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LETTER TO THE EDITOR

Molecular-field theory of interface pinning in an external potential

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Abstract. The behaviour of an interface subject to an external pinning force is studied in a molecular-field theory. In the case of a pinning force applied near the edge of the system, one finds a finite-temperature localisation–delocalisation transition in the SOS model but not in the Gaussian model.

Abraham (1980) has studied a localisation–delocalisation transition associated with the pinning of a domain wall in an inhomogeneous two-dimensional Ising model. In his model it is energetically favourable for the domain wall to pass near one edge of the system, where there is a row of weaker bonds. Below a transition temperature T_D, which is less than the bulk critical temperature T_c, the interface is bound a finite distance from this edge and is smooth, i.e. its root-mean-square width is finite. For $T_D < T < T_c$ the interface is no longer bound and is rough, i.e. the root-mean-square width diverges.

Stimulated by Abraham's work several authors (Burkhardt 1981, Chalker 1981, Chui and Weeks 1981, Kroll 1981, van Leeuwen and Hilhorst 1981) have studied the pinning of the one-dimensional interface in the planar solid-on-solid (SOS) model (Temperley 1952, Leamey *et al* 1975, Müller-Krumbhaar 1977), a simple special case of the Ising model, with various types of external potentials. In the case of a short-range pinning force applied a finite distance from one edge of the system, there is a localisation–delocalisation transition which is qualitatively the same as that discussed by Abraham. If the pinning force is applied an infinite rather than a finite distance from the edge, the interface remains smooth and pinned at all finite temperatures. Lajzerowicz and Vallade (1981) have reached similar conclusions for a continuum model with a one-dimensional interface.

It would be interesting to know more about such pinning phenomena in higher dimensions, where the interface fluctuations are weaker. In particular, possible pinning effects should be kept in mind in designing and analysing experiments (Balibar and Castaing 1980, Avron *et al* 1980) to look for the roughening transition (Leamy *et al* 1975, Müller-Krumbhaar 1977) in three dimensions. In this Letter, a modest step toward understanding the higher-dimensional behaviour is taken. SOS and Gaussian models with an interface subject to a pinning force are examined in a molecular-field theory which may be qualitatively correct in sufficiently high dimensions. Similar molecular-field theories have been considered by Temkin (1966) and Swendsen (1977) in the absence of pinning forces. In the case of a pinning force applied a finite distance

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from the edge of the system, the molecular-field theory predicts a localisation–delocalisation transition in the SOS model but not in the Gaussian model. Since molecular-field theory, which underestimates the interface fluctuations, and the exact solution for $d = 2$ dimensions, where the interface fluctuations are stronger than in $d > 2$, both predict a localisation–delocalisation transition in the SOS model, the model probably really has such a transition for all $d \geqslant 2$.

The systems considered here have the Hamiltonian

$$H = J \sum_{\langle ij \rangle} |x_i - x_j|^r + \sum_i U(x_i) \tag{1}$$

with $r = 1$ and 2 corresponding to the SOS and Gaussian models, respectively. x_i denotes the perpendicular distance of the interface from point i on a $d-1$ dimensional lattice, as shown for $d = 2$ in figure 1. The x_i vary continuously in the interval $0 < x_i < \infty$. It is straightforward to extend the molecular-field theory described below to an integer spectrum for the x_i. In $d = 2$ dimensions continuous and integer spectra lead to transitions in the SOS model which are qualitatively the same (Burkhardt 1981). The energy contribution from the first sum in (1), which only involves interactions between neighbouring height variables, is minimised by a flat horizontal interface. The quantity $U(x_i)$ is the pinning potential. The case of a square-well potential is considered explicitly below.

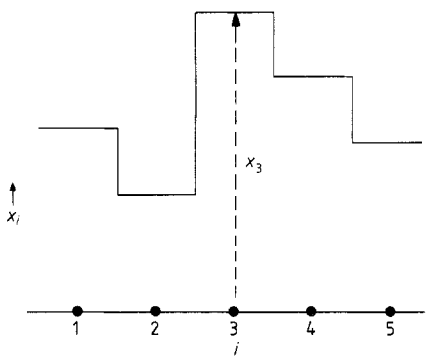

Figure 1. The SOS and Gaussian models in $d = 2$ dimensions.

