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1991 J. Phys. A: Math. Gen. 24 L1315

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LEITER TO THE EDITOR

The Ising model in a random boundary field

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Received 28 June 1991

Abstract. Random inagnetic fields acting on the boundary of a system are relevant if $\eta_{\parallel} < 1$ For the case of the two-dimensional Ising model they are marginal, giving rise to calculable logarithmic corrections to boundary quantities near the bulk critical point. These considerations may be important in the study of finite-size effects in the critical behaviour of adsorbed systems.

Consider the problem of a system near bulk criticality, in the presence of a quenched random field which couples to the order parameter, and which is confined to the vicinity of the surface or boundary of the sample. Such boundary fields should not affect the bulk critical behaviour, but may induence the surface properties. For a given bulk universality class, there may be several different types of surface critical behaviour possible [1], and the question arises as to whether new behaviour is possible when such random fields are present. We expect that similar effects should arise for random boundary conditions, that is, when the order parameter(s) are frozen in a fixed, but random, manner. The general problem has recently been analysed in some detail by Diehl and Nüsser [2]. In this letter we focus on the type-dimensional case.

Given a system represented by a Hamiltonian \mathcal{H}_0 , the surface terms we consider are, in a continuum notation, given by

$$\mathscr{X} = \mathscr{X}_0 \div \int_S h(x) \sigma(x) \, \mathrm{d}^{d-1} x \tag{1}$$

where σ is the local boundary magnetization. This is written for the case of Ising spins; appropriate generalizations to other types of order parameter are straightforward. The random fields h(x) are random variables with the properties that $\overline{h(x)} = h$ and $\overline{h(x)h(x')} = h^2 + \Delta\delta(x - x')$. The quenched average may be obtained by using the replica trick. The replicated Hamiltonian has the form

$$\mathscr{H} = \sum_{\alpha} \mathscr{H}_{0}^{\alpha} + n \int_{S} \sum_{\alpha} \sigma^{\alpha}(x) d^{d-1}x - \Delta \int_{S} \sum_{\alpha \neq \beta} \sigma^{\alpha}(x) \sigma^{\beta}(x) d^{d-1}x$$
(2)

where we have ignored higher cumulants, which may be shown to be irrelevant in the sense of the renormalization group. The terms in the last sum with $\alpha = \beta$ have also been dropped because they represent a local contribution to the energy density at the boundary; they do not affect the critical properties, although they may modify non-universal quantities such as the location of the special transition.

From equation (2) we may redezive the criterion of Diehl and Nüsser [2] for whether these boundary random fields are relevant. First we must have h=0 so that there is no net uniform boundary magnetization. When $\Delta = 0$ the two-point function of the operator $\mathcal{O} = \sum_{\alpha \neq \beta} s^{\alpha} s^{\beta}$ along the boundary behaves like $r^{-2(d-2+\eta_{\parallel})}$, where η_{\parallel} is the usual exponent describing the decay of correlations along the boundary [1]. Thus \mathcal{O} has a surface scaling dimension $x_{\mathcal{O}} = d - 2 + \eta_{\parallel}$ and therefore a renormalization group eigenvalue $y_{\mathcal{O}} = d - 1 - x_{\mathcal{O}} = 1 - \eta_{\parallel}$. We conclude that random boundary fields are relevant if $\eta_{\parallel} < 1$. This is equivalent [1] to having $\gamma_{11} > 0$. For the ordinary transition, the ε -expansion gives [1] $\eta_{\parallel} = 2 - O(\varepsilon)$, with $\eta_{\parallel} \approx 1.48$ for the Ising case in d = 3. Thus random boundary fields are generally irrelevant, and lead only to possible corrections to scaling in surface quantities. However, for the d = 2 Ising model [3], we have $\eta_{\parallel} = 1$, and thus such effects are marginal. For the special transition, $\eta_{\parallel} = O(\varepsilon)$, and in fact is estimated [1] to be negative in d = 3. Thus Δ is relevant in this case (the special transition does not arise in two dimensions).

