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LETTER TO THE EDITOR

Universal order-parameter profiles in confined critical systems with boundary fields

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Abstract. We consider systems at the bulk critical temperature with an ordering field applied at the boundary. For various boundary geometries, universal expressions for the spatial dependence of the order parameter are obtained by conformal mapping of the known results for the half space. Analytical results for strip, wedge and other two-dimensional geometries and for systems with spherical boundaries in arbitrary dimension are given.

Recognition of the constraints imposed by conformal invariance of correlations at critical points (Polyakov 1970, Wegner 1976) has resulted in considerable progress in both bulk critical phenomena (Belavin *et al* 1984, Dotsenko 1984, Friedan *et al* 1984) and in surface critical phenomena (Cardy 1984a, b, Cardy and Redner 1984). Conformal invariance restricts the form of bulk and surface correlation functions and in two dimensions completely determines both correlation functions and critical exponents.

The work of Cardy (1984a, b) and of Cardy and Redner (1984) on surface critical phenomena is primarily concerned with the 'ordinary' critical behaviour (Binder 1983) of two-point correlations at the bulk critical temperature. Conformally invariant Dirichlet boundary conditions, i.e., vanishing of the order-parameter density at the boundaries, are imposed.

In this letter we consider another conformally invariant boundary condition. At the boundaries the system is subject to an infinite ordering field. The ordering field induces a non-zero order parameter at the bulk critical temperature that increases to its maximum value at the boundaries of the system. We derive universal expressions for the spatial dependence of the order parameter for several different boundary geometries.

In the case of a magnetic system, the ordering field corresponds to a magnetic field applied only to the boundary spins. The ordering-field boundary condition is realised physically in a binary mixture bounded by walls that exert a short-range preferential attraction on one of the two species (Fisher and de Gennes 1978).

In a semi-infinite critical system with an infinite ordering field at the boundary, ordinary scaling completely determines§ the order-parameter profile at bulk criticality.

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§ We restrict our attention to the continuum limit $r_\perp \gg a$, where a is the lattice constant or equivalent microscopic length. For $r_\perp \sim a$ there is a crossover to a different $r_\perp$ dependence, with a finite limit as $r_\perp$ approaches zero.

The order parameter $\langle\phi(\boldsymbol{r})\rangle$ varies as

$$\langle\phi(\boldsymbol{r})\rangle_{\text{semi-infinite}} = Ar_{\perp}^{-x_b} \qquad (1)$$

(Fisher and de Gennes 1978, Rudnick and Jasnow 1982, Brézin and Leibler 1983). Here A is a constant amplitude, and $r_{\perp}$ is the perpendicular distance from the surface to point $\boldsymbol{r}$. The bulk scaling dimension x_b of the order-parameter density $\phi(\boldsymbol{r})$ is related to the conventional critical exponents by

$$x_b = \tfrac{1}{2}(d-2+\eta) = \beta/\nu. \qquad (2)$$

Cardy (1984a, b) and Cardy and Redner (1984) have determined the ordinary critical behaviour of two-point correlations in several two-dimensional boundary geometries by conformal mapping of the results for the half space. Below, the same procedure is followed, except that we consider the order-parameter profile instead of two-point correlations.

A mapping $\boldsymbol{r}\to\boldsymbol{r}'$ is conformal if it corresponds locally to a rotation and a dilation (Polyakov 1970, Wegner 1976). Under a conformal mapping the order parameter transforms according to

$$\langle\phi(\boldsymbol{r}')\rangle_{G'} = b(\boldsymbol{r})^{x_b}\langle\phi(\boldsymbol{r})\rangle_G \qquad (3)$$

at criticality (Cardy 1984a, b). Here $b(\boldsymbol{r})$ is a position-dependent length-rescaling factor corresponding to the local dilation, i.e., $b(\boldsymbol{r})^{-d} = |\partial\boldsymbol{r}'/\partial\boldsymbol{r}|$ is the Jacobian of the transformation. The ensemble averages in (3) are evaluated with original and transformed boundary geometries G and G', respectively.

