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Finite-size scaling close to the critical point: renormalisation group and ε expansion

A M Nemirovsky and Karl F Freed

The James Franck Institute, The University of Chicago, Chicago, Illinois 60637, USA

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Abstract. We present an effective free-energy functional formalism which allows systematic ε-expansion methods to be used deep inside the critical region. Applications are provided to a d-dimensional layered geometry with periodic boundary conditions, and calculations are presented for the shift of the critical temperature and its associated exponent λ. The theory shows how the $(d-1)$-dimensional physics emerges with power law dependences on the interlayer separation.

1. Introduction

Considerable interest exists in explaining finite-size effects on phase transitions. (A good review of the subject is given by Barber (1983).) Away from the critical region the finite size produces corrections to bulk thermodynamic variables and correlation functions. These corrections can be described in terms of the scaling variable $y = Lt^{\nu}$, where $t = (T - T_c^{\infty})/T_c^{\infty}$ is the reduced temperature, T_c^{∞} is the bulk critical temperature, L is a characteristic length scale for the finite system and ν is the usual d-dimensional exponent. In addition, finite size produces a shift in the critical (or pseudocritical) temperature from T_c^{∞} to T_c^L. The exponent λ describes the power law L dependence of this shift by

$$T_c^{\infty} - T_c^L \sim L^{-\lambda} \qquad L \to \infty. \tag{1}$$

The ε-expansion method is one of the most powerful renormalisation group techniques for studying the critical behaviour of bulk (see e.g. Amit 1978) and semi-infinite systems (Diehl and Dietrich 1981, Symanzik, 1981, Nemirovsky and Freed 1985a). Recently, it has been extended to consider systems of finite size (Nemirovsky and Freed (1985b), hereafter referred to as paper I). Paper I considers the N-vector ϕ^4 field theory for a layered geometry, i.e. infinite in $d-1$ dimensions and of thickness L in the remaining dimension, satisfying periodic boundary conditions. The ε expansion is shown to be well defined as long as $Lt^{\nu} \gtrsim 1$. The correlation function, susceptibility and correlation length to $O(\varepsilon)$ are explicitly evaluated in paper I where the critical exponents are found to be those of the d-dimensional theory for a system of infinite extent. When $t \lesssim L^{-1/\nu}$ the perturbation expansion of paper I breaks down, becoming an expansion in a large dimensionless parameter proportional to $(Lt^{\nu})^{-1}$. Hence, the methods of paper I do not allow a penetration deeper inside the critical region.

This difficulty is understood in terms of the usual argument (see e.g. Barber 1983) that $t \simeq L^{-1/\nu}$ should mark the beginning of a dimensional crossover from a d-dimensional behaviour away from the critical temperature to a $d-1$ one (for a layered geometry) very close to T_c^L. This difficulty is also partially the reason for the conclusion of Brézin (1982) that ε-expansion methods cannot be applied to evaluate finite-size scaling functions, a conclusion which arises from applying methods appropriate for $Lt^\nu \gg 1$ to the case of $Lt^\nu \ll 1$ (i.e. $t=0$) where they are not valid. A similar problem, which we discuss below in more detail, exists with the ε-expansion calculation by Bray and Moore (1978) of λ in (1). The rectification of this fundamental difficulty requires the development of a new ε-expansion formalism which is specifically designed for the deep critical region of $Lt^\nu \leqslant 1$.

