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LETTER TO THE EDITOR

Surface critical behaviour and local operators with boundary-induced critical profiles

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Abstract, We present a simple argument showing that the surface energy density of a semi-infinite d-dimensional spin system has, in general, a leading thermal singularity of the same form, $|T-T_c|^{2-\alpha}$, as the bulk free energy. At bulk criticality energy-energy correlations decay as r^{-2d} parallel to the surface. These results hold for both free and fixed boundary spins, i.e. the 'ordinary' and 'extraordinary' transitions. The extraordinary critical behaviour of the magnetisation is the same as that of the energy density. We also confirm and generalise these results in two dimensions with an independent approach based on conformal invariance.

In this letter we consider the surface critical behaviour of semi-infinite spin systems in d spatial dimensions, with either free or fixed boundary spins, on approaching the bulk critical temperature. In the terminology of surface critical behaviour these two boundary conditions correspond to the 'ordinary' and 'extraordinary' transitions, respectively (Binder 1983).

Evidence from a number of model calculations (McCoy and Wu (1973) and Cardy (1984b, 1986b) for the two-dimensional Ising model, Dietrich and Diehl (1981), Diehl *et al* (1983) and Ohno and Okabe (1984) for the d-dimensional n-vector model, and Cardy (1984b, 1986b) and Burkhardt (1985) for the two-dimensional q-state Potts model) seems to indicate that the ordinary and extraordinary surface critical behaviour of the energy density and the extraordinary surface critical behaviour of the magnetisation is of the same simple type. These local densities have surface thermal singularities of the same form, $|T-T_c|^{2-\alpha}$, as the bulk free energy and their two-point correlations decay as r^{-2d} parallel to the surface. This particular critical behaviour is characterised by the surface scaling† dimension $x^{(s)}=d$.

The first model-independent prediction of this type of surface critical behaviour was made by Bray and Moore (1977), who analysed the extraordinary critical behaviour of the magnetisation on the basis of a local free-energy hypothesis. With an entirely different approach, we confirm here the predictions of Bray and Moore for the surface magnetisation at the extraordinary transition and extend them to the energy density at both the ordinary and extraordinary transitions.

† A local operator $\Phi(\boldsymbol{r})$ with scaling dimension x rescales according to $\Phi(\boldsymbol{r}')=b^x\Phi(\boldsymbol{r})$, $\boldsymbol{r}'=b^{-1}\boldsymbol{r}$ in thermal averages. This relation, the corresponding temperature transformation $T'=T_c+b^{1/\nu}(T-T_c)$ and the hyperscaling relation $2-\alpha=d\nu$ imply

$$\langle\Phi(\boldsymbol{r})\rangle_T\sim|T-T_c|^{x\nu}=|T-T_c|^{(2-\alpha)x/d}$$

$$\langle\Phi(\boldsymbol{r}_1)\Phi(\boldsymbol{r}_2)\rangle_{T_c}\sim|\boldsymbol{r}_1-\boldsymbol{r}_2|^{-2x}.$$

Our letter consists of two parts. We first derive the leading thermal singularity $|T-T_c|^{2-\alpha}$ in the surface energy and magnetisation densities in general dimension d with a simple argument that considers the change in free energy of the system as it is extended by adding an extra layer of spins at the surface. We then confirm and generalise these results in $d=2$ dimensions with a different approach based on conformal invariance (Cardy 1986c). Conformal invariance implies that the surface scaling dimension $x_\psi^{(s)}$ of any local operator $\psi(\boldsymbol{r})$ with a non-vanishing boundary-induced critical profile ($\langle\psi(\boldsymbol{r})\rangle_{T_c}\neq 0$) is given, in general, by $x_\psi^{(s)}=2$ in two dimensions, independent of the bulk scaling dimension of the particular operator.

