Thermodynamic Casimir effects involving interacting field theories with zero modes

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Systems with an $O(n)$ symmetrical Hamiltonian are considered in a d-dimensional slab geometry of macroscopic lateral extension and finite thickness L that undergo a continuous bulk phase transition in the limit $L \to \infty$. The effective forces induced by thermal fluctuations at and above the bulk critical temperature $T_{c,\infty}$ (thermodynamic Casimir effect) are investigated below the upper critical dimension $d^* = 4$ by means of field-theoretic renormalization-group methods for the case of periodic and special-special boundary conditions, where the latter correspond to the critical enhancement of the surface interactions on both boundary planes. As shown previously [Europhys. Lett. **75**, 241 (2006)], the zero modes that are present in Landau theory at $T_{c,\infty}$ make conventional renormalization-group-improved perturbation theory in $4 - \epsilon$ dimensions ill-defined. The revised expansion introduced there is utilized to compute the scaling functions of the excess free energy and the Casimir force for temperatures $T \gtrsim T_{c,\infty}$ as functions of $\mathsf{L} \equiv L/\xi_\infty$, where ξ_∞ is the bulk correlation length. Scaling functions of the L-dependent residual free energy per area are obtained, whose $\mathsf{L} \to 0$ limits are in conformity with previous results for the Casimir amplitudes Δ_C to $O(\epsilon^{3/2})$ and display a more reasonable small-L behavior inasmuch as they approach the critical value Δ_C monotonically as $\mathsf{L} \to 0$. Extrapolations to $d = 3$ for the Ising case $n = 1$ with periodic boundary conditions are in fair agreement with Monte Carlo results. In the case of special-special boundary conditions, extrapolations to $d = 3$ are hampered by the fact that the one-loop result for the inverse finite-size susceptibility becomes negative for some values of L when $\epsilon \gtrsim 0.83$.

I. INTRODUCTION

When a classical or quantum fluid or an n-vector magnet, with $n = 1$, 2, and 3, is confined by macroscopic bodies such as two parallel plates, walls, surfaces, or interfaces, of area A, its free energy F depends on the distance L between these boundary planes. The L dependence implies a force

$$\mathcal{F}_C(T,L) = -k_B T \frac{\partial f_{\text{ex}}(T,L)}{\partial L} \tag{1.1}$$

between the plates, where $f_{\text{ex}} = (F/k_B T) - L f_b$ is the reduced excess free energy per unit area and f_b is the reduced bulk free-energy density, and the limit $A \to \infty$ has been taken.[1–5] By analogy with the familiar Casimir force[6] produced by vacuum fluctuations of the electromagnetic field between two metallic plates (and slight abuse of language), $\mathcal{F}_C$ is conventionally called "thermodynamic Casimir force."

Provided long-range interactions are either absent or negligible, this force decays exponentially for separations $L \gtrsim \xi_\infty(T)$, where $\xi_\infty(T)$ is the bulk correlation length. Near a continuous phase transition in d bulk dimensions, $\xi_\infty(T)$ diverges as $|T - T_{c,\infty}|^{-\nu}$ at the bulk critical temperature $T_{c,\infty}$. Therefore, the Casimir force $\mathcal{F}_C(T,L)$ extends to distances L much larger than the microscopic scale a ($\simeq$ radius of atoms, lattice constant).

Writing

$$f_{\text{ex}}(T,L) = f_s(T) + f_{\text{res}}(T,L), \tag{1.2}$$

let us decompose the excess free energy f_{ex} into an L-independent surface part $f_s(T) \equiv f_{\text{ex}}(T,\infty)$ and a residual finite-size contribution $f_{\text{res}}(T,L)$. The latter behaves as

$$f_{\text{res}}(T_{c,\infty},L) \underset{L \to \infty}{\approx} \Delta_C L^{-(d-1)} \tag{1.3}$$

at the bulk critical point $T = T_{c,\infty}$, and hence produces the long-ranged effective force

$$\frac{\mathcal{F}_C(T_{c,\infty},L)}{k_B T_{c,\infty}} \underset{L \to \infty}{\approx} (d-1)\Delta_C L^{-d}. \tag{1.4}$$

Here, Δ_C, the so-called Casimir amplitude,[2] is a universal quantity which depends on the bulk universality class of the phase transition considered and gross properties of the boundary plates, but is independent of microscopic details.