The fact that random boundary fields are marginal in the two-dimensional Ising case leads to some interesting predictions for the behaviour of surface quantities. Before analysing these, we remark that such boundary fields may be of direct physical relevance for some of the realizations of the Ising universality class. Consider, for example, the melting of a 2×1 commensurate phase of an adsorbed gas on a substrate. The adsorbed atoms are supposed to occupy sites on one of the two sublattices A or B of the substrate. In the bulk, there is no preference for either sublattice, which translates into the absence of any bulk magnetic field in the Ising mode!. The boundary sites, however, may be on either sublattice, and, if the shape of the boundary is irregular on scales of a few lattice spacings, the potential produced by the boundary will be equivalent to a random field, with zero mean, of the type we have been discussing.

In order to discuss the marginal case in more detail it is necessary to derive the renormalization group equations. This is most simply done within the replica formalism by analysing the operator product expansion of the operators \mathcal{O} and $S = \sum_{\alpha} \sigma^{\alpha}$. In fact, the calculation is very similar to that for the Ising model with random bonds [4], and the details will not be reproduced here. The result is

$$\frac{\mathrm{d}\Delta}{\mathrm{d}l} = 4(n-2)\Delta^2 + \dots \qquad \qquad \frac{\mathrm{d}h}{\mathrm{d}l} = \frac{1}{2}h + 4(n-1)\Delta h + \dots \qquad (3)$$

where the neglected terms do not affect the leading results given below. Although for the current problem one should set n=0 in (3), it is interesting to consider other values. In particular for n=2, we see that $d\Delta/dl=0$ to this order. In fact, this is so to all orders. This case corresponds to two semi-infinite Ising models coupled along their boundary, and we may 'unfold' this to obtain a single, infinite, Ising model with a defect line. It is well known that this exhibits a line of fixed points [5, 6], with a non-universal magnetic exponent varying continuously along this line. The existence of this line to all orders in Δ may be inferred using the conformal field theory methods of [7]. It turns out that all the correlation functions of the operator \mathcal{O} are identical with those of the operator $\partial_{\nu}\phi$ in the semi-infinite Gaussian model with Hamiltonian

$$\mathcal{H}_{G} = \frac{1}{2} \int (\partial \phi)^{2} d^{2}x + \Delta \int (\partial_{j} \phi) dx$$
(4)

and the scale invariance of this theory for all values of Δ is evident. For n > 2, equation (3) shows that Δ is marginally relevant, and will drive the system to a new type of behaviour. This may be investigated in the large-*n* limit. Consider *n* replicas of the Hamiltonian (1), and instead of tracing out the random field h(x), integrate over the Ising degrees of freedom. In a cumulant expansion, the resulting effective Hamiltonian

$$\mathcal{H}_{eff} = -\frac{1}{2\Delta} \int h(x)^2 dx + \frac{1}{2} \iint h(x_1)h(x_2) \langle S(x_1)S(x_2) \rangle dx_1 dx_2 + \frac{1}{4} \iiint h(x_1)h(x_2)h(x_3)h(x_4) \times \langle S(x_1)S(x_2)S(x_3)S(x_4) \rangle_c dx_1 dx_2 dx_3 dx_4 + \dots$$
(5)

where $S = \sum_{\alpha} \sigma^{\alpha}$. Each of the connected correlation functions is O(n), so that, as $n \to \infty$, we may rescale $h(x) \to n^{-1/2}h(x)$ and $\Delta \to \Delta/n$ in such a way that all cumulants beyond the second drop out, leaving

$$\mathscr{H}_{\text{eff}} = -\frac{1}{2\Delta} \int h(x)^2 \,\mathrm{d}x + \frac{1}{2} \int \int h(x_1) h(x_2 \langle \sigma(x_1) \sigma(x_2) \rangle \,\mathrm{d}x_1 \,\mathrm{d}x_2. \tag{5'}$$

This quadratic Hamiltonian may be diagonalized by going \circ Fourier modes. The q = 0 part of the second term is the local susceptibility χ_{11} , which diverges close to the bulk critical point as $\ln t$. Thus we see that, sufficiently close to bulk criticality, the coefficient of the q = 0 component of h changes sign, indicating an instability, and a non-zero expectation value for $\langle h \rangle$. This implies a non-zero magnetization at the boundary. Whether this transition is first or second order depends on the sign of the h^4 term, which seems difficult to determine. However, we may conclude that, for large n, the boundary actually orders at a temperature greater than that of the bulk. It is a reasonable guess that this occurs for all n > 2.

