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Field-theoretical approach to multicritical behavior near free surfaces

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The critical behavior of a semi-infinite n-vector model in $4-\epsilon$ dimensions near the special transition is studied. The renormalization of the relevant surface operators is discussed and explicitly carried out in two-loop order. It is found that the crossover exponent ϕ_s related to the square of the order parameter in the surface does not satisfy the relation $\phi_s = 1-\nu$ due to Bray and Moore.

Renormalization-group (RG) methods of field theory have been applied with considerable success in the study of bulk critical phenomena.[1,2] In a recent paper[3] (hereafter referred to as I) similar methods were used to investigate the effects of free surfaces on critical behavior. The analysis in I was based on a semi-infinite n-vector model and restricted to the ordinary transition.[4,5] This transition occurs in ferromagnetic systems when the coupling between the magnetic moments in the surface is less or only slightly stronger than in the bulk. However, if the surface coupling is sufficiently strong, the surface may order at a higher temperature than the bulk. The bulk then orders in the presence of the ordered surface. This is the extraordinary transition. The lines of ordinary, surface, and extraordinary transitions meet in a multicritical point that describes the special transition.

In this Communication we will analyze the critical behavior of the semi-infinite n-vector model in $d=4-\epsilon$ dimensions near the special transition. Previous work on this transition was based on mean-field theory,[4,5] position-space RG methods[6–10] (for the Ising case $n=1$), and ϵ-expansion techniques.[5,11–13] Bray and Moore[14] also discussed the $n=\infty$ case. In addition, they proposed[5] the scaling relation $\phi_s = 1-\nu$ (where ν is the bulk correlation-length exponent) for the crossover exponent ϕ_s related to the square of the order parameter in the surface. An analogous prediction $\gamma_{11}^{\text{ord}} = \nu - 1$ was made for the susceptibility exponent γ_{11}^{ord} at the ordinary transtition. Both relations are satisfied by the semi-infinite n-vector model to order ϵ. We will show that the relation $\phi_s = 1-\nu$ is in general *not* valid. For the other one this has been shown already.[3,15]

With the exception of Reeve's work,[13] previous analyses of the special transition based on the ϵ expansion were limited to first order. Reeve presented results to order ϵ^2 for surface exponents, but did not calculate ϕ_s. He renormalized the usual bulk operators and identified surface exponents by exponentiation. However, a systematic RG analysis of critical phenomena in semi-infinite systems requires that one incorporates *all* relevant, i.e., bulk *and* surface operators into the renormalization program. This requirement is less important in the case of the bulk-driven ordinary transition discussed in I where a single surface operator (the normal derivative of the order parameter) had to be renormalized. The inclusion of this operator into the RG was partly a matter of convenience only, but needed to derive the surface scaling laws. Since the special transition is described by a mulitcritical point that involves relevant surface operators, we believe that a careful study of these operators is *indispensable.*

An extension of the analysis in I to the special transition turns out to be nontrivial. New conceptual and technical difficulties appear. For example, the (Neumann) boundary condition, the two-point correlation function satisfied at the special point is destroyed already in first order of perturbation theory.[16] (The corresponding Dirichlet boundary condition at the ordinary transition holds to all orders.[3,16,17]) Thus an expansion of the order parameter in terms of eigenfunctions that satisfy the mean-field boundary condition is less advantageous. These difficulties are characteristic for systems in which translational invariance is broken by surfaces or defect planes. We therefore believe the present study to be of some general interest.

Our approach is based on recent work of Symanzik,[16] who discussed general aspects of the renormalization of surface operators. His work also shows that critical phenomena in semi-infinite systems are related to other problems in field theory. Once the relevant surface operators have been renormalized, the powerful machinery of Callen-Symanzik equations can be directly applied to surface quantities of interest. As we will see, critical exponents, transients, and crossover exponents follow in the usual straightforward way form the renormalization (Z) functions.

The model we consider is defined by the free-energy functional

$$F=\int d^{d-1}r\left[\int_0^\infty dz\left[\frac{1}{2}(\nabla\phi)^2+\frac{1}{2}\tau\phi^2+\frac{g}{4!}(\phi^2)^2\right]+\frac{1}{2}c^0\phi^2(r,0^+)\right] \tag{1}$$

for the n-component order parameter $\phi(x)$, where z measures the distance from the surface and $x=(r,z)$, with a $d-1$-dimensional parallel component r.

