Modified Extrapolation Length Renormalization Group Equation

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A modified renormalization group equation for the inverse extrapolation length \( c \) is derived by considering the phase shifts of order parameter fluctuations. The resulting non-linear equation is also derived using standard methods and some additional assumptions. The associated renormalized flow \( c(l) \) exhibits the correct behavior near both the special and ordinary fixed points and in particular yields a canonical scaling of \( c \) with cross-over exponent \( \phi_{\text{ot}} = -\nu \) near the ordinary transition.

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I. INTRODUCTION

Since the first renormalization group (RG) analysis of surface critical behavior by Lubensky and Rubin [1] a number of subsequent advances [2–5] in the technique have enabled computation of exponents to \( O(\epsilon^2) \), critical amplitudes, and various cross-over functions [6–9]. In particular, Diehl and Dietrich have systematically developed a formalism whereby the power and elegance of the field theoretic method has been fully exploited.

For the case of an \( O(1) \) system confined to the half-space \( z > 0 \) it suffices to consider the reduced Hamiltonian

\[
H[\phi] = \int d^4x \left[ \frac{1}{2} (\nabla \phi)^2 + \frac{r}{2} \phi^2 + \frac{u}{4!} \phi^4 \right] + \int dS \frac{c}{2} \phi^2
\]

(1.1)

the presence of the bounding surface manifesting itself as an additional surface interaction \[\frac{c}{2}\phi^2\]. The parameter \( c \) takes account of the local enhancement of the reduced temperature in the vicinity of the surface. At lowest order the surface term results in the boundary condition \( \phi'(0) = c\phi(0) \) and thus \( 1/c \) corresponds to the distance over which the order parameter falls to zero when extrapolated away from the surface. For \( c > 0 \) the surface orders with the bulk while for \( c < 0 \) there is an enhanced tendency to order at the surface. The “special” transition with \( c = 0 \) divides these two regimes whereas the “ordinary” transition with \( c = \infty \) corresponds to a state where ordering at the surface is completely suppressed.

An issue of considerable interest is the manner in which various quantities behave close to the ordinary transition and to this end an expansion in the \emph{bare} extrapolation length \( 1/c \) has been developed [1,3]. Among the results is the finding that at the ordinary point energy related quantities involving \( \phi^2 \) averages exhibit behavior characterized by relations involving \emph{bulk} exponents [13]. This in turn is a direct consequence of a vanishing anomalous exponent \( \eta_c \) associated with the extrapolation length.

The canonical scaling of \( c(l) \) near the ordinary point is interesting in light of the fact that all analyses addressing the cross-over behavior from the special to ordinary point [1,3] have utilized a \emph{linear} RG equation which in dimensional regularization reads

\[
\frac{dc}{dl} = (1 + \eta_c)c
\]

(1.2)

with \( \epsilon^l \) corresponding to the block spin size. For finite \( c(l) \) Eq. (1.2) results from a straightforward application of the field theoretic method to a bulk system with a planar bounding surface [3]. Clearly equation (1.2) yields a flow which is independent of the proximity to the special transition and thus does not display the expected classical behavior at large \( c(l) \). It is readily verified, however, that this disparity in scaling behavior from that inferred from the \( 1/c \) expansion is compensated for by the crossover functions exhibiting logarithmic singularities at large \( c(l) \). When exponentiated, these singularities lead to powers of \( c(l) \) that in effect undo the incorrect large \( c \) behavior of Eq. (1.2) and in turn lead to the appropriate exponents at the ordinary point.

With the above in mind a question of immediate interest is to what extent it is possible to deduce a flow for \( c(l) \) that correctly interpolates between the special and ordinary points. Constructing such a flow is not immediately obvious since for finite \( c \) the linear RG Eq. (1.2) results from the standard program of renormalizing all relevant surface operators. It has been pointed out [11], however, that near the ordinary point additional care must be used in categorizing operators as relevant or irrelevant in the RG sense. In particular, in the context of the \( 1/c \) expansion it happens that insertions of the formally irrelevant \( \partial_\nu \phi \) must be considered [11].