In $d=2$ dimensions, conformal mappings correspond to transformations of the form $z\to w$, where $w=u+\mathrm{i}v$ is an arbitrary analytic function of the complex variable $z=x+\mathrm{i}y$. In $d=2$, (3) becomes (Cardy 1984a, b)

$$\langle\phi(w)\rangle_{G'} = |w'(z)|^{-x_b}\langle\phi(z)\rangle_G. \qquad (4)$$

In higher dimensions the conformal group is less rich, its generators consisting of homogeneous translations, rotations and dilations, and special transformations of the form

$$\boldsymbol{r}'/r'^2 = \boldsymbol{r}/r^2 + \boldsymbol{R}/(2R^2), \qquad (5)$$

where $\boldsymbol{R}$ is an arbitrary constant vector, that map hyperspheres onto hyperspheres (Polyakov 1970, Wegner 1976).

We now turn to some specific examples. Consider, firstly, the order-parameter profile in a two-dimensional strip of width L and infinite length. The transformation

$$w = (L/\pi)\ln z \qquad (6)$$

maps the upper half plane $y=\mathrm{Im}\, z\geq 0$ conformally onto the infinite strip $0\leq v\leq L$, $v=\mathrm{Im}\, w$. Inserting equations (1) and (6), with $r_{\perp}=y$, into (4), one finds

$$\langle\phi(w)\rangle_{\text{strip}} = A[(L/\pi)\sin(\pi v/L)]^{-x_b}. \qquad (7)$$

The order parameter is independent of u, as expected†. The profile described by equation (7) is universal in a more general sense than the universality of critical exponents or scaling functions. The functional form (7) applies to any critical system with strip geometry and strong ordering-field boundary conditions. Only the amplitude A and the index x_b depend on the particular system under consideration.

† Reversing the above steps, one sees that equation (1) is implied by (4), (6), and the requirement that $\langle\phi(w)\rangle_{\text{strip}}$ be independent of u. Thus (1) is also a consequence of conformal invariance.

In the limit $v/L \ll 1$ equation (7) may be expanded in the form

$$\langle\phi(w)\rangle_{\text{strip}} = Av^{-x_b}[1+\tfrac{1}{6}x_b(\pi v/L)^2+\ldots]. \tag{8}$$

The first term on the right-hand side is consistent with the semi-infinite result (1), as expected. The correction term is compatible with the L^{-d} dependence of the contribution to the order parameter from a distant wall conjectured by Fisher and de Gennes (1978).

Next we derive an expression for the order parameter in a semi-infinite strip. The upper half z plane is conformally mapped onto the domain $u \geq 0$, $0 \leq v \leq L$ by the function

$$w = (L/\pi)\cosh^{-1} z. \tag{9}$$

Inserting (1) and (9) into (4), one obtains the universal profile

$$\langle\phi(w)\rangle_{\text{halfstrip}} = A\{[(L/\pi)\sinh(\pi u/L)]^{-2} + [(L/\pi)\sin(\pi v/L)]^{-2}\}^{x_b/2}. \tag{10}$$

In the limit $u \gg L$, (10) reduces to (7), as expected.

To obtain the order-parameter profile in a two-dimensional wedge geometry, we use the conformal transformation

$$w = z^{\alpha/\pi} \tag{11}$$

that maps the upper half z plane onto the open wedge $0 \leq \omega \leq \alpha$, where $w = |w|\exp(\mathrm{i}\omega)$. The corresponding order parameter is given by

$$\langle\phi(w)\rangle_{\text{wedge}} = A[(\alpha/\pi)|w|\sin(\pi\omega/\alpha)]^{-x_b}. \tag{12}$$

We now briefly consider two-dimensional systems bounded by closed curves of finite length. According to complex-variable theory (see, e.g., Fuchs and Shabat 1964), for any closed curve C there exist functions that conformally map the interior of C onto the upper half plane and the curve C onto the real axis. (This is physically clear from the connection between conformal mapping and two-dimensional electrostatics, see, e.g., Morse and Feshbach (1953).) Thus for each such boundary there is a corresponding order-parameter profile that is universal in the same sense as the profiles considered above. For examples of conformal transformations that map closed two-dimensional domains onto the half plane, we refer to standard texts on complex variables and on electrostatics. Here only rectangular and circular two-dimensional domains are considered.