Consider a spin system with L^d interacting spins and with free boundary conditions, shown schematically in figure 1. The number of interacting spins may be increased to $(L+\Delta L)^d$ by adding a layer of spins at the surface. The partition functions Z and free energies $F=\ln Z$ of the original and augmented systems are related by

$$Z_{L+\Delta L}=Z_L\langle\exp\Delta H\rangle_L \tag{1}$$

$$F_{L+\Delta L}-F_L=\ln\langle\exp\Delta H\rangle_L \tag{2}$$

where ΔH is, apart from an unimportant proportionality constant, the energy of the extra bonds added at the surface. Substituting

$$F_L=L^d f_b+L^{d-1}f_s \tag{3}$$

where f_b and f_s denote the intensive bulk and surface free energies, into equation (2) gives

$$f_b=(dL^{d-1}\Delta L)^{-1}\ln\langle\exp\Delta H\rangle_L+O(L^{-1}). \tag{4}$$

In a spin system defined on a spatial continuum, one can consider an extra layer of infinitesimal thickness. In the corresponding limit $\Delta L\to 0$, equation (4) becomes

$$f_b=\lim_{\Delta L\to 0}(dL^{d-1}\Delta L)^{-1}\langle\Delta H\rangle_L+O(L^{-1}). \tag{5}$$

Since the first term on the right is proportional to the surface energy density ε_1, equation (5) implies

$$\varepsilon_1\sim f_b\sim|T-T_c|^{2-\alpha}\qquad\text{ordinary transition} \tag{6}$$

in the thermodynamic limit. Thus the surface energy density at a free surface has a leading thermal singularity of the same form as the $|T-T_c|^{2-\alpha}$ singularity of the bulk free energy.

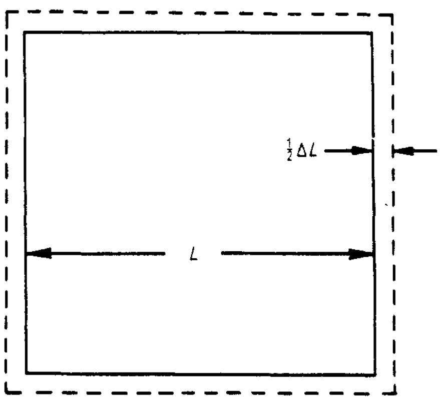

Figure 1. Systems with L^d and $(L+\Delta L)^d$ interacting spins.

In a spin system defined on a lattice†, one cannot take the limit $\Delta L \to 0$ in equation (4), since ΔL is restricted to integer values. However, in the limit $L \to \infty$ with ΔL a non-zero integer, one again expects the same thermal singularites in $(L^{d-1}\Delta L)^{-1} \ln \langle \exp \Delta H \rangle_L$ and $(L^{d-1}\Delta L)^{-1} \langle \Delta H \rangle_L$. Thus for the case of free boundary conditions (ordinary transition) result (6) should hold quite generally.

We now turn to the extraordinary transition (Bray and Moore 1977, Binder 1983), in which the bulk orders in the presence of a surface magnetisation due to sufficiently enhanced surface couplings or a surface field. If the boundary dimension is too low to support a spontaneous surface magnetisation above the bulk critical temperature, the surface field is essential for extraordinary critical behaviour.

In the case of a semi-infinite system with no enhancement of the surface couplings and with boundary spins oriented by a surface field h_1, we consider the change in free energy that results when an extra layer of interacting spins is added to the system and when the magnetic field is shifted from the original boundary spins to the new boundary spins. Equations (4) and (5) again apply, but now ΔH contains both single-spin magnetic-field energies and two-spin bond energies. A variety of heuristic arguments‡ suggests that both of these energies have the same leading thermal singularity in the extraordinary transition. Thus we conclude

$$m_1 \sim \varepsilon_1 \sim f_b \sim |T - T_c|^{2-\alpha} \qquad \text{extraordinary transition.} \tag{7}$$

Here m_1 denotes the component of the magnetisation that couples to the surface field and ε_1 is the energy density associated with the surface pair interactions.

