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A duality relation between an interface in a pinning potential and a modified Coulomb gas

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Abstract. The duality transformation between the discrete Gaussian model of a d-dimensional interface in a $(d+1)$-dimensional bulk system and the Coulomb gas in d dimensions is extended to include a pinning force which tends to localise the interface either in the centre or near the edge of the bulk system. Arguments are given for the probable phase diagrams of each system.

1. Introduction

The behaviour of a d-dimensional interface between oppositely magnetised, low-temperature phases of the $(d+1)$-dimensional Ising model varies considerably with dimensionality. In the case of a one-dimensional interface in the planar Ising model, exact calculations (Gallavotti 1972, Abraham and Reed 1974) show that, at all finite temperatures, capillary fluctuations result in a divergence with the linear system size of the mean-square displacement of the interface from its ground-state position. For a two-dimensional interface in the three-dimensional Ising model there is extensive evidence (Dobrushin 1972, Weeks *et al* 1973, van Beijeren 1977, Weeks and Gilmer 1979) that the mean-square displacement diverges more weakly (logarithmically) at high temperatures, whilst below the roughening temperature fluctuations are finite and there is a sharp domain wall. In higher dimensions a simple consideration of the density of states for fluctuations, as well as more sophisticated arguments (Kosterlitz 1977), predicts a sharp domain wall at all temperatures below the bulk transition. Recently there has been some interest in a variation on this problem. Abraham (1980) considered an inhomogeneous, planar Ising model with a row of weakened bonds next to one edge and showed by an exact solution that at low temperatures this pinning force localises the interface, and that at a transition temperature below the bulk critical point, the delocalised behaviour found in the homogeneous system is restored. Subsequently, several authors (Burkhardt 1981, Chalker 1981, Chui and Weeks 1981, Kroll 1981, van Leeuwen and Hilhorst 1981) have studied the solid-on-solid limit (Weeks *et al* 1973) of this system, which greatly simplifies calculations. Similar results are found in this approximation when a pinning force acts at the edge of the system, but it has been realised by the same authors that a pinning force of a similar kind acting in the bulk will localise the interface at any temperature below the two-dimensional critical point.

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In this paper, an attempt is made to understand the effects of such a pinning force in higher dimensions. The only previous work on this question of which we are aware, is a mean-field theory due to Burkhardt and Vieira (1981); the results presented here are in agreement with their main conclusions: that an interface will be localised by a bulk-pinning force, and will have an unbinding transition from an edge-pinning force, for all dimensionalities. However, a surprising difference which appears in mean-field theory between the behaviours of the solid-on-solid and Gaussian models is not found in the present work.

The method used is to extend the well established duality relation (Chui and Weeks 1976, José *et al* 1977, Kosterlitz 1977) between the d-dimensional discrete Gaussian model of an interface in $(d+1)$ bulk dimensions and a d-dimensional Coulomb gas to include either a bulk-pinning force (§ 2), or a form of edge-pinning force (§ 3). The resulting modified Coulomb gases contain, with a certain chemical potential, charges which take a continuous range of values and interact with the usual, integer charges. It is argued that, when present at a finite density, these continuous charges will have a sufficient screening effect to allow unbinding of integer charge pairs in the Coulomb gas, irrespective of dimensionality. The form of their chemical potential in the case of bulk pinning suggests that the continuous charges will be present at all temperatures in the related Coulomb gas, whilst for edge pinning their density will be zero below a transition temperature—corresponding to an unbound, high-temperature phase of the dual interface. Finally, the conclusions reached in this way are supported by very different reasoning applied directly to the interfacial models.

2. The duality relation for bulk pinning

A general form for the Hamiltonian of an interfacial model which includes a pinning force is:

$$\mathcal{H}_I = J \sum_{i,\delta} |h_i - h_{i+\delta}|^P + \sum_i V(h_i) \tag{1}$$

where $i, i+\delta$ label nearest-neighbour pairs of the N sites on a d-dimensional lattice (taken below to be cubical and subject to periodic boundary conditions) at which are columns of height h_i, $h_i = 0, \pm 1 \ldots \pm\infty$. The exchange energy parallel to the domain wall in the corresponding Ising model is proportional to J, and in the solid-on-solid model $P = 1$. It can be argued that excitations of the system for which $|h_i - h_{i+\delta}| > 1$ are unimportant, and hence that the value of P is not crucial. The value $P = 2$ gives the discrete Gaussian model to which the duality relations described here apply. Similar results for the roughening transition of a two-dimensional interface have been derived for $P = 1$ (Weeks *et al* 1973), $P = 2$ (Chui and Weeks 1976), $P = \infty$ (van Beijeren 1977) and $1 \leqslant P \leqslant \infty$ (Emery and Swendsen 1977). Exact solutions in one dimension for the unbinding of an interface from an edge-pinning force give the same behaviour for $P = 1$ and $P = \infty$ (Chui and Weeks 1981). The value $P = \infty$, the restricted solid-on-solid model, will be considered in § 4. A pinning potential is represented by $V(h)$: in the case of bulk-pinning, we take $V(h) = -\Delta\delta_{h,0}$ where $\delta_{h,0}$ is the Kronecker delta. The duality transformation follows that of Chui and Weeks (1976) closely. The partition function, Z, for the model can be written:

$$Z = \prod_{i=1}^{N} \int_{-\infty}^{\infty} \mathrm{d}h_i \, W(\{h_i\}) \, \mathrm{e}^{-\beta \mathcal{H}_0}$$

where

$$W(\{h_i\}) = \prod_{i=1}^{N} w(h_i), \qquad w(h) = \sum_{n=-\infty}^{\infty} \delta(h-n) + [e^{\beta\Delta} - 1]\delta(h) \tag{2}$$

and

$$\mathcal{H}_0 = \tfrac{1}{2} \sum_{i,\delta} (h_i - h_{i+\delta})^2 + 2dH \sum_i h_i^2.$$

We are concerned with the behaviour in the limit $H \to 0$. The integrations over $\{h_i\}$ can be performed after writing the delta functions in their Fourier integral representation; the partition function becomes:

$$Z = Z_u Z_C \tag{3}$$

where Z_u is the unrestricted partition function obtained by setting $W(\{h_i\}) = 1$ in equation (2), and Z_C is the grand partition function for a modified Coulomb gas.

$$Z_C = \sum_{\substack{\{P_i\} \\ P_i = 0,1}} \left[\prod_i \left(P_i \int_{-\infty}^{\infty} dq_i + (1 - P_i) \sum_{q_i=-\infty}^{\infty} \right) \right] e^{-\beta' \mathcal{H}_C}, \tag{4}$$

with

$$\mathcal{H}_C = -\sum_{\substack{i,j \\ i \neq j}}{}' q_i q_j U(i,j) + C\left(\sum_i q_i \right)^2 + \mu \sum_i P_i.$$

$$U(l,m) = \frac{\pi^2}{2dN} \sum_k \frac{1 - \exp[i\boldsymbol{k} \cdot (\boldsymbol{r}_l - \boldsymbol{r}_m)]}{1 - \phi(\boldsymbol{k}) + H},$$

$$C = \frac{\pi^2}{2dN} \sum_k \frac{1}{1 - \phi(\boldsymbol{k}) + H}$$

where $\mu = -\beta'^{-1} \ln(e^{\Delta/\beta'} - 1)$ and $\phi(\boldsymbol{k}) = d^{-1} \sum_{n=1}^{d} \cos k_n$. There are N allowed values of $\boldsymbol{k}$ lying in one Brillouin zone of the reciprocal lattice. The temperatures of the dual systems are inversely related $\beta' = \beta^{-1}$. The asymptotic behaviour of $U(l, m)$ for large $|\boldsymbol{r}_l - \boldsymbol{r}_m|$ in the limit $H \to 0$ is (Kosterlitz 1977) that of the d-dimensional Coulomb potential.

The quantities $\{P_i\}$ are annealed random variables, and in a given configuration the sites for which $P_i = 0$ are occupied by integer charges, q_i, while sites with $P = 1$ support charges with a continuous range of values. The scale for temperature in the Coulomb gas is set by the unit of charge (Kosterlitz 1977): if continuous charges are present their behaviour should be that of the usual (discrete) Coulomb gas at infinite temperature. They will therefore be in the metallic phase, in which charges are not bound together in pairs and correlations decay exponentially. Such a plasma of continuous charges will screen interactions between discrete charges so that these, too, are in a metallic phase. Since μ (equation (4)) is always finite for $\Delta > 0$, $\infty > \beta' > 0$, we expect this modified Coulomb gas to contain a finite concentration, $\langle P_i \rangle$, of continuous charges and hence to be in the metallic phase at all non-zero temperatures, independently of dimensionality. We expect, equivalently, that a bulk-pinning force will always localise the dual interface. It is straightforward to relate the concentration of continuous charges in the Coulomb gas to the probability of finding the dual interface in the attractive part of the pinning potential

$$\langle P_i \rangle_{\mathcal{H}_C} \propto \langle \delta_{h_i,0} \rangle_{\mathcal{H}_1}. \tag{5}$$

3. Edge pinning

The type of edge pinning studied by Abraham (1980) corresponds to the choice for $V(h)$ in equation (1)

$$V(h)=\begin{cases}\infty & h<-\frac{1}{2}\\ -\Delta & -\frac{1}{2}\leqslant h\leqslant\frac{1}{2}\\ 0 & \frac{1}{2}<h.\end{cases} \tag{6}$$

