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LETTER TO THE EDITOR

The pinning of an interface by a planar defect

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Abstract. The behaviour of a domain wall is examined in a three-dimensional Ising model which has weaker exchange interactions near the surface than in the bulk. It is proved, within the Onsager–Temperley approximation, that the domain wall has a phase transition, being bound to the surface at low temperatures but not at high temperatures.

The theorem due to Hohenberg (1967), Mermin and Wagner (1966), on the absence of long-range order in certain one- and two-dimensional systems, provides a helpful context in which to discuss phase separation. An interface between a liquid and its vapour, in the limit of zero stabilising gravitational field, has a continuous symmetry under vertical translations, and is disordered, in the sense that the mean-square height difference between two points on the interface diverges logarithmically with their horizontal separation. The fluctuations of a one-dimensional interface in an equivalent model with two bulk dimensions are still stronger, resulting in a linear divergence of the same quantity. The relevant Goldstone modes which give rise to this disorder are long-wavelength capillary ripples.

Domain walls in homogeneous Ising models have only a discrete translational symmetry, and so these considerations do not apply directly. Nevertheless, a domain wall in the planar Ising model behaves in a similar fashion, having unbounded fluctuations from its ground-state position in the thermodynamic limit (Abraham and Reed 1974). There is also a range of evidence (Weeks *et al* 1973, Chui and Weeks 1976, van Beijeren 1977) to suggest that, at temperatures only a little below the Curie point, interfacial fluctuations in the three-dimensional Ising model are not grossly affected by the lattice. However, it has been proved (Dobrushin 1972, Gallavotti 1972, Abraham and Heilmann 1976) that at low temperatures, excitations are sufficiently suppressed by the discrete nature of the system for the domain wall to have a finite intrinsic width. The phase transition between the two states of the interface is known as the roughening transition (reviewed by Weeks and Gilmer, 1979).

Recently, the effects of a more extreme breaking of translational symmetry have been studied in the planar Ising model. Abraham (1980) has shown that a row of weakened exchange bonds next to one edge of the model will bind an interface at low temperatures, and that there is an unbinding transition, at a temperature below the Curie point, to a diffuse phase in which the interfacial free energy is dominated by the entropy gain from wandering, rather than the pinning energy. The purpose of this letter is to describe a proof that there is a similar transition for a related interfacial model in three bulk dimensions. Previous work, using mean-field theory (Burkhardt

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and Vieira 1981) and a duality relation (Chalker 1982a), has anticipated the conclusion but not provided any rigorous information.

Consider a simple cubic lattice constructed from M horizontal, square planes, each containing $(N+2)^2$ sites, arranged in a vertical column. At each site there is an Ising spin, s, taking the values $s=\pm\frac{1}{2}$. The spins interact through nearest-neighbour, ferromagnetic exchange bonds which are of strengths J in the horizontal directions, and $J_\perp$ in the vertical direction, except for those joining the lowest two planes, which are weaker by an amount Δ. The spins in the lowest plane of the lattice are constrained to have the value $s=-\frac{1}{2}$, and those on the remainder of the lattice surface are limited to $s=+\frac{1}{2}$, thus ensuring the presence of an interface. At temperatures below the Curie point a spontaneous magnetisation is to be expected, which will be positive in the upper part of the system, and negative in the lower lattice planes. If the thickness of the negatively magnetised layer is finite in the thermodynamic limit, the domain wall may be said to be bound by the weakened bonds.

The Onsager–Temperley (Temperley 1952) sheet, or solid-on-solid approximation, provides a way of focusing attention on interfacial behaviour and ignoring bulk fluctuations; it has proved remarkably successful in treating the unbinding transition in two bulk dimensions (Burkhardt 1981, Chalker 1981, 1982b, Chui and Weeks 1981, Kroll 1981, van Leeuwen and Hilhorst 1981). The approximation consists of omitting all those configurations of the Ising model described above in which there is a down spin vertically above an up spin. The remaining, allowed configurations may be more conveniently specified by introducing a new set of variables, 'columns', instead of the original spins. The column variables, $\{h_i\}$, are defined on the sites, $\{i\}$, of the lowest plane of the original lattice: in each allowed configuration, σ, the value of h_i is the height, in lattice units, of the highest down spin vertically above the site i. Hence, on the $4(N+1)$ boundary sites the column heights are fixed at zero, but on the N^2 remaining, interior sites they may separately take any non-negative integer value (in the limit $M\to\infty$). The energy of a configuration, $E(\sigma)$, relative to that of the ground state, is