The molecular-field theory discussed here is based on the variational principle (see, for example, Falk 1970)

$$F \leqslant \Phi[\rho] = \mathrm{Tr}\, \rho H + k_B T\, \mathrm{Tr}\, \rho \ln \rho. \tag{2}$$

Here F is the exact free energy, and ρ is any trial density matrix satisfying $\mathrm{Tr}\, \rho = 1$. The symbol Tr represents integration over all N displacement variables x_i. The equality holds for the canonical distribution $\rho \propto \exp(-H/k_B T)$. With the variational ansatz $\rho = P(x_1)P(x_2) \ldots P(x_N)$, which neglects correlations between the x_i, (2) becomes

$$\Phi/k_B TN = \frac{K}{2} \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}y\, P(x)|x-y|^r P(y) + \int_0^\infty \mathrm{d}x\, P(x)(V(x) + \ln P(x)) \tag{3}$$

where $K = qJ/k_B T$, q being the coordination number of the $d-1$ dimensional lattice, and where $V(x) = U(x)/k_B T$. Requiring that the variational derivative of Φ with

respect to $P(x)$ vanish yields the integral equation

$$P(x) = \exp\left(A - V(x) - K\int_0^\infty \mathrm{d}y |x-y|^r P(y)\right) \tag{4}$$

for the optimal molecular-field distribution function. The quantity A is a Lagrange multiplier chosen to satisfy the normalisation condition $\mathrm{Tr}\,\rho = 1$. Equation (4) has an obvious molecular-field form and could have been written down directly without recourse to the variational principle.

In the Gaussian case $r = 2$ equation (4) is equivalent to

$$P(x) = \exp[B - V(x) - K(x - \langle x\rangle)^2] \tag{5}$$

where B is a normalisation constant and the mean value $\langle x\rangle$ satisfies the self-consistency condition

$$0 = \int_0^\infty \mathrm{d}x (x - \langle x\rangle) \exp[-V(x) - K(x-\langle x\rangle)^2]. \tag{6}$$

The integral in (6) can be readily evaluated for the square-well potential $U(x) = -U_0$, $0 < x < R$, and $U(x) = 0$, $x > R$, which corresponds to a pinning force at the edge of the system. Solving for $\langle x\rangle$, one obtains

$$\langle x\rangle = \frac{R}{2} - \frac{1}{2KR}\ln(1 - \mathrm{e}^{-V_0}) \tag{7}$$

where $V_0 = U_0/k_B T$.

According to (7) $\langle x\rangle$ increases monotonically with T but remains finite as long as T is finite. It is easy to verify that (5) with $\langle x\rangle$ given by (7) yields a lower free energy than any other choice for $\langle x\rangle$, including $\langle x\rangle = \infty$. Thus the molecular-field theory predicts a localised interface in the Gaussian model with a square-well pinning potential at the edge for all finite temperatures.

The corresponding molecular-field calculation for the SOS model leads to a different conclusion. Equation (4) with $r = 1$ implies the differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ln(\mathrm{e}^{V(x)}P(x)) + 2KP(x) = 0. \tag{8}$$

For the square-well potential considered above, the solution is

$$P(x) = (\alpha^2/K)[\cosh(\alpha x - a)]^{-2} \qquad x > R \tag{9}$$

$$P(x) = (\beta^2/K)[\cosh(\beta x - b)]^{-2} \qquad 0 < x < R. \tag{10}$$

The integration constants α, β, a, and b are uniquely determined by the normalisation condition $\int_0^\infty \mathrm{d}x\, P(x) = 1$ and by three additional requirements which follow from (4): $\mathrm{d}\ln(P(x)\exp V(x))/\mathrm{d}x = K$ at $x = 0$, and $P(x)\exp V(x)$ and its derivative with respect to x are continuous at $x = R$. These conditions imply

$$2\alpha/K = 1 \tag{11}$$

$$2\beta/K = \coth b = \tanh(KR/2 - a)/\tanh(\beta R - b) \tag{12}$$

$$(2\beta/K)^2 = \mathrm{e}^{V_0}\cosh^2(\beta R - b)/\cosh^2(KR/2 - a). \tag{13}$$