The upper half z-plane is mapped onto the rectangular domain $-\frac{1}{2}a \leq u \leq \frac{1}{2}a$, $0 \leq v \leq b$ by the transformation (see, e.g., Fuchs and Shabat 1964)

$$w = C\int_0^z \mathrm{d}t[(1-t^2)(1-k^2t^2)]^{-1/2}. \tag{13}$$

The constants C and k are fixed by the requirements that the points 1 and $1/k$ on the positive x-axis map onto $w = \frac{1}{2}a$ and $w = \frac{1}{2}a + \mathrm{i}b$, respectively. The elliptic integral in equation (13) precludes analytic evaluation of the corresponding order parameter in terms of elementary functions.

The order-parameter profile in a two-dimensional system with a circular boundary can be worked out analytically. It is a special case of the result for hyperspherical boundaries in general dimension d, which we now discuss.

From the remarks about the generators of the conformal group in the paragraph containing (5), it is clear that in more than two dimensions, the most general conformal transformation maps hyperspheres onto hyperspheres. The plane $\hat{R}\cdot r=0$, where $\hat{R}$ is an arbitrary fixed unit vector, corresponds to a hyperspherical surface of infinite radius. The special conformal transformation (5) maps this plane onto a hyperspherical surface of radius R with centre at $\boldsymbol{R}$. The half spaces $\hat{R}\cdot r>0$ and $\hat{R}\cdot r<0$ map onto the interior and exterior of this hypersphere, respectively. The homogeneous translation

$$r''=r'-\boldsymbol{R} \tag{14}$$

shifts the centre of the hypersphere to the origin of the double-primed coordinate system. The scale factor $b(r)=|\partial r''/\partial r|^{-1/d}$ corresponding to the conformal mapping $r\to r''$ is given by

$$b(r)=1+\boldsymbol{R}\cdot r/R^2+r^2/(4R^2)=4R^2/(r''-\boldsymbol{R})^2. \tag{15}$$

With the mapping $r\to r''$, $\hat{R}\cdot r>0$, we determine the order-parameter profile in a hypersphere of radius R with a strong ordering field at the surface from the profile (1) for semi-infinite geometry. Applied to the half space $\hat{R}\cdot r<0$, the mapping gives the order parameter in an infinite critical system with ordering-field boundary conditions at the walls of a spherical cavity of radius R. Combining equations (1), (3), (5), (14), (15), one obtains the formula

$$\langle\phi(r'')\rangle_{\text{sphere}}=A\{\tfrac{1}{2}R|1-(r''/R)^2|\}^{-x_b} \tag{16}$$

which holds for either geometry. Note that the spatial dimension d does not appear explicitly in equation (16).

In the asymptotic regime $|r''-R|\ll R$, i.e., close to the spherical wall, the order-parameter profile reduces to $A|r''-R|^{-x_b}$, consistent with the semi-infinite result (1). Far outside the spherical cavity, i.e., for $r''\gg R$, the order parameter decays as $A(2R)^{x_b}(r'')^{-2x_b}$, with the same critical exponent $2x_b=d-2+\eta$ as the bulk pair correlation function.

Thus far only infinite boundary fields have been considered. The following heuristic scaling argument suggests that sufficiently far from the walls of a sufficiently large system, the order-parameter profiles for finite and infinite boundary fields coincide.

At a distance x from the boundary of a critical system with characteristic size L, the order parameter m scales as

$$m(x, L, t_1(1), h_1(1))=b^{-x_b}m(x/b, L/b, t_1(b), h_1(b)) \tag{17}$$

(Fisher and de Gennes 1978). Here b is the length-rescaling factor, and $t_1(1)$, $h_1(1)$ and $t_1(b)$, $h_1(b)$ denote the original and rescaled surface couplings and surface fields. We assume in (17) that $x\gg a$, where a is the lattice constant or average intermolecular distance, so that the order parameter scales with the bulk index x_b of equation (2). We now consider values of x, L, and b so large that $t_1(b)$ and $h_1(b)$ may be replaced by fixed-point values. Since $m(x, L, t_1(1), h_1(1))$ is independent of $t_1(1)$ and $h_1(1)$ in this regime, the profiles for infinite and finite boundary fields are the same. Brézin and Leibler (1983) have shown this explicitly for the semi-infinite continuum Ising model in $4-\varepsilon$ dimensions. For distances $r_\perp$ much greater than surface correlation lengths $\xi(t_1)$ and $\xi(h_1)$, the order parameter is given by equation (1), with an amplitude A independent of t_1 and h_1.