In the following we outline an approach based on the physical notion of an extrapolation length that gives rise to a non-linear RG equation exhibiting the correct behavior both at the special and ordinary fixed points. As in the case of the \( 1/c \) expansion the operator \( (\partial_\nu \phi)^2 \) is found to play a important role in the analysis. In addition to yielding an RG flow with the sought-after behavior at both fixed points, the method further elucidates the connection between the extrapolation length and parameter \( c \). This insight is of interest in its own right since conventional wisdom holds that the connection loses meaning beyond mean-field theory [1]. Making use of an analysis based on phase shifts, we will demonstrate that there is a
means of extending the notion of an extrapolation length that remains intact when fluctuations are taken into account. This approach may have the potential for further development since the use of phase shifts in many-body systems is a concept often incorporated into perturbative analyses of arbitrary order \[12\].

II. SCATTERING FORMULATION

Our analysis begins with the reduced Hamiltonian of Eq. (1.1) with the understanding that all volume integrations are to be taken over the half-space \( z > 0 \). Within mean field theory, straightforward variation of the Hamiltonian (1.1) gives rise to the boundary condition

\[ c\phi(0) = \phi'(0) \]  

(2.1)

Beyond mean field theory there is an approach in which the connection between \( c \) and an extrapolation length is still apparent. The key observation is that the oscillatory nature of the modes leads to the extrapolation length manifesting itself as a phase shift. In particular, taking the free Hamiltonian \( H_0 \) to be

\[ H_0 = \int d^dx \frac{1}{2} [\nabla\phi]^2 + r\phi^2 + \int dS \frac{\phi^2}{2} \]  

(2.2)

the modes which diagonalize \( H_0 \) satisfy the boundary condition Eq. (2.1) and are of the form

\[ \phi_k = e^{-ikz} - f_k e^{ikz} \]  

(2.3)

where the scattering amplitude \( f_k \) and phase shifts are given by

\[ f_k = \frac{c + i k}{c - ik} = e^{2i\delta_k}, \quad \tan \delta_k = k/c \]  

(2.4)

At this level of approximation it is apparent that the presence of the surface interaction serves as an effective scattering potential characterized by phase shifts \( \delta_k \). Conversely, given phase shifts \( \delta_k \) the associated inverse extrapolation length satisfies

\[ \lim_{k \to 0} \frac{\delta_k}{k} = \frac{1}{c} \]  

(2.5)

The inclusion of fluctuations will alter the effective surface potential. To ascertain how fluctuations influence the extrapolation length one can appeal to the manner in which the phase shifts are modified and then use Eq. (2.6).

We now carry out this program by addressing the lowest order, one-loop corrections. For a given self energy \( \Sigma \) the modes satisfy

\[ -\frac{d^2\phi}{dz^2} + (t + q^2 - E_k)\phi = -\sigma(z)\phi \]  

(2.6)

where \( \sigma(z) = \Sigma(z) - \Sigma(\infty) \), and \( t = r + \Sigma(\infty) \) is the suitably shifted bulk reduced temperature. Since we will ultimately be implementing the RG, let us assume that \( \sigma \sim \epsilon \) which then permits Eq. (2.6) to be solved using standard perturbation theory. In the present circumstance in which results appropriate to one-loop order are sought, first order perturbation theory suffices. We are led to a modified scattering amplitude

\[ f_r = f - \frac{1}{2ik} \int dz [\phi_k^0(z)]^2 \sigma(z) \]  

(2.7)

The corresponding fluctuation corrected \( c_r \) is obtained by considering the small \( k \) limit of Eq. (2.6). Noting that \( f \approx 1 + 2ik/c \) it follows that

\[ \frac{1}{c_r} = \frac{1}{c} - \int dz (z + 1/c)^2 \sigma(z) \]  

(2.8)

which is valid to \( O(\epsilon) \). In the event that higher order corrections are desired it is necessary to take account of additional perturbative corrections to Eq. (2.6).

