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Critical Wall Perturbations: Scaling and Renormalization Group

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The influence *at criticality* of a "far" wall on the order parameter close to a "near" wall as discussed by Fisher and de Gennes is recast in a form more suitable for microscopic analysis. An argument beyond ordinary scaling is presented which yields the perturbation exponent $d^* = d$ for longitudinal perturbations and $d_\perp^* = d - 1$ for transverse perturbations. These results are consistent with explicit renormalization-group computations to $O(\epsilon = 4 - d)$ which involve solution of the nonlocal equation of state.

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The special theoretical challenges posed by surface-related inhomogeneities *at bulk criticality* include the necessity of simultaneously taking into account the inherent nonlinearity of these often sizable inhomogeneities, their nontrivial effect on critical fluctuations, and the fact that they give rise to a spatial variation in a system with no bulk length scale. Renormalization-group approaches have yielded a theoretical picture of the surface of a system at its bulk critical point that, while not complete, has been substantially filled in.

It is also possible to consider surface effects at criticality from a phenomenological point of view. In a short but seminal paper Fisher and de Gennes[1] combined general scaling considerations and a phenomenological free energy to obtain information on the behavior near bounding surfaces, and on the mutual influence of parallel bounding surfaces, in a system at its bulk critical point. While their particular focus was different, the approach applies to effects in magnets, simple fluids, and other systems. Their results point to possible experimental tests of surface scaling at bulk criticality.[2,3]

The phenomenological free energy utilized by Fisher and de Gennes[1] encompasses proper scaling in the limit of a homogeneous system and incorporates the novel idea of a "floating" correlation length, $\xi(\vec{x})$. It yields, among other predictions, a power law for the decay of surface perturbations into the bulk of a semi-infinite system and a power law describing the mutual influence of two well-separated plane parallel bounding surfaces. The former prediction is consistent with general scaling arguments and has been borne out by recent renormalization-group calculations.[4] The latter prediction will be the subject of this note.

The quantity calculated by Fisher and de Gennes[1] is the influence on a scalar order parameter profile $m(z)$ close to a "near" wall at $z = 0$ of boundary conditions at a "far" wall at $z = D$. For $a \ll D$, the shift in $m(z = a) \equiv m_1$ due to the presence of

the far wall is described by

$$\Delta m_1/m_1(D=\infty) \sim D^{-d^*}, \quad (1)$$

at bulk criticality. The specific prediction for the exponent d^* arising from the phenomenological approach of Fisher and de Gennes[1] is $d^*=d$, the dimensionality of the system. This prediction was later verified for the two-dimensional Ising model by Au-Yang and Fisher.[5]

The exponent d^* has some special interest because it does *not* follow from a general scaling hypothesis for the free energy. One may suppose that Δm_1 should vanish as a negative power of D, but the exact power seems to require more detailed information concerning the form of the free energy. The free energy of Fisher and de Gennes[1] supplies just such information, but it is afflicted by acknowledged pathologies and is, in addition, based on a *local* free-energy functional which, in the light of our current understanding[4,6] of critical correlations in inhomogeneous systems, is an inherently suspect form.

In this note we report the results of an investigation into the mutual influence of two bounding surfaces *at bulk criticality* from a renormalization-group point of view. We have found the following: (1) The equality $d^*=d$ can be justified on the basis of general arguments incorporating correlation function scaling at the critical point. (2) Similar arguments yield the equality $d_\perp{}^*=d-1$ where $d_\perp{}^*$ is the exponent describing the *transverse* effect of boundary conditions at the far wall on the order parameter close to the near wall in an isotropic n-vector system. (3) Both of these equalities agree with the $O(\epsilon)$ results of an explicit renormalization-group calculation in $4-\epsilon$ dimensions.[7] This calculation, in contrast to those of Fisher and de Gennes[1] and of Fisher and Au-Yang,[1] involves the solution of a *nonlocal* equation of state for the order-parameter profile.

