result as above, but with D replaced by $2 \sinh K_2$. This is, of course, a restricted version of the Onsager–Temperley string (Temperley 1952).

(2) De Gennes and Fisher (1978) have recently discussed scaling theory in systems of finite size and of surface properties of infinite systems. Several of their phenomenological predictions have been verified for the planar Ising model (Au Yang and Fisher 1979, Abraham 1980). The result reported here has the homogeneous form central to scaling theory. Since the inverse correlation length diverges as t^{-1} near the

critical point T_c, where $t=(T_c-T)/T_c$, we see that (8) is of the form

$$F(p, s/2|s) \sim t^{1/8} g[p/\xi/(s/\xi)^{1/2}] \tag{11}$$

when $p \sim s^{1/2}$.

(3) The results of (7), (8), (9) and (10) should be compared with those of Abraham and Reed (1976) for the following simpler phase separation geometry: suppose instead of (2) we have

$$\sigma_{1m}=\sigma_{Nm}=\begin{cases}1 & m \geqslant M/2 \\ -1 & m < M/2.\end{cases}$$

This means that the long contour runs from side to side of the system. The density profile along the line $(N/2, p-M/2)$, $p \geqslant 0$ after taking the limit $M \to \infty$ is of the form (7) and (8), but with $p=\alpha N^{\delta}$ now and $F(x)$ in (9) replaced by

$$F(x)=\frac{2}{\sqrt{\pi}}\int_0^x \mathrm{e}^{-u^2}\,\mathrm{d}u \tag{12}$$

and D replaced by

$$D=[\sinh 2(K_2-K_1{}^*)]^{1/2}. \tag{13}$$

(4) The techniques used in this calculation are those which gave the n-point functions in the bulk (Abraham 1978). A dispersion representation for $m_+(p)$ is given explicitly and will be published elsewhere with the details of this calculation; but in connection with the phenomenology of de Gennes and Fisher (1978), note that calculation of $m_+(p)$ is equivalent to applying a given surface field to the spins one column in. The boundary conditions considered in this Letter may also be interpreted in terms of surface fields which are reversed in sign between the pinning points.

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