III. RENORMALIZATION GROUP

The above results can now be used to determine the renormalization group equation for \( c(l) \). We proceed with a momentum-shell approach. To this end, we note that translational invariance in directions parallel to the surface allows one to write

\[ \phi(x) = \sum_q \phi_q(z)e^{iqy} \]  

(3.1)

Integrating out all modes with parallel momentum in the shell \( e^{-\Delta l} < q < 1 \) and using the result that the averages obey

\[ \langle \phi_q(z)\phi_{-q}(z') \rangle = \frac{1}{2\kappa} \left[ e^{-\kappa|z-z'|} - a e^{-\kappa(z+z')} \right] \]  

(3.2)

with

\[ a = \frac{c - \kappa}{c + \kappa} \]  

(3.3)

and \( \kappa^2 = q^2 + t \), one finds for the subtracted self energy

\[ \sigma(z) = -\frac{uKd-1}{4\kappa_1} \Delta l a \rightarrow e^{-2\kappa_1z} \]  

(3.4)

where the 1-subscript refers to all quantities being evaluated at \( q = 1 \). Rescaling lengths so that \( c \rightarrow c e^{\Delta l/c} \), one arrives at the RG equation

\[ \frac{dc}{dl} = c - \frac{u^*K_{d-1}}{8} \left[ \frac{c - \kappa_1}{\kappa_1^2} + \frac{c^2}{2\kappa_1^3} \right] \left( \frac{c - \kappa_1}{c + \kappa_1} \right) \]  

(3.5)

where \( u \) has now been set to its fixed point value \( u^*K_{d-1} = 8\epsilon/3 \). For comparison we note that the corresponding equation resulting from a standard momentum shell approach \[14\] in which only the interactions \( \phi^2, \phi\partial_n\phi \) are considered reads...
\[ \frac{dc}{dl} = c - \frac{u^s K_{d-1}}{8} \left[ \frac{c - \kappa_1}{\kappa_1^2} \right] \]  

(3.6)

Equation (refeq:rc1) is the hard cut-off version of the dimensionally regularized result (1.2). This latter equation being linear in \( c \) implies a flow

\[ c(l) = e^{l \phi / \nu} \]  

(3.7)

that is independent of the proximity to special transition. Deviations between equations (3.6, 3.5) begin to appear when \( c(l) \sim 1 \). The third non-linear term appearing in Eq. (3.5) for finite \( c \) is ultraviolet convergent and corresponds to the inclusion of contributions from the formally irrelevant \((\partial_\mu \phi)^2\) vertex. However, if this last term is expanded in \( 1/c \), it is clear that corrections to the shift and exponent of \( c \) occur, and that successive terms become increasingly ultraviolet divergent.

Equation (3.5) leads to some interesting results, which we now address. For the sake of illustration assume that the system is close enough to criticality so that crossover to the ordinary point has already occurred while \( r(l) \ll 1 \). In this case Eq. (3.5) reduces to

\[ \frac{dc}{dl} = c - \frac{u^s K_{d-1}}{8} \left[ c - 1 + \frac{c^2 (c - 1)}{2} \right] \]  

(3.8)

Although it is possible to solve Eq. (3.8) exactly, only results accurate to \( O(\epsilon) \) will be considered. There are several ways to go about solving Eq. (3.8), one of which proceeds by iteratively solving the differential equation to \( O(\epsilon) \). This leads to the explicit solution

\[ c(l) = b(l) - \frac{u^s K_{d-1}}{8} \left[ 1 + \frac{b(l)^2}{2} - b(l) \ln(1 + b(l)) \right] \]  

(3.9)

\[ b(l) = b(0) e^{(1+\eta_c)l} \]

with \( b(0) = c(0) + u^s K_{d-1}/8 \), and \( \eta_c = -\epsilon/3 \). Another method approximates the roots to the resulting cubic on the right hand side of Eq. (3.8) and leads directly to the implicit form

\[ \left( \frac{c(l) - \eta_c}{c(0) - \eta_c} \right)^{1-\eta_c} \left[ \frac{1 + c(l) + \eta_c}{1 + c(0) + \eta_c} \right]^{\eta_c} \left( \frac{2/\eta_c + c(0)}{2/\eta_c + c(l)} \right) = e^l \]  

(3.10)

which can also be shown to follow from exponentiation of (3.10). Inspection of the above results reveals that for \( c(l) \ll 1 \) the flow is characterized by \( \eta_c \neq 0 \) while close to the ordinary point \( c(l) \sim \epsilon \) thus implying a vanishing \( \eta_c \). Stated differently, the cross-over exponent for the extrapolation length \( \lambda(l) = 1/c(l) \) at the ordinary point is \( \phi_{ord} = -\nu \). Another interesting feature of Eq. (3.10) is that it yields an ordinary fixed point of order \( c(\infty) \sim 1/\epsilon \).