$$E(\sigma)=J\sum_{\langle ij\rangle}|h_i-h_j|-\Delta\nu(\sigma). \tag{1}$$

$\Sigma_{\langle ij\rangle}$ is a sum over all nearest-neighbour pairs of sites; and $\nu(\sigma)=\Sigma_i'\,\delta_{h_i,0}$, Σ_i' being a sum over all interior sites and $\delta_{h_i,0}$ the Kronecker delta. The set of all allowed configurations is denoted by $\mathscr{A}$. The canonical probability, p_σ, for the state σ is

$$p_\sigma=Z^{-1}\,\mathrm{e}^{-\beta E(\sigma)}, \qquad Z=\sum_{\sigma\in\mathscr{A}}\mathrm{e}^{-\beta E(\sigma)} \tag{2}$$

with β the inverse temperature.

An order parameter for the unbinding transition is

$$\rho_N=N^{-2}\sum_{\sigma\in\mathscr{A}}\nu(\sigma)p_\sigma \tag{3}$$

which measures the proportion of columns on internal sites taking the value zero: clearly $0\leqslant\rho_N\leqslant 1$. If $\lim_{N\to\infty}\rho_N=0$, the interface is unbound, whilst if $\lim_{N\to\infty}\rho_N>0$, it is bound. The exact results which will be proved are:

(i) if $(\mathrm{e}^{-\beta\Delta}+\mathrm{e}^{-4\beta J})>1$,

then $\lim_{N\to\infty}\rho_N=0$; (4*a*)

(ii) $$\text{if } e^{-\beta\Delta}\left(\frac{1+e^{-\beta J}}{1-e^{-\beta J}}\right) \equiv x < \tfrac{1}{16},$$

$$\text{then } \lim_{N\to\infty} \rho_N \geqslant [1+\ln(1-8x)] > 0. \tag{4b}$$

Thus, for any given pair of positive values for J and Δ, there is a temperature below which the interface is certainly bound and another, higher one above which it is certainly unbound.

Proof of (i)

Let $\mathscr{B}_M$ denote the set of configurations, σ, for which $\nu(\sigma) > M$. Then

$$\rho_N \leqslant \sum_{\sigma\in\mathscr{B}_M} p_\sigma + \frac{M}{N^2}. \tag{5}$$

From each state σ, $2^{\nu(\sigma)}$ different states, $\sigma[\alpha]$, $\alpha = 1, 2 \ldots 2^{\nu(\sigma)}$, may be constructed according to the following prescription: (a), increase the value of the column variable on every internal site by one, unless it has the value zero in the state σ; and (b), allow all possible combinations of the values zero and one for these $\nu(\sigma)$ remaining variables on internal sites, which were left unaltered under (a). Let $\mathscr{C}_M$ be the set of configurations constructed in this way from those in $\mathscr{B}_M$. Note that two states, $\sigma[\alpha]$ and $\sigma'[\alpha']$, constructed from different original states, σ and σ', are necessarily different. The energy of the state $\sigma[\alpha]$ satisfies the inequality

$$E(\sigma[\alpha]) \leqslant E(\sigma) + 4NJ + 4J\nu(\sigma[\alpha]) + \Delta[\nu(\sigma) - \nu(\sigma[\alpha])] \tag{6}$$

so that

$$\sum_{\alpha=1}^{2^{\nu(\sigma)}} \exp[-\beta E(\sigma[\alpha])] \geqslant \exp[-\beta(E(\sigma)+4NJ)](e^{-\beta\Delta}+e^{-4\beta J})^{\nu(\sigma)}. \tag{7}$$

When $(e^{-\beta\Delta}+e^{-4\beta J}) > 1$, equation (7) leads to a lower bound on Z

$$Z \geqslant \sum_{\sigma\in\mathscr{C}_M} e^{-\beta E(\sigma)} \geqslant (e^{-\beta\Delta}+e^{-4\beta J})^M\, e^{-4N\beta J} \sum_{\sigma\in\mathscr{B}_M} e^{-\beta E(\sigma)} \tag{8}$$

and hence an upper bound on ρ_N

$$\rho_N \leqslant e^{4N\beta J}/(e^{-\beta\Delta}+e^{-4\beta J})^M + M/N^2. \tag{9}$$

With, for example, the choice $M = N^{3/2}$ in equation (9), the result (i) is obtained.

