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Critical Behavior of a Semi-infinite System: n-Vector Model in the Large-n Limit

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The n-component Ginzburg-Landau-Wilson model for a semi-infinite system is solved exactly at $T=T_c$ in the limit $n\to\infty$. In the scaling regime the spin-spin correlation function is $G(\vec{\rho},z,z',T_c)=\mathrm{const}\{[\rho^2+(z-z')^2]^{-1}-[\rho^2+(z+z')^2]^{-1}\}^{(d-2)/2}$, for dimensionalities d in the range $2<d<4$, where z,z' are the distances of the two spins from the surface and $\vec{\rho}$ is their separation parallel to the surface. The critical exponents $\eta_\perp$ and $\eta_\parallel$ are $(d-2)/2$ and $(d-2)$, respectively.

The techniques of expansion in powers of $\epsilon=4-d$ and in powers of $1/n$ have proved useful tools for the study of critical phenomena in bulk systems.[1,2] In recent years increased attention has been devoted to the effects of surfaces on critical phenomena.[3-6] Order-parameter correlations near a surface have been studied within the ϵ expansion by Lubensky and Rubin[6] (LR hereafter) who calculated to order ϵ, for all n, the exponents $\eta_\perp$ and $\eta_\parallel$ introduced by Binder and Hohenberg.[3] In this Letter we present the first results for the limit $n\to\infty$, valid for all dimensionalities in the range $2<d<4$. In the region where the two calculations overlap, our results for $\eta_\perp$ and $\eta_\parallel$ agree with those of LR, and the form of the two-point correlation function is identical to that conjectured by LR on the basis of their $O(\epsilon)$ result. The reader should note that for the surface problem the large-n limit is *not* equivalent to the spherical model. The latter model has received some attention in the literature,[7] but to our knowledge the present Letter is the first investigation of the large-n limit for a surface problem.

We adopt the following continuum model Hamiltonian for a semi-infinite system

$$H_n=\int d^dx\,\{\tfrac{1}{2}[r+\Delta r+c\delta(z)]\sum_{i=1}^{n}\varphi_i^2+\tfrac{1}{2}\sum_{i=1}^{n}(\nabla\varphi_i)^2+(u/4n)(\sum_{i=1}^{n}\varphi_i^2)^2\},\qquad(1)$$

where $r\propto(T-T_c)/T_c$, with T_c the bulk transition temperature. The term Δr will be chosen to compensate for the shift in T_c introduced by the quartic term in Eq. (1). The surface is the plane $z=0$ and c^{-1} plays the role of an extrapolation length,[3,5,6] assumed nonnegative here. (For $c<0$ the surface may order at a higher temperature than the bulk.[3,5] We do not consider that possibility here.) We introduce the two-point correlation function $G(\vec{\rho},z,z',T)$ between points with z coordinates $z>0$, $z'>0$ and whose separation has projection $\vec{\rho}$ on a plane parallel to the surface:

$$G(\vec{\rho},z,z',T)\equiv\langle\varphi_i(\vec{\rho},z)\varphi_i(0,z')\rangle\equiv\int D\varphi\,\varphi_i(\vec{\rho},z)\varphi_i(0,z')e^{-H}/\int D\varphi\,e^{-H},$$

where $\int D\varphi$ represents a functional integration over all order-parameter configurations.

For $u=0=\Delta r$, the Fourier transform with respect to $\vec{\rho}$, $\hat{G}(\vec{k},z,z',T)$ is given by mean-field theory[3,5] and, in the limit $c\to\infty$ which corresponds to zero extrapolation length, it has at $T=T_c$ the particularly simple form

$$\hat{g}(\vec{k},z,z',T_c)=\frac{1}{2k}\{e^{-k|z-z'|}-e^{-k(z+z')}\}=\frac{1}{k}f(kz,kz'),\qquad(2)$$

where we have written $\hat{g}$ for the $u=0=\Delta r$ form of $\hat{G}$. In the limit $n\to\infty$, the quartic term in Eq. (1) may be "decoupled" in the usual way by writing $\varphi_i^2=\langle\varphi_i^2\rangle+(\varphi_i^2-\langle\varphi_i^2\rangle)$ and neglecting terms of second order in the curly brackets to give

$$(\sum\varphi_i^2)^2\to 2n\langle\varphi^2(z)\rangle\sum\varphi_i^2-(\sum\langle\varphi^2\rangle)^2 \tag{3}$$

and we have used the fact that $\langle\varphi^2\rangle=\langle\varphi_j^2\rangle$ is independent of j due to the "spin isotropy" of the model. Hence we obtain an effective Hamiltonian

$$H_\infty=\int d^dx\,\{\tfrac{1}{2}[r+c\delta(z)]\sum\varphi_i^2+\tfrac{1}{2}\sum(\nabla\varphi_i)^2+\tfrac{1}{2}V(z)\sum\varphi_i^2\}+\text{const}, \tag{4}$$

where

$$V(z)=u[\langle\varphi^2(z)\rangle-\langle\varphi^2(\infty)\rangle] \tag{5}$$

and we have chosen $\Delta r=-u\langle\varphi^2(\infty)\rangle$ to ensure that the bulk transition occurs at $r=0$. It is the z dependence of the potential $V(z)$ which renders this problem nontrivial.