Past analyses, employing the momentum-shell technique to surface related phenomena, have encountered various technical difficulties [14]. We, therefore, first consider how this method leads to the standard linear equation (1.2) before attempting an alternate derivation of the modified RG equation (3.5). As degrees of freedom are integrated out, additional interactions are generated. This is accommodated by taking the surface interaction to be of the form

\[ V(z) = \sum_m v_m \delta^{(m)}(z) \]  

(3.11)

with \( \delta^{(m)}(z) \) referring to a \( m^{th} \) derivative. For given \( V(z) \) the coefficients \( v_m \) are determined by

\[ v_m = -\frac{m!}{m} \int_0^\infty z^m V(z) dz \]  

(3.12)

Consider the one-loop contribution, which results in the surface interaction \( V(z) = \sigma(z) \) given by Eq. (3.4). After rescaling the surface spins by a factor \( e^\Delta r/(1-m)^2/2 \) one finds that the coefficients \( v_m \) satisfy the recursion relations:

\[ \frac{dv_m}{dl} = (1 - m - \eta_1) v_m - \frac{u^s K_{d-1}}{2} \frac{(-)^m a_1}{(2\kappa_1)^{m+2}} \]  

(3.13)

The vertex involving \( \phi^2 \delta(z) \), or equivalently \( \delta(z) \phi \partial_\mu \phi \) results from the boundary term associated with \( (\nabla \phi)^2 \). Analogous to what is done in bulk phenomena the factor \( \eta_1 \) is chosen so that \( \nu_1 = 1/2 \) remains fixed. This leads to the result

\[ \eta_1 = \frac{u^s K_{d-1}}{8\kappa_1} a_1 \]  

(3.14)

When this value for \( \eta_1 \) is inserted into Eq. (3.13) for \( v_0 \), one ends up with the linear RG equation (1.2). It is interesting that the non-linearity associated with the factor \( a_1 \) is entirely cancelled. Inspection of Eq. (3.13) governing \( v_m \) reveals that all interactions with \( m \geq 2 \) are irrelevant. However, in the context of calculating various scaling functions, these interactions with \( m \geq 2 \) must, in fact, be considered to account for all \( O(\epsilon) \) contributions [10].

It is possible under certain circumstances to interpret the contribution to \( c \) from \( \eta_1 \) as feeding in from the \( \nu_1 \) vertex. This becomes evident upon considering the contribution each surface term makes when inserted into a propagator with legs off the surface. Recall that the \( m^{th} \) vertex involves a factor \( \delta^{(m)}(z) \), which leads, after an integration by parts, to an interaction \( \delta(z) \partial_\mu^m \phi^2 \). The boundary condition then effectively relates this to a term proportional to \( \delta(z) \partial_\mu^m \phi^2 \) and leads to a contribution from \( v_m \) feeding into the recursion for \( c \). In such case it is possible that the higher order surface interactions will influence the behavior of \( c \).

To see how the above reasoning leads to the modified RG Eq. (3.3) assume that all two point interactions ultimately will modify a propagator with legs off the surface and that these legs each carry a transverse momentum \( q \) with associated factor \( \kappa_0 = \sqrt{q^2 + r(l)} \). The assumption
that the legs are off the surface effectively leads to the replacements:

\begin{align}
\partial_{\kappa_0 n}^{2m+1} \phi &\rightarrow \kappa_{0}^{2m} \phi \\
\partial_{\kappa_0 n}^{2m} \phi &\rightarrow \kappa_{0}^{2m} \phi
\end{align}

in all surface interactions. Note that the $\delta$ function singularity associated with two or more derivatives makes no contribution because of the fact that the legs are off the surface. When momenta in a thin shell are integrated out, each $v_m$ receives a contribution

$$
\Delta v_m = \frac{\Delta l}{2} a_{1} \left(\frac{-m c}{2\kappa_0}\right)^{m+2}
$$