Such thermodynamic Casimir forces have been the subject of much interest recently.[7–11] Clear experimental evidence for their existence has been found in the thinning of wetting layers of liquid ^{4}He as a function of temperature on approaching the lambda line.[10,11]

Near the bulk critical point, the residual free-energy density and Casimir force are expected to have the scaling forms

$$f_{\text{res}}(T,L) \approx L^{-(d-1)} \Theta(L/\xi_\infty) \tag{1.5}$$

and

$$\frac{\mathcal{F}_C(T_{c,\infty},L)}{k_B T} \approx L^{-d} \Xi\left(\frac{L}{\xi_\infty}\right), \tag{1.6}$$

where Θ and

$$\Xi(\mathsf{L}) = (d-1)\Theta(\mathsf{L}) - \mathsf{L}\Theta'(\mathsf{L}) \tag{1.7}$$

should be universal functions of $\mathsf{L} \equiv L/\xi_\infty$. These expectations rest on the assumption that ξ_∞ and L are large compared to other lengths, which means, in particular, that the symmetry breaking field h vanishes and long-range interactions are either absent or negligible.

In studies of the Casimir effect in QED, matter usually is taken into account only through the choice of appropriate boundary conditions on the surfaces of macroscopic bodies. Hence, they involve *free* field theories under given boundary conditions. Systematic theoretical investigations of the Casimir effect at *critical points* are a much greater challenge in that one has to deal with *interacting* field theories in finite and bounded systems.[12,13]

A first fairly detailed study of the thermodynamic Casimir effect was made about 15 years ago by Krech and Dietrich (KD) for the ϕ^4 theory on a slab $\mathbb{R}^{d-1} \times [0, L]$ of thickness L.[7,8] Building on Symanzik's work[14] in the 1980s and the simultaneously emerging field-theory approach to critical behavior of systems with boundaries,[12,13,15–18] these authors considered five different boundary conditions $\wp$, namely, periodic ($\wp$=per), antiperiodic ($\wp$=ap), and the three non-equivalent combinations (D, D), (D, sp), and $(\mathrm{sp}, \mathrm{sp})$ of Dirichlet (D) and special (sp) boundary conditions on the slab's two boundary planes. Here, the former (D) means $\boldsymbol{\phi}=\mathbf{0}$ as usual, while the latter (sp) is the case of a Robin boundary condition $\partial_n \boldsymbol{\phi} = \mathring{c} \boldsymbol{\phi}$, for which $\mathring{c}$ takes the special value $\mathring{c}_{\mathrm{sp}}$ corresponding to the critical enhancement of the surface interactions on the respective boundary plane.

Restricting themselves to temperatures $T \geq T_{c,\infty}$, KD performed two-loop calculations for $(4-\epsilon)$-dimensional slabs under these boundary conditions $\wp$ and determined the ϵ expansions of the Casimir amplitudes $\Delta_C^{(\wp)}$ as well as those of the corresponding scaling functions $\Theta^{(\wp)}$ to first order in ϵ.

In a recent paper with Shpot,[19] we have shown that conventional renormalization-group (RG) improved perturbation theory, on which both Symanzik's[14] and KD's[7,8] analyses are based, becomes ill-defined at $T_{c,\infty}$ beyond two-loop order due to infrared singularities for those boundary conditions that involve a zero mode at $T_{c,\infty}$ in Landau theory. This applies to both $\wp$=per and $\wp$=(sp,sp). To remedy these deficiencies, we performed a reorganization of field theory such that the resulting RG-improved perturbation theory remained meaningful at $T_{c,\infty}$. It was found that the small-ϵ expansions of the corresponding Casimir amplitudes $\Delta_C^{(\wp)}$ involved fractional powers $\epsilon^{k/2}$, with $k \geq 3$, and powers of $\ln \epsilon$. Furthermore, explicit results for these series to order $\epsilon^{3/2}$ were given.

In this paper, we will utilize this approach to compute the scaling functions $\Theta^{(\wp)}$, and hence $\Xi^{(\wp)}$ for $\wp$=per and (sp,sp) to the same order of RG-improved perturbation theory. The results are consistent with and reproduce those of Ref. 19 when $T = T_{c,\infty}$.

Let us note that KD's two-loop results for these boundary conditions, though well defined down to $T_{c,\infty}$, gave clear indications of existing problems. To see this, consider the scaling functions $\Theta^{(\mathrm{per})}$ for $n=1, 2, 3,$ and ∞ displayed in Fig. 1, which were obtained by extrapolating their $O(\epsilon)$ results to $d=3$.