Proof of (ii)

If the interface is strongly bound to the defect plane, so that in a typical configuration most column heights have the value zero, then it is more natural to describe configurations by specifying heights and positions of non-zero columns, rather than the heights of all columns. To this end, we introduce some definitions.

The lth n-site connected cluster, $C_{l,n}$, is a particular group of n interior lattice sites with the property that any site in the cluster can be reached from any other, along a path of nearest-neighbour bonds, without crossing a site which is not part of the cluster. Let $C^*_{l,n}$ be the sites which are nearest neighbours to those in $C_{l,n}$, but which

are not members of $C_{l,n}$. It will be useful to associate with each cluster n nearest-neighbour bonds. Of these, $(n-1)$ are to be chosen so that they interconnect all sites in the cluster, in the sense of forming the paths described above, and the remaining one is to join a site in $C_{l,n}$ to one in $C^*_{l,n}$.

For a given configuration of the model, the cluster $C_{l,n}$ is said to be excited if and only if: $h_i > 0, \forall i \in C_{l,n}$, *and* $h_i = 0, \forall i \in C^*_{l,n}$; the variable $X_{l,n}(\sigma)$ takes the value one in this case and is zero otherwise. A state is completely defined by the values of $X_{l,n}(\sigma)$, for all l and n, together with, for each excited cluster, $C_{l,n}$, n values of $(h_i - h_j)$, where the n pairs of sites, i and j, are those at the ends of the bonds associated with that cluster. The energy, $E(\sigma)$, of the state σ satisfies the inequality

$$E(\sigma) \geqslant J \sum_{\langle ij \rangle}{}' |h_i - h_j| + J \sum_{\langle ij \rangle}{}'' |h_i - h_j| - \Delta\nu(\sigma) \tag{10}$$

where $\Sigma'_{\langle ij \rangle}$ is a sum over all nearest-neighbour pairs of sites, excepting those where one or both sites belong to a particular cluster, $C_{l,n}$, and $\Sigma''_{\langle ij \rangle}$ is a sum over the n pairs of sites joined by the bonds associated with that given cluster. A crucial stage of the argument is to find an upper bound on the thermal expectation value of $X_{l,n}(\sigma)$. Let $\mathscr{D}_{l,n}$ be the set of states in which $h_i = 0, \forall i \in C_{l,n} \cup C^*_{l,n}$. Then, using equation (10)

$$\sum_{\sigma \in \mathscr{A}} \mathrm{e}^{-\beta E(\sigma)} X_{l,n}(\sigma) \leqslant \sum_{\sigma' \in \mathscr{D}_{l,n}} \mathrm{e}^{-\beta E(\sigma')} \left(\mathrm{e}^{-\beta\Delta} \sum_{h=-\infty}^{\infty} \mathrm{e}^{-\beta J|h|} \right)^n \tag{11}$$

since all the states for which $X_{l,n}(\sigma) = 1$ can be obtained from those in the set $\mathscr{D}_{l,n}$ by altering just the values of the column variables on the sites belonging to the cluster $C_{l,n}$. A lower bound on Z is $Z \geqslant \Sigma_{\sigma \in \mathscr{D}_{l,n}} \mathrm{e}^{-\beta E(\sigma)}$ so that

$$\sum_{\sigma \in \mathscr{A}} p_\sigma X_{l,n}(\sigma) \leqslant x^n \tag{12}$$

where x is defined in equation (4*b*).

The order parameter can be expressed in terms of the variables $X_{l,n}(\sigma)$

$$\rho_N = 1 - N^{-2} \sum_{\sigma \in \mathscr{A}} \sum_{n,l} n p_\sigma X_{l,n}(\sigma). \tag{13}$$

Finally, a crude upper limit to the number, $\mathscr{N}_n$, of n-site connected clusters on the lattice is, from consideration of a Cayley tree of the same coordination number (Leath 1976), $N^2 8^n n^{-2} \geqslant \mathscr{N}_n$, leading to

$$N^{-2} \sum_{\sigma \in \mathscr{A}} \sum_{n,l} n p_\sigma X_{l,n}(\sigma) \leqslant \sum_{n=1}^{\infty} n^{-1} (8x)^n. \tag{14}$$

The result (ii) follows immediately.

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