From Eq. (4) one sees that the function $\hat{G}(\vec{k},z,z',T)$ satisfies the integral equation

$$\hat{G}(\vec{k},z,z,'T)=\hat{g}(\vec{k},z,z',T)-\int_0^\infty dx\,V(x)\hat{g}(\vec{k},z,x,T)\hat{G}(\vec{k},x,z',T), \tag{6}$$

and, from Eq. (5), that $V(x)$ can be expressed as

$$V(x)=u\sum_{p<\Lambda}[\hat{G}(\vec{p},x,x,T)-\hat{G}(\vec{p},\infty,\infty,T)], \tag{7}$$

where Λ is a large-momentum cutoff. Since the cutoff has been taken as infinite for wave vectors q perpendicular to the surface, the Brillouin zone employed is an infinitely long right circular cylinder of radius Λ. The integral equation may be converted to a differential equation by taking two derivatives with respect to z and noting that

$$d^2\hat{g}(\vec{k},z,z',T_c)/dz^2=k^2\hat{g}(\vec{k},z,z',T_c)-\delta(z-z'). \tag{8}$$

Thus one obtains, for $T=T_c$,

$$[d^2/dz^2-k^2-V(z)]\hat{G}(\vec{k},z,z',T_c)=-\delta(z-z'). \tag{9}$$

By analogy with Eq. (2), we seek a solution having the scaling form

$$\hat{G}(\vec{k},z,z',T_c)=k^{-1}F(kz,kz'). \tag{10}$$

(We have specialized here to the case of zero extrapolation length. One expects that critical exponents, etc., will be independent of the value of c for $c>0$.) Dimensional analysis of Eq. (9) shows that such a solution is only possible if $V(z)\propto z^{-2}$. Therefore, we write

$$V(z)=(\nu^2-\tfrac{1}{4})/z^2, \tag{11}$$

with ν as yet undetermined, but turning out to lie in the range $-\frac{1}{2}<\nu<\frac{1}{2}$. Equation (9) may then be solved in terms of modified Bessel functions:

$$\hat{G}(\vec{k},z,z',T_c)=(zz')^{1/2}I_\nu(kz)K_\nu(kz'),\quad z<z', \tag{12a}$$

$$=(zz')^{1/2}K_\nu(kz)I_\nu(kz'),\quad z>z'. \tag{12b}$$

In principle, a term like $(zz')^{1/2}I_\nu(kz)I_\nu(kz')$ could be added to both Eqs. (12a) and (12b). It is excluded by the boundary condition that the bulk correlation function $\hat{G}(\vec{k},\infty,\infty,T_c)=1/2k$ is recovered as $z,z'\to\infty$. It might also be thought that a term like $(zz')^{1/2}K_\nu(kz)K_\nu(kz')$ could be added to both equations since it satisfies the boundary condition at infinity and the surface boundary condition appropriate to the infinite-c limit, $\hat{G}(\vec{k},z,z',T)=0$ for z or z' zero, provided $|\nu|<\frac{1}{2}$. [Note that $K_\nu(x)\sim x^{-|\nu|}$ as $x\to 0$.] Addition of such a term is precluded, however, by a rather subtle point, which is most easily made by examining the eigenfunctions $\psi(\vec{k},\vec{\rho},q,z)$ of the linear operator in Eq. (9). These satisfy the equation

$$[\nabla^2+k^2+q^2-(\nu^2-\tfrac{1}{4})/z^2]\psi=0.$$

The eigenfunctions corresponding to the eigenvalue (k^2+q^2) are $(\pi qz)^{1/2}\exp(i\vec{k}\cdot\vec{\rho})J_{\nu}(qz)$ and $(\pi qz)^{1/2}\times\exp(i\vec{k}\cdot\vec{\rho})J_{-\nu}(qz)$. Notice that *any* linear combination of these eigenfunctions satisfies the boundary condition appropriate to infinite c, viz. $\psi(\vec{k},\vec{\rho},q,0)=0$ provided $|\nu|<\frac{1}{2}$. This somewhat unusual situation seems to leave the problem indeterminate. The difficulty, however, can be resolved by noting that linear combinations with different q values are not orthogonal, so that *mixtures* of the eigenfunctions form an over-complete set of states. The only satisfactory orthonormal functions are the given pure eigenfunctions. This situation occurs generally for potentials as singular or more singular than z^{-2}.[8] The expression for $\hat{G}(\vec{k},z,z',T_c)$ in Eq. (12) then results from the use of the standard relation between the Green's function and the eigenfunctions,