We have been unable to perform the duality transformation with this form for $V(h)$. However, it has been shown (Chalker 1981), following the general relationship between the statistical mechanics of a d-dimensional system and the quantum-mechanical ground state of a $(d-1)$-dimensional system (Kogut 1979), that the behaviour of a one-dimensional interface in a potential $V(h)$ is related to that of a quantum-mechanical particle moving in one dimension with position h, in the same potential. A more tractable choice for an edge-pinning potential with the same property as that of equation (6), that a quantum-mechanical particle only has a bound state for sufficiently large values of Δ, is

$$V(h)=\lim_{H\to 0}\{H(h-H^{-1/2})^2-\Delta\delta(h)\}. \tag{7}$$

The transformation of the previous section can be repeated when $\mathcal{H}_0$ (equation (2)) is replaced by

$$\mathcal{H}_0=\tfrac{1}{2}\sum_{i,\delta}(h_i-h_{i+\delta})^2+2dH\sum_i(h_i-H^{-1/2})^2. \tag{8}$$

The result is given by equation (4), but with $\beta'\mathcal{H}_C$ replaced by

$$\left(\beta'\mathcal{H}_C-2\pi iH^{-1/2}\sum_i q_i\right).$$

This change affects only the contributions to Z_C in which there are continuous charges. (If the limit $H\to 0$ is taken in such a way that $H^{-1/2}$ is integer, then $\exp(2\pi iH^{-1/2}\Sigma_i q_i)=1$ whenever $\Sigma_i q_i$ is integer.) For these configurations, in which $\Sigma_i P_i\equiv\rho N>0$, we change variables in the integrals for Z_C and consider first integration over the net charge, defined as $S\equiv(\rho N)^{-1}\Sigma_i q_i$; the factor this contributes to Z_C is

$$I=\int_{-\infty}^{\infty}dS\,\exp\left\{2\pi iH^{-1/2}\rho NS-\beta'S^2\sum_{j,k}[C-U(j,k)]p_jp_k+2\beta'S\sum_{j,k}p_jq'_ku(j,k)\right\} \tag{9}$$

where $q'_i\equiv q_i-Sp_i$, so that $\Sigma_i q'_i=0$.

In all configurations of $\{q'_i\}$ for which $\lim_{H\to 0}\lim_{N\to\infty}(\mathcal{H}_C/N)$ is finite,

$$\lim_{H\to 0}\lim_{N\to 0}(I^{1/N})=\exp(-2d/\beta'). \tag{10}$$

When $\Sigma_i P_i=0$ there are no continuous charges and so this factor does not appear. The edge-pinning model is therefore described by equation (4), with the restriction $\Sigma_i q_i=0$ and a concentration-dependent chemical potential, μ', for continuous charges of

$$\rho\mu'=\begin{cases}0, & \rho=0\\ 2d/\beta'^2-\rho[\beta'^{-1}\ln(e^{\Delta/\beta'}-1)] & \rho>0.\end{cases} \tag{11}$$

The divergence of μ' as $\rho\to 0$ provides a clear driving mechanism, apparently similar

in all dimensionalities, for a transition at which the continuous charges disappear as temperature is lowered in the modified Coulomb gas. This corresponds to an unbinding at high temperatures of the dual interface from an edge-pinning potential.

4. Discussion

We now outline arguments applied directly to the interface models in support of the behaviour which has been suggested for their dual, modified Coulomb gases. Bulk pinning is treated first.

A two-dimensional interface below the roughening transition, and interfaces of higher dimensionality, have a finite width, $\langle h_i^2 \rangle^{1/2}$, and so can have a lower energy (by $-\Delta\langle\delta_{h_i,0}\rangle$) per site, refering to canonical averages with respect to the Hamiltonian of equation (1), in a pinning potential, at no cost in entropy (per site, in the thermodynamic limit). A two-dimensional interface in a bulk-pinning potential above the roughening temperature will have a lower entropy, as well as a lower energy, than the free interface, since fluctuations must be restricted in order for $\langle\delta_{h_i,0}\rangle$ to be non-zero. To compare the importance of each we represent the restriction on fluctuations by a minimum wavenumber, q_o, for these and calculate within the Gaussian model (Chui and Weeks 1976). The reduction in free energy in a bulk-pinning potential is, taking $\langle\delta_{h_i,0}\rangle \sim \langle h_i^2\rangle^{-1/2}$,

$$f(q_0) \sim -k_B T q_0^2 \ln(1/q_0) + \Delta[\ln(1/q_0)]^{-1/2} \tag{12}$$

for $d = 2$. Since $f(q_0)$ is positive at all temperatures for $\Delta > 0$ and sufficiently small q_0, bulk pinning will always localise an interface.