The behavior of these curves at small L differs in a qualitative fashion from that of the exact scaling function for $n=\infty$ and $d=3$, which follows from the exact solution of the mean spherical model under periodic boundary conditions.[5,21,22] Unlike the latter, which decreases monotonically to its critical value
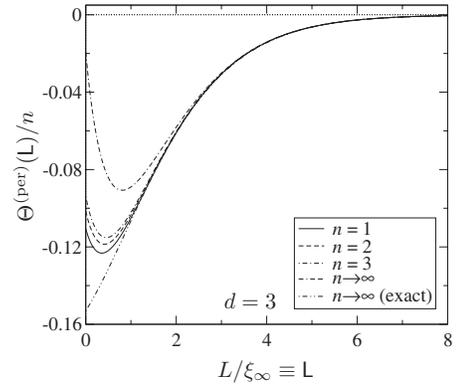

FIG. 1. Scaling functions $\Theta^{(\mathrm{per})}$ for $n=1, 2, 3,$ and ∞ obtained by extrapolating the $O(\epsilon)$ results of Ref. 8 to $d=3$, compared with the exact large-n result for $d=3$ (Refs. 5 and 20).

$$\Delta_C^{(\mathrm{per,SM})} = \frac{-2\zeta(3)}{5\pi} \simeq -0.153\,05 \qquad (1.8)$$

at $\mathsf{L}=0$, the former go through a minimum at small $\mathsf{L}>0$ and then increase as $\mathsf{L} \to 0$. Such a minimum is neither expected at $\mathsf{L}>0$ nor in conformity with the Monte Carlo results of Ref. 23 and announced more recent ones.[24–26] Note also that as n increases, the extrapolations actually move away from the exact $n=\infty$ curve since the deviations at small L get bigger.

A second problem was pointed to by KD: Since for finite L no phase transition takes place at $T_{c,\infty}$, the free energy per unit area must be an analytic function of temperature at $T_{c,\infty}$, which imposes conditions on the small-L behavior of the scaling functions $\Theta^{(\wp)}(\mathsf{L})$ (which will be recalled in Sec. IV C). KD found their $O(\epsilon)$ results to be consistent with these conditions only in the considered cases of nonzero-mode boundary conditions $\wp$=ap, (D, D), and (D, sp). In the remaining cases of the zero-mode boundary conditions $\wp$ =per and (sp,sp), these conditions turned out to be violated by terms of first order in ϵ.

The results our approach yields for the scaling functions $\Theta^{(\mathrm{per})}$ do better in two regards. First, the small-L behavior is improved inasmuch as the Casimir amplitudes $\Delta_C^{(\mathrm{per})}$ are approached in a monotonically decreasing manner as $\mathsf{L} \to 0$. Second, the order of the terms violating the analyticity condition is increased from $O(\epsilon)$ to $O(\epsilon^{3/2})$. In the case of sp-sp boundary conditions, our results raise questions whose answers might require a generalization of our analysis in which the surface enhancement variables are allowed to vary. As we shall see, the one-loop expression for the scaling function of the inverse finite-size susceptibility becomes negative in a small interval of $\mathsf{L}=L/\xi_\infty$ when evaluated at $\epsilon=1$. This probably simply means that this extrapolation to $d=3$ is not sufficiently accurate. In any case, this violation of a necessary stability condition of the disordered phase is a problem even for KD's original $O(\epsilon)$ results.

The remainder of this paper is organized as follows. In the next section, we specify the model utilized in our analysis—the ϕ^4 theory in slab geometry. We briefly recapitulate the general fluctuating Robin boundary conditions it involves, its

renormalization, the fixed points that are relevant for the subsequent analysis, and the renormalization of its free energy. In Sec. III, we first recall the conventional theory of the Casimir effect based on RG improved perturbation theory in $4-\epsilon$ bulk dimensions, and then discuss the problems into which it runs when a zero mode appears in Landau theory. This is followed by a detailed exposition of how these problems can be overcome through an appropriate reformulation of field theory. In Sec. IV, our results for the residual free energies and their scaling functions are presented. In Sec. V, we employ the solution of the mean spherical model under periodic boundary conditions[5,20,21] for $d<4$ to show that our small-ϵ results are in conformity with these exact ones in the limit $n\to\infty$. A brief summary and discussion of our work are given in Sec. VI. Finally, there are four appendixes in which technical details are described.

II. CONTINUUM MODEL, BOUNDARY CONDITIONS, AND BACKGROUND

A. Definition of model

We consider a d-dimensional slab of finite thickness L occupying the region $\mathfrak{V}=\mathbb{R}^{d-1}\times[0,L]$ of d-dimensional space. Let x_j, $j=1,\ldots,d$, be Cartesian coordinates, with $x_d \equiv z$ taken along the finite direction. We write the position vector $\boldsymbol{x}=(x_1,\ldots,x_d)$ as $\boldsymbol{x}=(\boldsymbol{y},z)$, where $\boldsymbol{y}=(x_1,\ldots,x_{d-1})$ is the component along the slab.