Although it is well known that the $L \to 0$ limit for a layered geometry should produce $(d-1)$-dimensional physics, the parameter L does not disappear from the problem. By small L ($L \to 0$) we mean the limits that $L/a \to \infty$ and $\zeta_\parallel/a \to \infty$, such that $L/\zeta_\parallel \to 0$, where a and $\zeta_\parallel$ are the lattice spacing and the correlation length perpendicular to the layer thickness, respectively. (For instance, in experiments on critical phenomena in thin films (Meadows *et al* 1979, Scheibner *et al* 1979) $L \geqslant 0.4\ \mu$m.) Even in this $L \to 0$ limit, critical amplitudes can depend on L in a power law fashion such as the shift in the critical temperature (equation (1)). Important problems, which have previously not been solved, involve showing how the powerful field-theoretical techniques, used to calculate exponents and scaling functions in infinite systems, can be employed to study (a) the d-dimensional region ($L > \zeta_\infty(t)$, $\zeta_\infty \to \infty$ where $\zeta_\infty(t)$ is the bulk correlation length), (b) the d'-dimensional region where $d' = d-1$ for a layered geometry ($\zeta_\infty > L$, $L \to \infty$) and (c) the dimensional crossover from d to d'. Paper I discusses the d-dimensional case (a) where finite-size effects produce small corrections to bulk quantities. This paper presents ε-expansion techniques that allow a penetration deep inside the critical region where the L-dependent $d-1$ physics emerges. We note that it was previously believed that ε-expansion methods were not suitable to study any of the finite-size problems (a), (b) or (c) (Brézin 1982, Barber 1983).

In this paper we use the same model of paper I, i.e. an N-vector ϕ^4 theory for a layered geometry with periodic boundary conditions, and consider the limit where the temperature approaches close to T_c^L. In this limit there are, in fact, two small parameters present in the theory, the renormalised coupling constant and the thickness L, or, more properly, the ratio $(L/\zeta_\parallel)$. The presence of two small parameters then forms the basis for a new ε-expansion method that is designed especially for this region.

The order parameter $\phi(x)$ is periodic along the dth direction (parallel to the thickness) and can be expanded in Fourier series. When L is small compared with coarse graining length scales, i.e. near T_c^L, only the lowest homogeneous mode ϕ_0 is relevant, while shorter wavelength modes ϕ_j ($j = 1, 2, \ldots$) provide some corrections. This conclusion is substantiated by the calculations. Because calculations close to T_c^L have L and g appearing in the combination gL^{-2}, the formal assignment of $L^2 \sim g$ provides a consistent ordering recipe for the expansion in both small parameters. Then, an effective free-energy functional F_{eff} can be systematically constructed as a series in powers of the coupling constant. We evaluate F_{eff} formally to $O(g)$ within this scheme, and show it to have the same structure as the Landau free-energy functional for a $(d-1)$-dimensional infinite-volume ϕ_0^4 field theory. This automatically implies that critical exponents near T_c^L are those of a $d-1$ system of infinite extent. However, F_{eff} has non-trivial dependences on L. In the process of determining and renormalising F_{eff}, the shift in the critical temperature is calculated to provide the 'shift' exponent λ to $O(\varepsilon'^2)$ where $\varepsilon' = 4-(d-1)$.

The calculation proceeds in two steps. First, we use ε-expansion techniques (valid only for $d \leqslant 4$) to construct an L-dependent effective $(d-1)$-dimensional free-energy functional. In lowest order it has the same form as the Landau free-energy functional for a $(d-1)$-dimensional ϕ_0^4 field theory in full space. Secondly, we study this $d-1$ field theory. Here, we utilise ε'-expansion methods with $\varepsilon' = 4-(d-1)$ though this is not required, and other approaches (such as real space renormalisation group, etc) could have been employed. The techniques we utilise here to construct the effective free-energy functional follow analogous ones developed in the context of finite-temperature field theories (Ginsparg 1980).