To discuss edge pinning of a type more closely related to the problem considered by Abraham (1980) than that for which the duality relation was demonstrated, we compare two systems on identical lattices, both described by Hamiltonians of the form of equation (1), with $P = \infty$. For system (a), $V(h) = 0$, and for system (b), $V(h)$ is given by equation (6); the condition $h_i = 0$ is imposed on the boundaries of both. Every configuration, S, of (a), with energy E_s, will consist of m_s unconnected regions, within each of which all h_i have the same sign, separated from one another by n_s sites where $h_i = 0$. A state S is completely specified by the value of $|h_i|$ on every site, together with the sign of h_i in each region. All configurations, S', of (b) with finite energy have $h_i \geqslant 0$ for all i, so that 2^{m_s} states of (a) are associated with one of (b). Define Z_a, Z_b to be the partition functions for (a), (b) respectively. Then

$$\begin{aligned} Z_b/Z_a &= Z_a^{-1} \sum_s \exp(-\beta E_s + \beta \Delta n_s - m_s \ln 2) \\ &= \langle \exp(\beta \Delta n_s - m_s \ln 2) \rangle_a \\ &\geqslant \exp(\beta \Delta \langle n_s \rangle_a - \langle m_s \rangle_a \ln 2) \end{aligned} \tag{13}$$

where $\langle\ \rangle_a$ denotes a thermal average in the system (a). Whenever the free interface width is finite, $\langle n_s \rangle_a$ and $\langle m_s \rangle_a$ are extensive quantities, so it then appears plausible that the equality holds in equation (13), in the thermodynamic limit. The edge-pinning model, (b), will therefore show an unbinding transition as Δ is varied with β fixed, at a critical value

$$\Delta_C = \beta^{-1} \ln 2 \lim_{N \to \infty} \left(\frac{\langle m_s \rangle_a}{\langle n_s \rangle_a} \right), \tag{14}$$

provided $\lim_{N\to\infty}(1/N)\langle n_s\rangle_a$ is finite. When the width of the free interface is unbounded, fluctuations are stronger and so an unpinned phase at high temperatures is also expected for a rough, two-dimensional interface.

The inequality (equation (11)) can be illustrated by comparison with the exact solution for the one-dimensional restricted solid-on-solid model. In one dimension, it is clear that $n_s \geq m_s$ for every state s. Hence the interface will certainly be pinned when $\beta\Delta > \ln 2$, although that only provides a bound on the transition point since the equality cannot be assumed in this example. The actual transition point, from Chui and Weeks (1981) is

$$\beta\Delta_C = \ln[(1+2R)/(1+R)] < \ln 2 \qquad R = e^{-\beta J}. \tag{15}$$

To summarise: the extension of a duality transformation on interfacial models to include pinning forces leads to modified forms for the dual Coulomb gases. The suggested behaviour of these Coulomb gases is borne out in one dimension by previous exact solutions of the interfacial models, and supported for higher dimensions by qualitative arguments which become quantitative if the unpinned interface has a finite width.

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References

Abraham D B 1980 *Phys. Rev. Lett.* **44** 1165–8
Abraham D B and Reed P 1974 *Phys. Rev. Lett.* **33** 377–9
van Beijeren H 1977 *Phys. Rev. Lett.* **38** 993–6
Burkhardt T W 1981 *J. Phys. A: Math. Gen.* **14** L63–8
Burkhardt T W and Vieira V R 1981 *J. Phys. A: Math. Gen.* **14** L223–7
Chalker J T 1981 *J. Phys. A: Math. Gen.* **14** 2431–40
Chui S T and Weeks J D 1976 *Phys. Rev.* B **14** 4978–82
—— 1981 *Phys. Rev.* B **23** 2438–42
Dobrushin R L 1972 *Theory of Probability and its Applications* (USSR) **17** 582–600
Emery V J and Swendsen R H 1977 *Phys. Rev. Lett.* **39** 1414–7
Gallavotti G 1972 *Commun. Math. Phys.* **27** 103–36
José J V, Kadanoff L P, Kirkpatrick S and Nelson D R 1977 *Phys. Rev.* B **16** 1217–41
Kogut J B 1979 *Rev. Mod. Phys.* **51** 659–713
Kosterlitz J M 1977 *J. Phys. C: Solid State Phys.* **10** 3753–60
Kroll D M 1981 *Z. Phys.* B **41** 345–8
van Leeuwen J M J and Hilhorst H J 1981 *Physica* A **107** 319–29
Weeks J D and Gilmer G H 1979 *Adv. Chem. Phys.* **40** 157–228
Weeks J D, Gilmer G H and Leamy H J 1973 *Phys. Rev. Lett.* **31** 549–51