The Hamiltonians of the ϕ^4 models we are concerned with are sums of a bulk and a boundary term,

$$\mathcal{H}[\boldsymbol{\phi}]=\int_{\mathfrak{V}}\mathcal{L}_{\mathfrak{V}}(\boldsymbol{x})dV+\int_{\partial\mathfrak{V}}\mathcal{L}_{\partial\mathfrak{V}}(\boldsymbol{x})dA, \qquad (2.1)$$

where $\mathcal{L}_{\mathfrak{V}}(\boldsymbol{x})$ and $\mathcal{L}_{\partial\mathfrak{V}}(\boldsymbol{x})$ depend on $\boldsymbol{\phi}(\boldsymbol{x})$ and its derivatives.

We either consider periodic or free boundary conditions along the z direction. In the first case, where

$$\boldsymbol{\phi}(\boldsymbol{x}+L\hat{\boldsymbol{e}}_d)=\boldsymbol{\phi}(\boldsymbol{x}), \qquad (2.2)$$

there is no boundary, $\partial\mathfrak{V}=\varnothing$, and the boundary term $\int_{\partial\mathfrak{V}}\ldots$ is absent. In the case of free boundary conditions, the boundary $\partial\mathfrak{V}=\mathfrak{B}_1\cup\mathfrak{B}_2$ is the union of $\mathfrak{B}_1$, the $z=0$ plane, and $\mathfrak{B}_2$, the $z=L$ plane.

The bulk density is always given by

$$\mathcal{L}_{\mathfrak{V}}[\boldsymbol{\phi}]=\frac{1}{2}\sum_{\alpha=1}^{n}(\nabla\phi_\alpha)^2+\frac{\mathring{\tau}}{2}\phi^2+\frac{\mathring{u}}{4!}\phi^4, \qquad (2.3)$$

where $\boldsymbol{\phi}(\boldsymbol{x})=(\phi_\alpha(\boldsymbol{x}))$ is the n-component order parameter field and ϕ denotes its absolute value $|\boldsymbol{\phi}|$.

The boundary density we utilize when considering free boundary conditions reads

$$\mathcal{L}_{\partial\mathfrak{V}}[\boldsymbol{\phi}]=\frac{\mathring{c}(\boldsymbol{x})}{2}\phi(\boldsymbol{x})^2, \qquad (2.4)$$

where $\mathring{c}(\boldsymbol{x})$, the surface enhancement variable, is allowed to have different values on $\mathfrak{B}_1$ and $\mathfrak{B}_2$, i.e.,

$$\mathring{c}(\boldsymbol{x})=\begin{cases}\mathring{c}_1 & \text{for } \boldsymbol{x}\in\mathfrak{B}_1 \\ \mathring{c}_2 & \text{for } \boldsymbol{x}\in\mathfrak{B}_2.\end{cases} \qquad (2.5)$$

B. Boundary conditions

Using well-known arguments,[12,13] one concludes from the boundary terms in the classical equations of motion $\delta\mathcal{H}=0$ that the derivative $\partial_n\boldsymbol{\phi}$ along the inner normal $\boldsymbol{n}$ on $\partial\mathfrak{V}$ satisfies

$$\partial_n\phi_\alpha(\boldsymbol{x})=\mathring{c}_j\phi_\alpha(\boldsymbol{x}) \quad \text{for } \boldsymbol{x}\in\mathfrak{B}_j. \qquad (2.6)$$

This is a boundary condition for Landau theory, which holds beyond it in an operator sense (inside of averages).

C. Renormalization of correlation functions

To absorb the ultraviolet (uv) singularities of the $(N+M)$-point cumulant functions

$$G^{(N,M)}_{\alpha_1,\ldots,\beta_M}(\boldsymbol{x}_1,\ldots,\boldsymbol{y}_M)=\left\langle\prod_{j=1}^{N}\phi_{\alpha_j}(\boldsymbol{x}_j)\prod_{k=1}^{M}\phi_{\beta_k}(\boldsymbol{y}_k)\right\rangle^{\text{cum}} \qquad (2.7)$$

involving N interior points $\boldsymbol{x}_j\notin\partial\mathfrak{V}$ and M boundary points $\boldsymbol{y}_k\in\partial\mathfrak{V}$ for dimensions $d\leq4$, bulk and boundary counterterms are needed, which can be chosen to correspond to the reparametrizations

$$\boldsymbol{\phi}=Z_\phi^{1/2}\boldsymbol{\phi}_R,$$

$$\mathring{\tau}-\mathring{\tau}_{c,\infty}\equiv\delta\mathring{\tau}=Z_\tau\mu^2\tau,$$

$$\mathring{u}N_d=\mu^\epsilon Z_u u, \qquad (2.8)$$

and

$$\delta\mathring{c}_j\equiv\mathring{c}_j-\mathring{c}_{\text{sp}}=\mu Z_c c_j,$$

$$\boldsymbol{\phi}|_{\partial\mathfrak{B}}=(Z_\phi Z_1)^{1/2}\,\boldsymbol{\phi}|_{\partial\mathfrak{B}}^R. \qquad (2.9)$$