For the moment, we will ignore any contribution from an anomalous surface spin rescaling factor $\eta_1$. Integrating by parts and invoking the correspondence (3.16), the $v_1$ interaction leads to a term $\Delta v_1 \delta(z) c \phi^2$. Similarly, the $v_2$ vertex involves $\partial^2 [\phi^2]$ and thus leads to a term $2\Delta v_2 \delta(z)(c^2 + \kappa_0^2) \phi^2$. It follows that the total effective contribution from the $v_1$, $v_2$ interactions to $v_0$ is

$$
\Delta v_0 = \Delta v_1 c + 2\Delta v_2 (c^2 + \kappa_0^2)
$$

Rescaling spins and lengths, using Eq. (3.17), and for the moment ignoring the last term involving $\kappa_0$, one arrives at the modified RG Eq. (3.18). Alternatively, identifying $\Delta v_m$ with the moments of $V(z)$ using Eq. (3.12), one recovers Eq. (2.8) derived from the scattering theory approach. Though $\eta_1$ was ignored, the final result is the same when anomalous spin rescaling is included. If spins are rescaled so that $v_1$ remains fixed, while there is no contribution to $v_0$ in the form of $\Delta v_1$, there is a contribution from $\eta_1$, which, because of Eq. (3.14), yields an identical result.

The above analysis arbitrarily neglected the contributions from the $v_2$ vertex in addition to all interactions with $m > 2$. To determine under what circumstances this is justified note that the vertex $v_m$ makes a contribution to $\Delta v_0$ of order

$$
\frac{\kappa_0^{m-2}}{\kappa_1^{m+2}} \left[ (c + \kappa_0)^2 + (-)^m (c - \kappa_0)^2 \right] a_1
$$

and becomes increasingly negligible for $\kappa_0 \ll \kappa_1 \sim 1$. This latter condition is satisfied close to the critical point when leg momenta $q \ll 1$. For the current situation of interest here this condition is well satisfied. However, in view of this assumption, our derivation strictly applies only to the RG Equation (3.8), in which $r(l)$ was neglected.

Generally, when $r(l)$ is not negligible it is possible to sum the higher order corrections that were neglected in the above analysis. However, the resulting equation differs from that found using phase shifts (3.3). The differences arise from the two methods reflecting different conventions on the finite part of $c(l)$. This is, of course, compensated for by making a correspondingly different subtraction, depending on which flow is used.

### IV. CONCLUDING REMARKS

We have presented a method for identifying an effective surface enhancement $c(l)$ which utilizes the scattering phase shifts of the localized part of the self energy $\sigma(z)$. The resulting cross-over behavior in $c(l)$ is found to arise from the inclusion of contributions of various higher order surface interactions, in particular $(\partial_n \phi)^2$. It is interesting that the relatively simple connection involving phase shifts implicitly includes such higher order corrections. Furthermore, the method appeals to characteristics of the entire (smooth) surface interaction rather than its constituent localized (delta function) pieces and thus may lead to further insights into surface phenomena. Indeed, though often convenient, the use of hyper-localized surface distributions is somewhat unphysical and occasionally leads to pathological quantities requiring special limiting procedures and interpretations.

The task of determining a scaling field with the correct scaling behavior at both fixed points is important in its own right. We have performed a preliminary analysis of the scaling functions for the surface susceptibility and surface free energy and find, as expected, that the use of a modified flow similar to Eq. (3.10) eliminates the logarithmic singularities otherwise found in these quantities (11). This in turn suggests that the logarithmic singularities in these two quantities are due entirely to the cross-over in $c(l)$.

Within his calculation of the local susceptibility Goldschmidt (7) also addressed the exponentiation of the logarithmic singularities appearing in this quantity. In this particular scaling function, however, the introduction of our modified flow is not sufficient to eliminate the singularity. We have also verified this is also the case for the layer susceptibility (10). This is to be expected, however, since both these quantities involve at least one external point on the surface.

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