We now rederive these results in two dimensions in a somewhat more general form, as a consequence of the conformal invariance (Cardy 1986c) of critical correlations. The surface critical indices of several two-dimensional models have been determined (Cardy 1984b, 1986b) with the conformal invariance approach. It is interesting to see how results (6) and (7), which are expected to hold independent of the details of particular models, also follow from conformal invariance.

Consider any local operator $\psi(\boldsymbol{r})$ that has a non-vanishing boundary-induced profile $\langle \psi(\boldsymbol{r}) \rangle_{T_c}$ at the bulk critical temperature in a semi-infinite system with free or fixed-spin boundary conditions. The energy density $\varepsilon(\boldsymbol{r})$ is clearly such an operator, and a second example is the magnetisation component $m(\boldsymbol{r})$ singled out by the boundary coondition in a system with fixed boundary spins.

In the half space, the profile $\langle \psi(\boldsymbol{r}) \rangle_{T_c}^{\text{half space}}$ is given by

$$\langle \psi(\boldsymbol{r}) \rangle_{T_c}^{\text{half space}} = A r_\perp^{-x_\psi^{(b)}} \tag{8}$$

as follows from ordinary scaling (Fisher and de Gennes 1978). Here $r_\perp$ is the perpendicular distance from the surface to point $\boldsymbol{r}$ and $x_\psi^{(b)}$ is the bulk scaling dimension of

† For lattice spin systems in two dimensions, equation (6) can also be derived by considering helical boundary conditions and adding one extra spin.

‡ One can separate the one and two-spin contributions by considering the spins inside the full line in figure 1 to be coupled with short-range interactions but not subject to a magnetic field and the exterior spins to be coupled and also subject to a uniform field. Removing the field from the spins in a layer of thickness $\Delta L/2$ leads to equations similar to (4) and (5) with only single-spin terms in ΔH.

Consider (Burkhardt 1985), for example, the semi-infinite classical n-vector model with spins $\boldsymbol{S}$ of unit length and an infinite surface field h_1 in the z direction. It is clear that $\langle S_k^z \rangle = \langle \boldsymbol{S}_k \cdot \boldsymbol{S}_b \rangle$, where spin b is on the boundary and spin k is not. In a finite field h_1, the two thermal averages are no longer equal, but the critical behaviour of each is presumably unchanged. In the extraordinary transition the spontaneous surface magnetisation or an applied surface field breaks the rotational symmetry and the distinction between local operators with the symmetry of the magnetisation density and the energy density disappears.

the operator $\psi(\boldsymbol{r})$. In terms of conventional critical exponents, the bulk scaling dimensions of the energy and magnetisation densities are $x_\varepsilon^{(b)} = d - \nu^{-1}$ and $x_m^{(b)} = \beta/\nu = (d - 2 + \eta)/2$, respectively.

In two dimensions the profile $\langle\psi(z)\rangle_{T_c}^G$ transforms according to

$$\langle\psi(w)\rangle_{T_c}^{G'} = |\mathrm{d}w(z)/\mathrm{d}z|^{-x_\psi^{(b)}}\langle\psi(z)\rangle_{T_c}^G \tag{9}$$

under a conformal mapping generated by the analytic function $w = w(z)$. Here we use complex variables $w = u + \mathrm{i}v$, $z = x + \mathrm{i}y$ to specify position. The superscripts G' and G refer to the boundary geometry, which is modified, in general, by the mapping. Making use of equations (8) and (9) and of the conformal mapping

$$w = (L/\pi)\cosh^{-1} z \tag{10}$$

of the half space $y > 0$ onto the half strip $u > 0$, $0 < v < L$, Burkhardt and Eisenriegler (1985) obtained the explicit expression

$$\langle\psi(w)\rangle_{T_c}^{\text{half strip}} = A\{[(L/\pi)\sinh(\pi u/L)]^{-2} + [(L/\pi)\sin(\pi v/L)]^{-2}\}^{x_\psi^{(b)}/2} \tag{11}$$

for the profile in the half strip.