2. The model

Consider an N-component scalar ϕ^4 theory for a d-dimensional (valid only for $d \leqslant 4$) layered system of thickness L satisfying periodic boundary conditions along the dth direction, i.e. the local (renormalised) order parameter $\phi(\boldsymbol{\rho}, z)$ satisfies

$$\phi(\boldsymbol{\rho}, z) = \phi(\boldsymbol{\rho}, z+L) \tag{2}$$

where $\boldsymbol{\rho}$ is a $(d-1)$-dimensional vector perpendicular to the layer thickness. The Landau free-energy functional for the model is given by

$$F\{\phi\} = \int_0^L \mathrm{d}z \int \mathrm{d}^{d-1}\rho \left(\tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}t\phi^2 + \frac{(2\pi)^d}{S_d}\mu^{\varepsilon/2}\frac{g}{4!}(\phi^2)^2 + \textsc{ct} \right) \tag{3}$$

where t and g are the renormalised reduced temperature and coupling constant, respectively. The parameter μ has dimensions of temperature and is introduced to define a dimensionless coupling constant. The numerical factors $(2\pi)^d$ and $S_d = 2\pi^{d/2}/\Gamma(d/2)$ are placed before the quartic coefficient for later convenience. CT denotes the renormalisation counterterms which, as discussed in paper I, are the usual bulk ones.

The periodicity of $\phi(\boldsymbol{\rho}, z)$ in the interval $[0, L]$ permits it to be expanded in a Fourier series

$$\phi(\boldsymbol{\rho}, z) = L^{-1} \sum_{j=-\infty}^{\infty} \int \frac{\mathrm{d}^{d-1}k}{(2\pi)^{d-1}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\rho} + \mathrm{i}\kappa_j z)\phi_j(\boldsymbol{k}) \tag{4}$$

with $\boldsymbol{k}$ the Fourier variable conjugate to $\boldsymbol{\rho}$, and $\kappa_j = 2\pi j/L$. The partition function Z is given by

$$Z = \int D[\phi] \exp(-F\{\phi\}) \tag{5}$$

where $D[\phi]$ represents the sum over all configurations of the order parameter that satisfy the periodic boundary conditions of (2). Using equations (3) and (4) and rescaling the fields $\phi_j(\boldsymbol{k})$ by a factor $L^{-1/2}$ enables equation (5) to be written as

$$\begin{aligned} Z = \int D[\phi] \exp\Bigg\{ &\frac{1}{2}\int \frac{\mathrm{d}^{d-1}}{(2\pi)^{d-1}}(k^2+t)\phi_0(\boldsymbol{k})\phi_0(-\boldsymbol{k}) \\ &- \sum_{\substack{j=-\infty \\ j\neq 0}}^{\infty}{}' \frac{1}{2}\int \frac{\mathrm{d}^{d-1}k}{(2\pi)^{d-1}}\left[k^2 + t + \left(\frac{2\pi j}{L}\right)^2\right]\phi_j(\boldsymbol{k})\phi_j(-\boldsymbol{k}) \\ &- \frac{(2\pi)^d}{S_d}\mu^{\varepsilon/2}\frac{g}{4!}L^{-1}\sum_{j_1,j_2,j_3=-\infty}^{\infty}\int\frac{\mathrm{d}^{d-1}k_1}{(2\pi)^{d-1}}\int\frac{\mathrm{d}^{d-1}k_2}{(2\pi)^{d-1}}\int\frac{\mathrm{d}^{d-1}k_3}{(2\pi)^{d-1}} \\ &\times \phi_{j_1}(\boldsymbol{k}_1)\phi_{j_2}(\boldsymbol{k}_2)\phi_{j_3}(\boldsymbol{k}_3)\phi_{-j_1-j_2-j_3}(-\boldsymbol{k}_1-\boldsymbol{k}_2-\boldsymbol{k}_3)\Bigg\}. \end{aligned} \tag{6}$$

When rescaling fields, the measure $D[\phi]$ acquires a multiplicative factor which is irrelevant for most purposes; it cancels when evaluating correlation functions, susceptibilities, correlation lengths, etc, and is therefore dropped in equation (6). To aid in integrating over the $j \neq 0$ modes, it is convenient to use diagrammatic techniques. The theory of equation (6) is described in terms of two propagators, one for the $j = 0$ mode and the other for the sum of the $j \neq 0$ modes, along with four 4-point vertices with 4, 2, 1 and 0 $j = 0$ legs and 0, 2, 3 and 4 $j \neq 0$ ones, respectively. They are depicted in figures 1(a) and (b), and 2(a), (b), (c) and (d), respectively. The effective free-energy functional includes all diagrams with $j = 0$ external legs and $j \neq 0$ internal lines. Some examples are shown in figure 3.