We begin by posing the problem of the mutual influence of the two walls in terms of perturbations of the pure power-law decay of the order parameter in a semi-infinite critical system. This power-law decay follows from general scaling considerations and from explicit renormalization-group analysis.[4] When z is large enough in a semi-infinite system,[4] we have

$$m(z) \propto (z+z_0)^{-(d-2+\eta)/2}, \quad (2)$$

with η the standard correlation-function exponent and z_0 determined by the behavior of $m(z)$ when z is small. This result is significant. It tells us not only that the asymptotic decay of $m(z)$ is as $z^{-(d-2+\eta)/2}$ but also that the term of next-to-leading order goes as $z^{-(d+\eta)/2}$. The latter prediction goes somewhat beyond the most elementary scaling considerations and follows from the fact that contributions to the equation of state, while nonlocal, are sufficiently short ranged that surface effects do not influence the corrections to asymptotic decay into the bulk.

When the system is not semi-infinite, the order parameter will not be purely decaying. In fact, we may expect a small correction near $z=0$ to grow in relation to the decaying exponent and ultimately cause the order parameter to switch from decay to behavior that matches the boundary conditions at $z=D$. If, for $z \ll D$, we write $m(z) = Az^{-(d-2+\eta)/2} + \delta m$, it is plausible that the contribution to δm that grows does so as a power so that $\delta m \approx Bz^p$ (where we have left out the correction decaying as $z^{-(d+\eta)/2}$). The amplitude B determines how far away from $z=0$ the order-parameter profile deviates significantly from pure power-law *decay*. If this is to occur at $z \sim D$ then we must have $BD^p \sim AD^{-(d-2+\eta)/2}$ or

$$B \sim D^{-(d-2+\eta+2p)/2}. \quad (3)$$

The quantity Ba^p represents the perturbing effect of the surface at $z=D$ on the order-parameter profile at $z=a$. The result (3) along with Eq. (1) clearly implies

$$d^* = (d-2+\eta+2p)/2. \quad (4)$$

The value of d^* is controlled by p.

This latter exponent can be obtained from the equation of state for the order parameter which is of the generic form $\delta F/\delta m(\vec{x}) = 0$, where F is the free energy[8] expressed in terms of the order parameter $m(\vec{x})$. This equation of state predicts the leading-order power-law decay of $m(z)$. Suppose that we write $m(z) = M_0(z) + M_1(z)$, where $M_0(z)$ is the order-parameter profile in a semi-infinite system and M_1 represents the small perturbation associated with a finite D. The equation of state, expanded to first order in $M_1(z)$, takes the form (for $z \ll D$)

$$\int \Sigma(z,z')M_1(z')dz' = 0, \quad (5)$$

where $\Sigma(z,z')$ is the second functional derivative $[\delta^2 F/\delta m(z)\,\delta m(z')]_{m=M_0}$. Neglecting effects associated with surface scaling,[9] we expect this equation to admit of two solutions, one growing and the other decaying as a power of z. The decaying solution goes as $z^{-(d+\eta)/2}$, according to the arguments above,[10] and the growing one goes as z^p.

The quantity $\Sigma(z,z')$ has additional significance.

As the second functional derivative of the free energy with respect to the order parameter it is also the inverse of the kernel describing the static linear response of the semi-infinite system to an ordering field varying in the z direction only. Because of the connection between fluctuations and linear response $\Sigma(z,z')$ is also the inverse of $g(z,z')$, the following integral of the two-point correlation function, $G(\vec{x},\vec{x}')$:

$$g(z,z') = \int G(\vec{x},\vec{x}')d^{d-1}\rho \quad [\vec{x}=(z,\vec{\rho})]. \tag{6}$$