As mentioned above, ordering-field boundary conditions are realised in binary mixtures near container walls that adsorb one of the components preferentially. Recent optical experiments (Beysens and Leibler 1982, Franck and Schnatterly 1982) indicate critical anomalies in the boundary fluorescence and reflectivity of such systems. As far as we known, the power-law decay (1) of the order parameter at criticality near a planar wall has not been verified experimentally. The experimental determination of order-parameter profiles of the type we have considered is very difficult. The characteristic size L of the system should be large enough so that the order parameter can be probed locally and there is scaling behaviour. However, if L exceeds the maximum correlation length $\xi = \xi_0|T - T_c|^{-\nu}$ fixed by the temperature resolution, the order-parameter profile deviates significantly from the critical profile.

As mentioned in the first footnote, there is a crossover in the order-parameter profile at a microscopic distance a from the boundary. From equations (7) and (16) one sees that the order parameters at central and boundary points in a confined geometry of characteristic size L have the ratio $(a/L)^{x_b}$. It is interesting to note the strong dimensional dependence of this ratio. Choosing $a = 1$ Å and $L = 1$ cm, we find $(a/L)^{x_b} = 10^{-1}$ for the index $x_b = \frac{1}{8}$ of the $d = 2$ Ising model. In $d = 3$, $x_b \approx \frac{1}{2}$ and $(a/L)^{x_b} \approx 10^{-4}$.

Scattering experiments yield information about two-point correlations as well as the order-parameter profile. We conclude with a brief discussion of the ordinary critical behaviour of the two-point correlation function in hyperspherical geometry with zero surface field and Dirichlet boundary conditions.

In semi-infinite geometry, conformal invariance implies the form (Cardy 1984b)

$$\langle\phi(\boldsymbol{r}_1)\phi(\boldsymbol{r}_2)\rangle_{\text{semi-infinite}} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|^{-2x_b} Y\left(\frac{4r_{1\perp}r_{2\perp}}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|^2}\right) \tag{18}$$

for the corresponding correlation function, with $r_\perp$ defined as in (1). The function $Y(y)$ has the asymptotic behaviour

$$Y(y) \to \begin{cases} By^{x_s - x_b}, & y \to 0 \qquad (19a) \\ C, & y \to \infty. \qquad (19b) \end{cases}$$

Here $x_s = \frac{1}{2}(d - 2 + \eta_\|)$ and x_b is given by (2), consistent with standard definitions of the ordinary surface exponent $\eta_\|$ and the bulk exponent η (Binder 1983). Making use of the mapping that led from (1) to (16) and the analogue of (3) for two-point correlations, we obtain

$$\langle\phi(\boldsymbol{r}_1'')\phi(\boldsymbol{r}_2'')\rangle_{\text{sphere}} = |\boldsymbol{r}_1'' - \boldsymbol{r}_2''|^{-2x_b} Y(y) \tag{20a}$$

$$y = [1 - (r_1''/R)^2][1 - (r_2''/R)^2]|\boldsymbol{r}_1''/R - \boldsymbol{r}_2''/R|^{-2} \tag{20b}$$

for both of the hyperspherical geometries discussed in connection with (16).

For the $d = 2$ Ising model (Cardy 1984b), the $n \to \infty$ vector model in $2 < d < 4$ (Bray and Moore 1977), and the Gaussian model, the functions $Y(y)$ are known explicitly. In the limits $y \to 0$ and $y \to \infty$, with y defined by (20*b*), the asymptotic forms (19) apply, and the correlation function in the hyperspherical geometry is universal in the same sense as the order-parameter profiles considered above.

Presumably (18)-(20) also hold in the case of ordering-field boundary conditions. The scaling function is not the same, of course, and in (19*a*) x_s is the appropriate surface index for the extraordinary transition (Binder 1983) instead of the ordinary transition.

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