A diagram with E external lines and V vertices has the formal order g^N associated with it (Ginsparg 1980) where

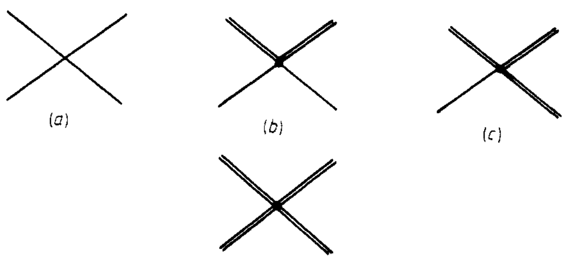
$$N = \tfrac{3}{4}(E-2) + \tfrac{1}{2}(V_c + 2V_d) \tag{7}$$

with $V = V_a + V_b + V_c + V_d$, where V_a, V_b, V_c and V_d are, respectively, the number of vertices of type (a), (b), (c) and (d) of figure 2. The formal ordering relation $L^2 \sim g$ is employed to derive (7). It is readily found that the diagram of figure 3(a) is 0th order in g, while figures 3(b) and (c) are first order, and the remaining diagrams are of higher order.

The lowest-order contribution to the effective free-energy functional comes from the diagram 3(a). It produces a shift in the coefficient of the term quadratic in the

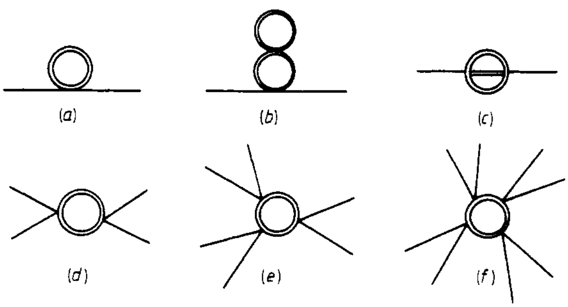
(a) (b)

Figure 1. Diagrammatic representation of the two propagators present in the theory of equation (6): (a) $j = 0$ mode, (b) sum of all the $j \neq 0$ modes.



(a) (b) (c) (d)

Figure 2. Diagrammatic representation of the four types of vertices present in the theory of equation (6).



(a) (b) (c) (d) (e) (f)

Figure 3. Some typical diagrams that arise in the construction of the effective free energy functional for the $j = 0$ mode.

field $\phi_0(\boldsymbol{k})$ from t to $(t+\Delta t)$ where Δt is calculated from diagram 3(a) to be

$$\Delta t = -g(2\pi)^d S_d^{-1}\mu^{\varepsilon/2}L^{-1}[(N+2)/3] \times \sum_{\substack{j=-\infty \\ j\neq 0}}^{\infty} \int \frac{\mathrm{d}^{d-1}q}{(2\pi)^{d-1}}\left[q^2+t+\left(\frac{2\pi j}{L}\right)^2\right]^{-1}. \tag{8}$$

The integration over $\boldsymbol{q}$ can be performed using standard rules (Amit 1978). After some algebra it is found that

$$\Delta t = -g[(N+2)/3](2\pi/L)^{2-\varepsilon}\mu^{\varepsilon/2}\Gamma(-\tfrac{1}{2}+\varepsilon/2)\pi^{-1/2}\sum_{j=1}^{\infty}[j^2+(t^{1/2}L/2\pi)^2]^{-\alpha} \tag{9}$$

with $\alpha = -\frac{1}{2}+\varepsilon/2$. Since $tL^2 \ll 1$, we use the expansion

$$\sum_{j=1}^{\infty}(j^2+a^2)^{-\alpha} = \zeta(2\alpha) - a^2\zeta(2\alpha+2) + \tfrac{1}{2}\alpha(\alpha-1)a^4\zeta(2\alpha+4) + \mathrm{O}(a^6) \tag{10}$$