The critical behavior of the Gaussian model that results when $g=0$ is well known[4,5,12]: special and ordinary transitions correspond to $c^0=0$ and $c^0>0$, respectively, surface and extraordinary transitions to $c^0<0$. At the special point ($\tau=0$, $c^0=0$) the parallel Fourier transform of the correlation function $G(x,x')$ for spins at sites $x=(r,z)$ and $x'=(r',z')$ becomes in this approximation

$$G_p^{(0)}(z,z')=\{\exp(-|p||z-z'|)+\exp[-|p|(z+z')]\}/(2|p|) \quad , \tag{2}$$

$G_p^{(0)}$ satisfies the Neumann boundary condition

$$\lim_{z'>0,\, z\to 0}\partial_z G_p^{(0)}(z,z')=0 \quad .$$

To include the effects of the ϕ^4 interaction, we use perturbation theory. The ultraviolet (uv) singularities can be regularized with the help of a momentum cutoff Λ. (One can work in a pz representation and cut off parallel momenta only.) However, for calculational purposes, dimensional regularization is preferable.

In the conventional translationally invariant ϕ^4 theory the uv divergences can be absorbed by a few counterterms related to order-parameter, temperature, and coupling-constant renormalization.[1,2] These divergences originate from the singular behavior of the bulk propagator $G_b^{(0)}(x)\sim|x|^{-2+\epsilon}$ at short distances. If translational invariance is broken by a surface, the propagator $G^{(0)}(x,x')$ differs from $G_b^{(0)}$ by an image term which in our case is equal to the bulk propagator $G_b^{(0)}(x-\tilde{x}')$ between x and the mirror image $\tilde{x}'=(r',-z')$ of x'. This term becomes singular when $x\to\tilde{x}'$ and gives rise to new divergences.[3,16] As discussed in detail in Ref. 16 one can therefore absorb these divergences by local surface counterterms.

One-particle irreducible (1PI) parts can be defined in terms of Feynman graphs. However, their renormalization does *not* render the correlation functions finite.[3,16] This is a *general new feature* of systems in which translational invariance is broken by surfaces and related to the fact that points in the surface are *exceptional* in a similar sense as $x-x'=0$ is for $G(x,x')$ in the translationally invariant theory. In both cases the counterterms that cure the divergences at nonexceptional points are insufficient, and additional counterterms with support at the exceptional points are needed. This means, in particular, that the order parameter $\phi(r,0^+):=\phi_1(r)$ on the surface must be treated as a separate operator whose anomalous dimension does *not* follow from bulk exponents.

We add bulk and surface magnetic field terms to F and define connected correlation functions by

$$G^{(N,L)}(\{x_i\};\{r_j\})=\left\langle\prod_{i=1}^N\prod_{j=1}^L\phi(x_i)\phi_1(r_j)\right\rangle_{\rm conn} \quad ,$$

where the average $\langle\cdots\rangle$ is meant with respect to the Boltzmann factor

$$\exp\left[-F+h^0\int d^dx\,\phi+h_1^0\int d^{d-1}r\,\phi_1\right] \quad .$$

Next we introduce renormalization functions Z_κ ($\kappa=\phi,t,u,1,c$) as follows:

$$\begin{aligned}&\phi=Z_\phi^{1/2}\phi^R,\quad \tau=\mu^2Z_tt+\Delta_t \quad , \quad g=\mu^\epsilon 2^d\pi^{d/2}Z_uu \quad ,\\ &\phi_1=(Z_\phi Z_1)^{1/2}\phi_1^R \quad , \quad c^0=\mu Z_cc+\Delta_c \quad .\end{aligned} \tag{3}$$

Here μ is an arbitrary momentum scale. Z_ϕ, Z_t, and Z_u are the usual bulk Z factors and can be found in I. The new features mentioned above are described by the other functions. $\Delta_t\sim\Lambda^2$ and $\Delta_c\sim\Lambda$ specify the shift of the Gaussian special point and are needed to absorb quadratic and linear divergences, respectively. They vanish in (minimal) dimensional renormalization. As noted by Symanzik, $\langle\phi_1\phi_1\rangle_{\rm 1PI}$ requires an additional counterterm $\sim\delta(z)\phi(r,0^+)\partial_z\phi$. However, this counterterm is annihilated in correlation functions due to the Neumann condition, provided the derivative is taken at $z=0$ and the arguments of the ϕ_1 fields approach the surface afterwards. (The renormalization of $\langle\phi^2\rangle$, $\langle\phi_1^2\rangle$, $\langle\phi^2\phi^2\rangle$, etc., would also require further counterterms, but will not be considered here.) Z_1 and Z_c can be calculated by minimally subtracting the poles of $G^{(1,1)}$ and $\langle\phi\phi\phi_1^2\rangle_{\rm conn}$. Our results[18] are

$$\begin{aligned}Z_1&=1+\frac{n+2}{3\epsilon}u+\left[\frac{(n+2)(n+5)}{9}-\frac{n+2}{3}\epsilon\right]\epsilon^{-2}u^2+O(u^3) \quad ,\\ Z_c&=1+\frac{n+2}{3\epsilon}u+\left[\frac{(n+2)(n+5)}{9}+\frac{n+2}{36}\epsilon(1-4\pi^2)\right]\epsilon^{-2}u^2+O(u^3) \quad .\end{aligned} \tag{4}$$