Scaling of correlations at criticality can be applied, conjecturally, to the inhomogeneous system of interest here.[11] These considerations yield for $G(\vec{x},\vec{x}')$

$$G(\vec{x},\vec{x}') \sim z^{-(d-2+\eta)} f(z'/z, |\vec{\rho}-\vec{\rho}'|/z), \tag{7}$$

and hence for $g(z,z')$

$$g(z,z') \sim z^{1-\eta} f(z/z'). \tag{8}$$

As remarked, $g=\Sigma^{-1}$ and so $g(z,z')$ satisfies an equation similar to (5) with g in place of M_1. Now, if $z' \gg z$, we expect $g(z,z')$ to go to zero. At criticality we should have power-law decay $g(z,z') \sim z'^{-q}$ as $z' \to \infty$. Furthermore, $g(z,z') \sim z^{p}$ as $z \to 0$, or

$$g(z,z') \sim z'^{-q} z^{p}, \quad z' \gg z. \tag{9}$$

The powers p and q are determined by Eq. (5) with $M_1(z) = z^{p}$ or z^{-q}. This tells us that $q=(d+\eta)/2$ and that p is the power in which we are interested. Referring back to the scaling form (8) we see that p and q must also satisfy

$$p - 1 + \eta = q = \tfrac{1}{2}(d+\eta), \tag{10}$$

or $p=(d+2-\eta)/2$.[10] Inserting this result into (3) we obtain

$$d^* = \tfrac{1}{2}(d+2-\eta) + \tfrac{1}{2}(d-2+\eta) = d, \tag{11}$$

and the desired equality results.

We can define a $d_\perp{}^*$ in the same way by asking for the transverse effect on the *vector* order parameter $\vec{m}(z)$ near $z=0$ induced by boundary conditions at $z=D$ that require $\vec{m}(z)$ to rotate. If we assume an isotropic n-vector model the arguments proceed straightforwardly. The scaling arguments for the correlation function ought to go through as before; we may assume no *essential* distinction between transverse and longitudinal correlations at criticality, even though there is a nonzero $\vec{M}_0(z)$. The connection between the kernel in the expanded equation of state and the inverse of the integrated transverse correlation function is the same as in the longitudinal case. The only difference between the two cases lies in the power law of the decaying correction to the dominant semi-infinite decay $z^{-(d-2+\eta)/2}$. To obtain a small transverse correction we simply perform a small uniform rotation on $\vec{m}(z)$. This yields a transverse perturbation decaying with the *same* power law. Thus $q_\perp=(d-2+\eta)/2$, so that, by the correlation-function scaling argument, the power $p_\perp$ for a small growing transverse correction is given by

$$p_\perp = q_\perp + 1 - \eta = (d-2+\eta)/2 + 1 - \eta = (d-\eta)/2,$$

and

$$d_\perp{}^* = q_\perp + p_\perp = \tfrac{1}{2}(d-2+\eta) + \tfrac{1}{2}(d-\eta) = d-1. \tag{12}$$

While the arguments above are all highly plausible, they rely on some assumptions concerning the behavior of correlation functions at the critical point when there is surface order.[11,12] We have checked the value of d^* and $d_\perp{}^*$ by performing $O(\epsilon)$ calculations in the field-theoretical renormalization group and find that $d^*=d$ and $d^*=d-1$ to order $\epsilon=4-d$. The details of the explicit calculation are sketched in the following.

We seek the growth of longitudinal and transverse corrections to the pure power-law decay $z^{-(d-2+\eta)/2}$ in the isotropic n-vector model. When $n=1$ this reduces to the Ising model, and so the calculation refers to scalar order parameters as well. In this single-loop calculation the longitudinal kernel $\Sigma_L(z,z')$ is given at order ϵ by

$$\Sigma_L(z,z') = \delta(z-z')[-d^2/dz^2 + 12u^* M_0(z)^2 z^{-\epsilon} + 12u^* G_L{}^{(s)}(\vec{x},\vec{x}) + 4u^*(n-1)G_T{}^{(s)}(\vec{x},\vec{x})]$$
$$-288\,u^{*2} S_{LL}(z,z')M_0(z)M_0(z') - 32(n-1)u^{*2} S_{TT}(z,z')M_0(z)M_0(z'). \tag{13}$$