To return to the case of interest with n = 0, the solution of (3) is

$$\Delta(l) = \frac{\Delta}{1+8\Delta l} \qquad h(l) = h e^{l/2} (1+8\Delta l)^{-1/2}.$$
 (6)

The critical behaviour of the various thermodynamic quantities may now be obtained in a standard fashion. Note that the bulk temperature variable t does not couple to the surface fields so that its renormalization group equation dt/dl = t is unaffected. For example, we find that the surface magnetization m_s acquires logarithmic corrections:

$$m_{\rm s} \sim \frac{(-t)^{1/2}}{(-\ln t)^{1/2}} \tag{7}$$

and so on. The analysis of the surface free energy is somewhat more subtle (as in the case of the analogous random bond problem [8, 9]) because d/y_r is an integer. Instead of using simple scaling, one must express the surface free energy as an integral along the renormalization group trajectory

$$f_{s}(t,\Delta) = \int_{0}^{\infty} e^{-l} g(t(l),\Delta(l)) dl$$
(8)

where g is expected to be an analytic function of its arguments. The singular behaviour may be extracted by changing variables to u = t(l) and cutting off the integral at some fixed value $u = t_1$:

$$f_0 \sim t \int_{t}^{t_1} \frac{\mathrm{d}u}{u^2} g(u, \dot{\Delta}(u)). \tag{9}$$

g may now be expanded as a sum of powers of the form $u^N \Delta(u)^M$. The term with N = 1, M = 0 leads to the usual [1] t ln t singularity in f_s , and the other terms with M = 0 are analytic. There is no first-order contribution with M = 1, but the higher-order terms in M do lead to further singular corrections. The most singular may be shown to be of the form t ln ln t. Note that, in contrast to the random bond case [8, 9], these are non-leading corrections, and the nature of the leading t ln t singularity is not modified.

The marginality of Δ also has an important effect on the manner in which the local magnetization $\langle s(y) \rangle$ decays with the distance y from the boundary. The quenched average $\overline{\langle s(y) \rangle}$ vanishes, but the typical value of this quantity may be estimated by evaluating the Edwards-Anderson order parameter $\overline{\langle s(y) \rangle^2}$. To lowest order in perturbation theory in Δ this has the form

$$\overline{\langle s(y) \rangle^2} \sim \Delta \int \frac{\mathrm{d}x}{r^{\eta+\eta_{\parallel}}} \sim y^{-(\eta+\eta_{\parallel}-1)}.$$
 (10)

Note that if $\eta_{\parallel} = 1$, this fall-off is the same as would be expected when the boundary spins are all fixed to the same value. Similar considerations are valid for the correlation function $\overline{\langle s(r)s(r')\rangle}$, whose Fourier transform is the structure factor. In fact these considerations shed some doubt on the applicability of finite-size calculations of the structure factor [10], which assume free boundary conditions. In the latter case, the above correlation function decays as y^{-1} when r and r' are far from the boundary, while the above calculation shows a weaker fall-off like $y^{-1/4}$ when random boundary fields are present. Presumably random boundary fields would also have a pronounced effect on finite-size behaviour of thermodynamic quantities at criticality. We have not yet performed a detailed analysis of this.

Finally we comment on some situations when random boundary fields are actually relevant, that is, $\eta_{\parallel} < 1$. This occurs in two dimensions for the q-state Potts model when q < 2, since, in that case [11], $\eta_{\parallel} = 2(m-1)/(m+1)$ where $q = 2\cos(\pi/m+1)$. Thus the case of percolation (q=1) should be interesting, if a suitable physical interpretation of the random field may be given. For q close to 2, it is possible to proceed in analogy with [4] and find a new fixed point of the renormalization group equations to first order in (2-q), and to compute the corrections to η_{\parallel} at this fixed point.

As was pointed out earlier, random boundary fields are always relevant at the special surface transition. We expect that, in general, they lead to a new type of boundary universality class. Diehl and Nusser [2] have argued that for d = 3, since random fields are known to destroy the surface-ordered phase, the special transition should also be absent. For d > 3, the problem may be analysed within perturbation theory in the ϕ^4 Landau-Ginzburg model much as in the usual case of a bulk random field. It turns out that the upper critical dimension for this problem is d = 5 (as opposed to 6 for the bulk random field problem). Despite the unphysical dimensionality, it would be very interesting to pursue this further, as it may help shed light on the failure of this approach for the bulk random field.

This work was supported by NSF Grant PHY 86-14185.

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