Conformal invariance provides a great deal of information on the structure of the transfer matrices of two-dimensional systems (Cardy 1986a, b). In an infinitely long strip of width L, the pair correlation function formed with the operator $\psi(w)$ is given by

$$\langle\psi(w_1)\psi(w_2)\rangle_{T_c}^{\text{infinite strip}} = \sum_n \langle 0|\hat{\psi}(v_1)|n\rangle\langle n|\hat{\psi}(v_2)|0\rangle \exp[-(E_n - E_0)|u_1 - u_2|]. \tag{12}$$

Here the $|n\rangle$ are eigenstates of the transfer matrix $\hat{T} = \exp(-\hat{H})$ of a slice of the strip with unit length and width L. The eigenstates satisfy $\hat{H}|n\rangle = E_n|n\rangle$ and $|0\rangle$ denotes the ground state of $\hat{H}$. The energy gaps $E_n - E_0$ are related to surface scaling dimensions $x_n^{(s)}$ by

$$E_n - E_0 = \pi x_n^{(s)}/L. \tag{13}$$

This follows from the mapping $w = (L/\pi)\ln z$ of the half space onto the infinite strip (Cardy 1984a). The smallest non-zero energy difference with non-vanishing matrix element $\langle n|\hat{\psi}(v)|0\rangle$ determines the surface scaling dimension $x_\psi^{(s)}$ of the operator $\psi(w)$.

In terms of the same eigenstates $|n\rangle$, the profile of $\psi(w)$ in the half-strip geometry is given by

$$\langle\psi(w)\rangle_{T_c}^{\text{half strip}} = \sum_n M_n\langle n|\hat{\psi}(v)|0\rangle \exp[-(E_n - E_0)u]. \tag{14}$$

The amplitude M_n specifies the compatibility of eigenstate $|n\rangle$ with the boundary condition at the end $u = 0$ of the semi-infinite strip.

The right-hand side of equation (11) has the expansion

$$\begin{aligned}\langle\psi(w)\rangle_{T_c}^{\text{half strip}} &= A[(L/\pi)\sin(\pi v/L)]^{-x_\psi^{(b)}} \\ &\quad\times \sum_{M,N,\bar{N}=0}^{\infty} a_M(x_\psi^{(b)})a_N(-x_\psi^{(b)}/2)a_{\bar{N}}(-x_\psi^{(b)}/2) \\ &\quad\times \exp[-2\pi(M + N + \bar{N})u/L + 2\pi\mathrm{i}(N - \bar{N})v/L]\end{aligned} \tag{15}$$

in powers of $\exp(-2\pi u/L)$, where

$$a_n(x) = \Gamma(n + x)/[n!\Gamma(x)]. \tag{16}$$

Comparing equations (14) and (15), one learns that the only gaps that appear in (14) are integral multiples of $2\pi/L$. These same energy gaps are also present in equation (12). Without explicit knowledge of the eigenstates $|n\rangle$ and amplitudes M_n, one cannot rule out the possibility that other energy gaps, which are not integral multiples of $2\pi/L$, appear in (12) but are excluded from (14) by the boundary condition at the end of the strip. Whenever this exceptional situation does not arise in connection with the smallest non-zero gap in (12), the gap necessarily has the value $\Delta E = 2\pi/L$, which through (13) implies the surface scaling dimension

$$x_{\psi}^{(s)} = 2 \tag{17}$$

for the local operator ψ.

As discussed in the first footnote, in a two-dimensional semi-infinite system the surface scaling dimension $x_{\psi}^{(s)} = 2$ corresponds to a surface thermal singularity in $\langle\psi(\boldsymbol{r})\rangle_T$ of the same form $|T-T_c|^{2-\alpha}$ as in the bulk free energy and to a pair correlation function $\langle\psi(\boldsymbol{r}_1)\psi(\boldsymbol{r}_2)\rangle_{T_c}$ that decays as $|\boldsymbol{r}_1-\boldsymbol{r}_2|^{-2d}$ parallel to the surface at criticality. Conformal invariance predicts this type of critical behaviour, barring the exceptional situation referred to in the previous paragraph, for any local variable with a non-vanishing boundary-induced profile of the form (8).