The interface described by (9) and (10) is pinned if the values of the constants a and b are finite. Combining (11) and (12) for $a, b \gg 1$, one finds that a and b diverge as

$-\frac{1}{2}\ln\{[e^{KR}(1-e^{-V_0})]^{1/2}-1\}$ on approaching the critical surface of localisation–delocalisation transitions

$$K_c(V_0, R)R = -\ln(1-e^{-V_0}) \tag{14}$$

where the argument of the logarithm vanishes. The exact (Burkhardt 1981) critical coupling $K_c(V_0, R)$ for $d = q = 2$ is larger than the molecular-field result (14), as expected.

The logarithmic divergence of a and b on approaching the critical surface implies that the mean distance $\langle x\rangle$ of the interface from the edge of the system diverges as $-\ln(T_D - T)$ on approaching the transition temperature T_D from below at fixed J, U_0, and R. In the exact results for $d = q = 2$ one finds the stronger divergence $\langle x\rangle \propto (T_D - T)^{-1}$. A lengthy calculation shows that the specific heat in the molecular-field theory is discontinuous at T_D, as in the exact solution for $d = q = 2$.

For $T > T_D$ the distribution function which minimises the mean-field free energy has the form

$$P(x) = (K/4)[\cosh(Kx/2)]^{-2} \tag{15}$$

where the origin of coordinates has now been chosen so that $x = \pm\infty$ correspond to edges of the system. $P(x)$ vanishes at the edges of the system and is independent of $U(x)$. If the regions above and below the interface are defined to be regions of spin 1 and -1 respectively, (15) implies the magnetisation profile

$$m(x) = \int_{-\infty}^{x} dy\, P(y) - \int_{x}^{\infty} dy\, P(y) = \tanh(Kx/2) \tag{16}$$

which is familiar from mean-field theories (Temkin 1966, Swendson 1977, Landau 1965) of the interface without a pinning potential. The mean-square width $\langle x^2\rangle$ of the interface calculated with (15) is finite. Thus the molecular-field theory predicts a smooth interface for $T > T_D$. This is not surprising. From quite general arguments (Buff *et al* 1980, Chui and Weeks 1976, Kosterlitz 1977) one expects the unbound interface to be rough for $d < 3$ and smooth for $d > 3$. Molecular-field theories generally become qualitatively correct in sufficiently high dimensions, if at all.

It is straightforward to carry out a molecular-field calculation for the SOS model with the square-well potential infinitely far from the edge. One finds a smooth localised interface for all finite temperatures. This is to be expected, since the exact solution for $d = 2$ indicates that the interface is always localised, and in higher dimensions the interface fluctuations are weaker. A similar molecular-field calculation for the Gaussian model also always indicates a pinned interface.

As mentioned in the introductory paragraphs, one can argue on the basis of the molecular-field theory discussed here and the exact results for $d = 2$ that there really is a finite-temperature localisation–delocalisation transition in the SOS model with a pinning potential at the edge for all $d \geqslant 2$. At sufficiently low but non-zero temperatures the interface is certainly localised, since it is localised in $d = 2$, where the fluctuations are strongest. Since molecular-field theory, which underestimates fluctuations, nonetheless predicts a transition to a delocalised state, the transition probably does indeed exist for all $d \geqslant 2$. Whether the absence of a similar transition in the Gaussian model is a real effect or an erroneous prediction of the molecular-field theory remains to be seen.

The most interesting dimension in which to study the localisation–delocalisation transition is, of course, $d = 3$, where in the absence of a pinning potential one expects finite-temperature roughening transitions in the discrete SOS and Gaussian models

(Leamy *et al* 1975, Müller-Krumbhaar 1977). If a strong pinning force is included near the edge of the SOS system, there is probably just a single transition from a smooth localised interface to a rough delocalised interface. In the case of a weak pinning force, the interface may remain smooth during the localisation–delocalisation transition and undergo a separate roughening transition at a higher temperature. However, the subtleties of the marginal dimension $d = 3$ are clearly beyond the capabilities of the simple molecular-field approach considered here.

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