where $\zeta(z)$ is Riemann's zeta function. Then equation (9) can be rewritten as

$$\Delta t = g(2\pi/L)^2[(N+2)/3][\tfrac{1}{12}+\tfrac{1}{4}(\ln 4\pi - \gamma - 2\ln \mu L)(tL^2/4\pi^2) + \mathrm{O}(tL^2)^2] \tag{11}$$

where γ is Euler's constant, properties of $\zeta(z)$ (Gradshteyn and Ryzhik 1965) have been used and the divergence associated with $\zeta(2\alpha+2)$ as $\alpha \to -\frac{1}{2}$ has been cancelled by the usual bulk counterterms. More generally, the analogy between this problem and ones in finite-temperature field theory (Nemirovsky and Freed 1985b) can be used in conjunction with results of Ginsparg (1980) for finite-temperature field theory to show that the renormalised effective free-energy functional is finite to all orders in the coupling constant g and that the renormalisation constants are the same as in the full space theory.

Inspecting equation (11) and using the formal ordering prescriptions $L^2 \sim g$ we find that (11) contains zeroth-, first-, second-, etc, order contributions to Δt. The lowest-order contributions to Δt arise solely from the diagram of figure 3(a). Diagrams 3(b) and (c) provide first-order contributions, so consistency dictates inclusion of these diagrams when keeping the second term in the square brackets of equation (11). Hence, the effective free-energy functional is given to lowest order by

$$\begin{aligned} F_{\mathrm{eff}}\{\phi_0\} = {} & \frac{1}{2}\int \frac{\mathrm{d}^{d-1}k}{(2\pi)^{d-1}}(k^2+t+\Delta t)\phi_0(\boldsymbol{k})\phi_0(-\boldsymbol{k}) \\ & + \frac{(2\pi)^d}{S_d}\mu^{\varepsilon/2}L^{-1}\frac{g}{4!}\int \frac{\mathrm{d}^{d-1}k_1}{(2\pi)^{d-1}}\int \frac{\mathrm{d}^{d-1}k_2}{(2\pi)^{d-1}} \\ & \times \int \frac{d^{d-1}k_3}{(2\pi)^{d-1}}\phi_0(\boldsymbol{k}_1)\phi_0(\boldsymbol{k}_2)\phi_0(\boldsymbol{k}_3)\phi_0(-\boldsymbol{k}_1-\boldsymbol{k}_2-\boldsymbol{k}_3) \end{aligned} \tag{12}$$

with

$$\Delta t = g(2\pi/L)^2[(N+2)/36]. \tag{12a}$$

3. Discussion

The F_{eff} of equation (12) has the same form as the Landau free-energy functional for an infinite-volume ϕ_0^4 field theory in $d-1$ dimensions, but it depends in a non-trivial manner on L. It then follows that critical exponents produced by F_{eff} are those of a $(d-1)$-dimensional system. The fixed point g^* in this case is (Amit 1978)

$$g^* = [6\varepsilon'/(N+8)] + O(\varepsilon'^2) \tag{13}$$

where $\varepsilon' = 4-(d-1)$, and the shift in the critical temperature, evaluated at the fixed point, is

$$t_c = -\Delta t = -\tfrac{1}{6}[(N+2)/(N+8)](2\pi/L)^2\varepsilon' + O(\varepsilon'^2). \tag{14}$$