$$\hat{G}(\vec{k},z,z',T_c)=\int_{-\infty}^{\infty}\frac{dq}{2\pi}\frac{1}{k^2+q^2}\psi(\vec{k},\vec{\rho},q,z)\psi^*(\vec{k},\vec{\rho},q,z'),$$

when the eigenfunction associated with the Bessel function of index ν is substituted for ψ. Only improper linear combinations of eigenfunctions give rise to terms in $\hat{G}$ like $(zz')^{1/2}K_\nu(kz)K_\nu(kz')$, so that we can conclude that such terms are absent.

It is convenient to rewrite the expression for the potential $V(z)$ in Eq. (7) as the sum of two terms $V_1(z)$ and $V_2(z)$. $V_1(z)$ is the potential which would be found if the cutoff Λ were infinite:

$$V_1(z)=uK_{d-1}\int_0^\infty dk\,k^{d-2}[zI_\nu(kz)K_\nu(kz)-\tfrac{1}{2}k^{-1}]=\frac{uK_{d-1}}{z^{d-2}}\int_0^\infty dt\,t^{d-3}[tI_\nu(t)K_\nu(t)-\tfrac{1}{2}]. \quad (13)$$

$K_{d-1}=2/\{(4\pi)^{(d-1)/2}\Gamma[\frac{1}{2}(d-1)]\}$ and $\epsilon=4-d$ as usual.

In order that $V(z)\propto z^{-2}$ it is necessary that the coefficient of $1/z^{d-2}$ in Eq. (13) be zero, which means that the integral must vanish. This condition determines ν as[9]

$$\nu=(d-3)/2,\quad 2<d<4. \quad (14)$$

Since ν has been chosen to make $V_1(z)$ zero, $V(z)=V_2(z)$; $V_2(z)$ is just the potential resulting from the finiteness of the cutoff:

$$V_2(z)=-uK_{d-1}\int_\Lambda^\infty dk\,k^{d-2}[zI_\nu(kz)K_\nu(kz)-\tfrac{1}{2}k^{-1}]=\frac{uK_{d-1}}{z^{d-2}}\int_{\Lambda z}^\infty dt\,t^{d-3}\left\{\frac{4\nu^2-1}{16t^2}+O(t^{-4})\right\}=\frac{uK_{d-1}}{4\epsilon\Lambda^\epsilon}\frac{\nu^2-\frac{1}{4}}{z^2}+O(u/\Lambda^{2+\epsilon}z^4). \quad (15)$$

The asymptotic expansion of $I_\nu(t)K_\nu(t)$ for large argument[10] has been used in Eq. (15). The terms of $O(u/\Lambda^{2+\epsilon}z^4)$ in Eq. (15) will be neglected for the moment. Comparison of Eqs. (11) and (15) shows that for consistency one has to choose a special value of the coupling constant

$$u=u_w=4\epsilon\Lambda^\epsilon/K_{d-1}. \quad (16)$$

This value removes "slow transients" of relative order $(k/\Lambda)^\epsilon$ and its choice is analogous to the special choice of the coupling constant in Wilson's ϵ-expansion technique for bulk systems.[1] It can be shown to coincide with the large-n limit of Wilson's result if allowance is made for the cylindrical Brillouin zone used in this paper.

Fourier transformation of Eq. (12), with ν given by Eq. (14), yields the correlation function in real space[11]:

$$G(\vec{\rho},z,z',T_c)=\tfrac{1}{2}\Gamma(d-2)K_{d-1}\left\{\frac{4zz'}{[\rho^2+(z-z')^2][\rho^2+(z+z')^2]}\right\}^{(d-2)/2}=\tfrac{1}{2}\Gamma(d-2)K_{d-1}\left\{\frac{1}{\rho^2+(z-z')^2}-\frac{1}{\rho^2+(z+z')^2}\right\}^{(d-2)/2}. \quad (17)$$