The renormalized functions

$$G_R^{(N,L)}=Z_\phi^{-N/2}(Z_\phi Z_1)^{-L/2}G^{(N,L)}$$

satisfy the RG equations

$$\{\mu\partial_\mu+\beta_u\partial_u-(2+\eta_t)t\partial_t-(1+\eta_c)c\partial_c+[\eta_\phi(N+h\partial_h)+(\eta_\phi+\eta_1)(L+h_1\partial_{h_1})]/2\}G_R^{(N,L)}=0, \quad (5)$$

with $h=Z_\phi^{1/2}h^0$, $h_1=(Z_\phi Z_1)^{1/2}h_1^0$, and the Wilson functions $\beta_u=\mu\partial_\mu|_0 u$, $\eta_\kappa=\mu\partial_\mu|_0\ln Z_\kappa$ $(\kappa=\phi,1,t,c)$, where $\partial_\mu|_0$ denotes a derivative at fixed bare parameters. β_u, η_ϕ, and η_t are the same as in I. η_1 and η_c follow from Eq. (4). At the infrared stable fixed point u^*, η_1 becomes to $O(\epsilon^2)$

$$\eta_1^*=-(n+2)(n+8)^{-1}\epsilon-3(n^2-4)(n+8)^{-3}\epsilon^2 \ . \quad (6)$$

Using Eq. (5) one can study the scaling properties of $G_R^{(N,L)}$ as usual. Setting $u=u^*$ we find, for example, that $G_R^{(0,2)}$ can be written in the form

$$G_R^{(0,2)}(r,r';u^*,t,c,h_1,h,\mu)=\mu^{d-2}(\mu\rho)^{-(d-2+\eta_\parallel)}f(\mu\rho t^\nu,ct^{-\phi_s},\mu^{-d/2}h_1t^{-\Delta_1},\mu^{-(d+2)/2}ht^{-\Delta}) \ ,$$

where $\rho=|r-r'|$, $\eta_\parallel=\eta+\eta_1^*$ with $\eta=\eta_\phi(u^*)$, $\nu=[2+\eta_t(u^*)]^{-1}$, $\phi_s=\nu[1+\eta_c(u^*)]$, $\Delta_1=\nu(d-\eta_\parallel)/2$, and $\Delta=\nu(d+2-\eta)/2$. The exponents introduced here are bulk (η,ν,Δ) and surface exponents $(\eta_\parallel,\Delta_1)$ in the commonly used notation.[19] Our result for $\eta_\parallel$ which follows from Eq. (6) is consistent with the one given in Ref. 13. The result for Δ_1 establishes a well-known scaling law.[19] The scaling laws $\eta_\perp=(\eta+\eta_\parallel)/2$, $\gamma_{11}=\nu(1-\eta_\parallel)$, $\gamma_1=\nu(2-\eta_\perp)$, $\beta_1=\nu(d-2+\eta_\parallel)/2$ for the correlation function exponent $\eta_\perp$,[20] the susceptibility exponents γ_{11}, γ_1, and the exponent β_1 for the magnetization in the surface follow similarly.

Our result for the crossover exponent ϕ_s is

$$\phi_s=\frac{1}{2}-\frac{n+2}{4(n+8)}\epsilon+\frac{n+2}{8(n+8)^3}\times[8\pi^2(n+8)-(n^2+35n+156)]\epsilon^2+O(\epsilon^3) \ ,$$

which differs from $1-\nu$ at order ϵ^2. As a result of the asymptotic nature of the ϵ expansion the numerical value $\phi_s=0.68$ for $n=1$ obtained by setting $\epsilon=1$ cannot be trusted. It is, however, closer to the position-space results ≈ 0.55 of Ref. 9 and 0.67 of Ref. 10 than $1-\nu\approx 0.36$.

By a similar analysis one can study the corrections to scaling near the ordinary fixed point that result when c differs from the corresponding fixed-point value ∞.[21]

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