The transverse kernel, $\Sigma_T(z,z')$, is given by an analogous expression. $S_{\alpha\beta}(z,z')$ is given by

$$S_{\alpha\beta}(z,z') = \int G_\alpha(\vec{x},\vec{x}')G_\beta(\vec{x},\vec{x}')d^{d-1}\rho' - S, \quad \alpha,\beta = L,T, \tag{14}$$

where $G_{L(T)}$ is the "bare" longitudinal (transverse) correlation function in the presence of $\vec{M}_0(z)$. The term S refers to subtractions that remove divergences from the integral and account for contributions to renormalized quantities. Similar subtractions have been made from $G_{L(T)}{}^{(s)}(\vec{x},\vec{x})$. The leading-order solution $M_0(z)$

decays as $z^{-(2-\epsilon)/2} \sim z^{-(d-2+\eta)/2}$.[4] The quantity u^* in (13) is the fixed-point value of the renormalized four-spin coupling, and controls the magnitude of $M_0(z)$ for fixed z, which enters in an important way in Eqs. (13) and (14).

Equation (13) (and the analog for Σ_T) differ from those derivable from the free energy of Fisher and de Gennes[1] in that they are *nonlocal*. Nevertheless the solutions $M_{L(T)}(z)$ of the equation $\int \Sigma_{L(T)}(z,z')M_{L(T)}(z')dz' = 0$ are

$$M_L(z) \sim z^{3-\epsilon/2}, \quad M_T(z) \sim z^{2-\epsilon/2}, \tag{15}$$

which yields $d^* = 4 - \epsilon = d$ and $d_\perp{}^* = 3 - \epsilon = d - 1$.

In summary, we have recast the question of mutual influence of a "far" wall on the behavior of the order parameter in the vicinity of a "near" wall in a form more suitable for microscopic analysis. An argument beyond ordinary scaling and utilizing features of the semi-infinite system obtained in Ref. 4 has been presented which yields the wall perturbation power (as introduced by Fisher and de Gennes[1]) $d^* = d$ for longitudinal perturbations and $d_\perp{}^* = d - 1$ for transverse ones.[13] These results are shown to be consistent with an explicit renormalization-group calculation to $O(\epsilon)$ which involves solution of the nonlocal equation of state.

We conclude by noting that the Fisher–de Gennes functional[1] is an uncommonly good local approximation to the nonlocal equation of state. There are known difficulties with the local functional such as when boundary conditions require that the order parameter vanish within the sample. Further, the functional cannot give surface exponents in the appropriate regime[4] and cannot give logarithms in $d = 4$. Nonetheless the asymptotic decay $z^{-(d-2+\eta)/2}$ is given correctly as is the relation $d^* = d$. This is nontrival since other local equations of state will satisfy the former but not the latter. For experimental interpretations the Fisher–de Gennes functional, perhaps patched up to include the surface exponent regime, would seem an ideal starting point. Detailed questions would of course have to be answered within the framework of the nonlocal equation of state.

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[7]For $d > 4$ one obtains mean-field results $d^* = 4$, $d_\perp{}^* = 3$. The arguments below apply to $2 < d < 4$.

[8]The functional F contains fluctuation corrections and is in general nonlocal.

[9]Here we refer to special exponents corresponding to behavior near the surface; see, e.g., Ref. 4.

[10]This has been explicitly verified to $O(\epsilon)$, $\epsilon = 4 - d$.

[11]The results of Ref. 4 show explicitly that scaling of the equation of state holds in the semi-infinite system. No new exponents are required to discuss asymptotic behavior (away from $z = 0$). Physically the boundary introduces a spatially dependent correlation length $\xi(z) \propto z$. Similar arguments and analysis can be applied to the two-point function and other correlations.

[12]Further evidence has been provided by the work of K. Symanzik [Nucl. Phys. B190 (FC3), 1 (1981)], in which formal renormalization procedures are discussed for systems with boundaries. See also the work of Diehl and Dietrich, Ref. 6.

[13]Experiments on superconducting films might yield information on $d_\perp{}^*$.