Three limiting cases are of special interest: (i) For $z,z'\to\infty$, with ρ, $z-z'$ fixed, $G^{-1}\propto[\rho^2+(z-z')^2]^{(d-2)/2}$, the usual bulk result with bulk exponent $\eta=0$; (ii) for $z'\to\infty$, with ρ, z fixed, $G^{-1}\propto z'^{3(d-2)/2}\equiv z'^{d-2+\eta_\perp}$ giving $\eta_\perp=\frac{1}{2}(d-2)$; (iii) for $\rho\to\infty$, with z, z' fixed, $G^{-1}\propto\rho^{2(d-2)}\equiv\rho^{d-2+\eta_\parallel}$ giving $\eta_\parallel=d-2$. The results for $\eta_\perp$ and $\eta_\parallel$ agree with the $\eta=\infty$ limit of those of LR,[6] and the structure of the correlation function is identical to the $\eta=\infty$ limit of that conjectured by LR on the basis of their $O(\epsilon)$ result.

We conclude by discussing some of the limitations of the present calculation. Firstly, terms of relative order $(k/\Lambda)^\epsilon$ (corrections to scaling) were eliminated by our special choice of coupling constant. We have been unable to determine them explicitly. Secondly, terms of order $1/\Lambda^2z^4$ (taking $u\sim\Lambda^\epsilon$) and higher were dropped from the potential $V_2(z)$ in Eq. (15). The influence of these higher-order terms is presumably negligible in the scaling regime $\rho\Lambda$, $z\Lambda$, $z'\Lambda\gg1$, $k/\Lambda\ll1$, but again we have been unable to verify this directly. The following argument suggests, however, that such terms are probably of no importance in the scaling regime. Suppose that the surface potential were not just $c\delta(z)$ with $c\to\infty$, but included a contribution $v(z)$, so chosen as to cancel the higher terms which arise in Eq. (15), i.e., $v(z) = (\nu^2 - \frac{1}{4})/z^2 - V_2(z)$ when $u = u_w$. A simple form for $v(z)$ cannot be given, but when $\Lambda z \gg 1$ it will obviously fall off as $1/\Lambda^2 z^4$, and in fact is repulsive in this regime. Our expression for $\hat{G}(\vec{k}, z, z', T_c)$, Eq. (12) is exact in the presence of this modified surface potential. The question which must now be considered is whether the modified potential $v(z)$ and the original potential $c\delta(z)$ with $c \to \infty$ belong to the same universality class. The chief danger is that a surface potential falling off as only z^{-4} might constitute a long-range interaction which could modify critical exponents, etc. If both potentials give rise to the same critical exponents in mean-field approximation then it is probably safe to assume that both potentials belong to the same universality class outside mean-field theory. While it is not possible to derive closed-form expressions for $\hat{g}(\vec{k}, z, z', T_c)$ for a general (repulsive) potential of the form $1/\Lambda^{-p} z^{2-p}$ with p arbitrary, it is possible to find the critical value of p for which mean-field exponents associated with short-range potentials like δ functions first occurs. For example, it is readily shown that[12]

$$\hat{g}(\vec{0}, z, z, T_c) \sim \begin{cases} z & p < 0 \\ z(\Lambda z)^{-p/2}, & p > 0 \end{cases}, \quad \Lambda z \to \infty.$$

Linear z dependence of $\hat{g}$ at $\vec{k} = 0$ is found for the $c\delta(z)$ potential as can be verified from Eq. (2). We have investigated other special cases of the correlation function $\hat{g}$. The borderline between short-range exponents and long-range exponents was at $p = 0$ in every case. We therefore conclude that surface potentials falling off faster than z^{-2} belong to the same universality class as a short-range potential such as a δ function and hence that the neglected terms in Eq. (15) are of no significance for behavior in the scaling regime. Thirdly, we have not discussed the changes which might arise if c were finite rather than infinite. In most applications to spin systems c will be of order Λ. It is worth noting that for $k/c \ll 1$ the infinite-c expression for $\hat{g}$, Eq. (2), is recovered. It thus seems likely that once again in the scaling regime (where $k/\Lambda \ll 1$) the detailed form of the surface interaction is irrelevant, except in the interesting situation where the surface potential is sufficiently attractive to split off a surface phase. Exact results for finite c cannot be obtained using the present techniques, because the existence of an extra length scale renders the scaling *Ansatz* Eq. (10) inappropriate. Similar difficulties arise in the case $T \neq T_c$, where the finite correlation length introduces an extra length scale. At present these difficulties seem insurmountable.

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[10]Reference 9, p. 962, Nos. 5 and 6.

[11]The angular integral is straightforward, the radial integral may be found in Ref. 9, p. 697, No. 16.

[12]The calculation is trivial if use is made of Ref. 9, p. 972, No. 10.