We conclude with a brief discussion of the 'special' or 'multicritical' transition (Binder 1983). This transition takes place at the bulk critical temperature in semi-infinite systems with critically-enhanced surface couplings too strong for ordinary surface critical behaviour but too weak for extraordinary behaviour.

In the special transition the surface free energy has the scaling form (Binder 1983)

$$f_s(t, t_1) = t^{2-\alpha-\nu} G(t_1 t^{-\phi}). \tag{18}$$

Here t and t_1 are relevant variables proportional to the deviations of the bulk and surface couplings, respectively, from the multicritical values. The function G is a universal scaling function and ϕ is a positive crossover exponent. Equation (18) implies the thermal singularity

$$\varepsilon_1 \sim \partial f_s/\partial t_1 \sim |T-T_c|^{2-\alpha-\nu-\phi} \qquad \text{special transition} \tag{19}$$

in the surface energy density at the special transition, which is stronger than the $|T-T_c|^{2-\alpha}$ singularity† derived above for the ordinary and extraordinary transitions.

It is interesting to see whether or not the methods of this letter give information on the special transition. If the number of spins in a multicritical system is increased as in figure 1 by adding an extra layer of interacting spins at the surface, equations (4) and (5) still hold. Now, however, ΔH is not just the energy of the new critically-enhanced surface bonds. Adding ΔH to H also replaces the critically-enhanced couplings of the original surface spins with normal unenhanced couplings. Thus ΔH represents a difference of energies. Since the left-hand sides of equations (4) and (5) have the singular form $|T-T_c|^{2-\alpha}$ instead of the stronger singularity $|T-T_c|^{2-\alpha-\nu-\phi}$, the leading thermal singularities from the opposing contributions in ΔH apparently cancel. No information on the crossover exponent ϕ is obtained.

Some two-dimensional semi-infinite systems do exhibit special surface critical behaviour despite the low dimensionality of the boundary. For example, the Gaussian and classical $n\to 0$ vector models, which correspond to ordinary and self-avoiding

† At the ordinary and extraordinary transitions the corresponding crossover exponent has the value $\phi = -\nu$. The negative sign reflects the irrelevance of changes in the surface coupling strength.

walks, respectively, have special transitions in two dimensions. For two-dimensional self-avoiding walks in the presence of a critically absorbing wall, the crossover crossover exponent ϕ has been estimated by real-space renormalisation (Kremer 1983) and by enumerations (Ishinabe 1983). Thus there is reason to ask whether conformal invariance yields any information on the special transition in two dimensions.

It would appear that the arguments from conformal invariance given above should apply equally well to the special transition, giving a result contradicting (19). One possible resolution of this paradox is as follows. The amplitude A of the energy-density profile in equation (8) may vanish at the special transition. This is reasonable since one may see on physical grounds that, far from the multicritical point, $A>0$ for the ordinary transition (i.e. the energy density is enhanced at the surface), while for the extraordinary transition $A<0$. In that case, one should consider the correction to the behaviour given in (8), which will be proportional to $r^{-2+1/\nu-\lambda}$, where $\lambda>0$. The result of expanding the energy-density profile in the half strip is now different, since the first factor on the right-hand side of (9) will involve only the bulk scaling dimension $x_\varepsilon^{(b)}=2-\nu^{-1}$, while the second factor will depend on λ. We then find that the energy decays as $\exp(-\pi\lambda u/L)$ in the half strip, with corrections which are down by integer powers of $\exp(-2\pi u/L)$, corresponding to the existence of an energy gap $\pi\lambda/L$ in the spectrum of $\hat{H}$. This is consistent with the energy density having a surface scaling dimension $1-\phi/\nu$ (and hence with a surface energy-density singularity as in equation (19)) if $\lambda=1-\phi/\nu$. However, this argument places no constraint on the value of ϕ.

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