This result agrees with that obtained in paper I, equation (16), up to the replacement of ε by ε'. Finally, we consider the 'shift' exponent λ. Equation (14) predicts $\lambda = 2$ formally to $O(\varepsilon')$. However, from the results of our calculations it is possible to evaluate λ formally to $O(\varepsilon'^2)$ as follows: only $\ln \mu L$ contributions to Δt can produce a modification in the exponent λ. A $\ln \mu L$ portion appears in the second term in square brackets of equation (11). As discussed above, diagrams 3(b) and (c) are of the same formal order in g. However, it can be shown that they do not produce $\ln \mu L$ terms to order g. (They do in higher orders in g.) This occurs because the divergences are L independent (see e.g. Kislinger and Morley 1976), so the divergent contributions from figures 3(b) and (c) are of the form $(g^2/L^2)(tL^2) \sim g^2$. Thus, using equation (11), we can write

$$\Delta t = g(2\pi/L)^2[(N+2)/3]\{\tfrac{1}{12} - (tL^2/4\pi^2)(\tfrac{1}{2}\ln \mu L + \text{FT}) + O[(tL^2)^2, g^2]\} \tag{15}$$

where FT designates finite terms which do not contain $\ln \mu L$. Combining (13) and (15) yields

$$\lambda = 2 - [(N+2)/(N+8)]\varepsilon' + O(\varepsilon'^2). \tag{16}$$

Bray and Moore (1978) consider a d-dimensional layered geometry with Dirichlet boundary conditions and evaluate the shift exponent λ to $O(\varepsilon)$. A problem with their approach is the fact that the first-order corrections $\delta\mu_{1,0}$ (in their notation) to mean-field temperature shifts is complex (see for instance their equations (4.7) and (4.8)). However, the leading contribution to $\delta\mu_{1,0}$ in the limit $L \to \infty$ is real, and it is in this approximation that the exponent λ is extracted by them. Because the original expression for $\delta\mu_{1,0}$ is complex, this approach is questionable. Similar difficulties have been noted by Dolan and Jackiw (1974) in the context of finite-temperature field theories where the standard perturbation theory breaks down close to the shifted critical temperature T_c^L (Ginsparg 1980). The calculation of Bray and Moore attempts to calculate λ using the limit ($kb \gg 1$ in their notation) $t \to 0$, $L \to \infty$ such that $tL^2 \gg 1$, whereas we employ the limit $t \to 0$, $L \to \infty$ such that $tL^2 \ll 1$ which is more appropriate to the deep critical region.

The effective free-energy functional method enables the description of the L dependence of a finite-size system very close to its critical temperature T_c^L where a $(d-1)$-dimensional behaviour emerges. The methods of paper I describe the system away from criticality where the d-dimensional physics takes over. Both approaches provide the first systematic ε-expansion techniques for exponents and critical amplitudes. The crossover between these two regimes remains to be explored. More details and expanded discussions of these topics will be given elsewhere.

After the submission of this manuscript we received preprints by Brézin and Zinn-Justin (1985) and Rudnick *et al* (1985) discussing ε-expansion techniques close to T_c^L for cubic and cylindrical geometries with periodic boundary conditions. Their approaches are similar to ours in the deep critical regions, although these authors consider cases where no true critical point exists, and they do not discuss the existence of the three regions of different effective dimensionality, presented here, and the fact that standard ε techniques can be applied away from the critical point in the region of quasi-d-dimensional physics (Nemirovsky and Freed 1985b).

It is still unclear if the fixed point g^* to be employed, together with equation (15) to evaluate the shift exponent λ, is the d-dimensional one as utilised by Brézin *et al* (1985) and Rudnick *et al* (1985) or the $(d-1)$-dimensional fixed point of equation (13) which follows the work of Ginsparg (1980) in the context of finite-temperature field theory. To first order in $\varepsilon(\varepsilon')$ the first assumption produces $\lambda = \nu_d^{-1}$ while the second one gives $\lambda = \nu_{d-1}^{-1}$. The effective free-energy functional of (12) is obtained from the original d-dimensional functional of (3) by integrating out the 'heavy' modes, and by using the usual d-dimensional counterterms to render F_{eff} finite. On the other hand, the effective $d' = d-1$ field theory of (12) should itself be renormalised by $(d-1)$ counterterms. We have studied F_{eff} only to lowest order. A systematic study of the effective field theory in higher orders, which we plan to pursue, should resolve this important question.

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