Here, $\boldsymbol{\phi}|_{\partial\mathfrak{B}}$ means $\boldsymbol{\phi}(\boldsymbol{y}_k)$ at a boundary point $\boldsymbol{y}_k$, and μ is an arbitrary momentum scale. Further, $\delta\mathring{\tau}$ is the deviation of $\mathring{\tau}$ from $\mathring{\tau}_{c,\infty}$, the critical-point value of $\mathring{\tau}$ of the bulk system. In a theory regularized by a large-momentum cutoff Λ, $\mathring{\tau}_{c,\infty}$ would diverge $\sim\Lambda^2$. We prefer to use dimensional regularization; then $\mathring{\tau}_{c,\infty}$ vanishes in perturbation theory. The renormalization factors Z_ϕ, Z_τ, and Z_u are standard bulk quantities. The renormalization factors Z_1 and Z_c are properties of the semi-infinite system that results in the limit $L\to\infty$ when $c_1=c_2$ with $|c_1|<\infty$.

We choose the factor that is absorbed in the renormalized coupling constant as[27]

$$N_d=\frac{2\Gamma(3-d/2)}{(d-2)(4\pi)^{d/2}}=\frac{1}{16\pi^2}\left[1+\frac{1-C_E+\ln(4\pi)}{2}\epsilon+O(\epsilon^2)\right], \qquad (2.10)$$

where C_E is the Euler-Mascheroni constant. It differs from the one advocated by Schloms and Dohm (see, e.g., Ref. 28

and references therein) by a trivial factor of 2. Ours agrees to zeroth order in ϵ with $(2^{-d}\pi^{-d/2})$, the one employed in Ref. 12 and by KD. Therefore, all of the above bulk and surface renormalization factors $Z_\phi, \dots, Z_1$ remain the same as in Refs. 8 and 12 when determined by minimal subtraction of poles at $\epsilon = 0$. Explicit two-loop expressions for these functions can be found in Eqs. (3.42a)–(3.42c) and Eqs. (3.66a) and (3.66b) of Ref. 12 or in Refs. 17 and 18. The advantage of our choice of N_d is that it simplifies the resulting expressions for renormalized one-loop bulk vertex functions while leaving the renormalization factors of Ref. 12 and KD unchanged.

The quantity $\mathring{c}_{\mathrm{sp}}$ is the special value of $\mathring{c}_1$ corresponding to the critical enhancement of the surface interactions in a semi-infinite system with surface plane $\mathfrak{B}_1$, i.e., the value at which the so-called special transition occurs (provided the surface dimension $d-1$ is large enough to allow long-range surface order above $T_{c,\infty}$). Analogous to $\mathring{\tau}_{c,\infty}$, it would diverge $\sim \Lambda$ as $\Lambda \to \infty$ in a cutoff regularized theory, but vanishes in a perturbative approach based on dimensional regularization.[29–31]

D. Fixed points

Let u^* be the infrared-stable zero of the beta function $\beta_u(u) \equiv \mu \partial_\mu|_0 u$, where $\partial_\mu|_0$ means a derivative at fixed bare parameters $\mathring{u}$, $\mathring{\tau}$, $\mathring{c}_1$, and $\mathring{c}_2$ of the theory. In the enlarged space $\{\tau, u, c_1, c_2\}$ of bulk and surface variables, the RG yields fixed points on the hyperplane $(\tau, u) = (0, u^*)$ located at the nine pairs (c_1^*, c_2^*) of the fixed-point values

$$c_j^* = \begin{cases} c_{\mathrm{ord}}^* = \infty \\ c_{\mathrm{sp}}^* = 0 \\ c_{\mathrm{ex}}^* = -\infty. \end{cases} \quad (2.11)$$

These values pertain to the fixed points describing the critical behavior at the ordinary, special, and extraordinary transitions of the semi-infinite system. Each one of these fixed points is specified by a pair (κ_1, κ_2) with $\kappa_1, \kappa_2 =$ ord, sp, and ex of the respective surface universality classes. Universal finite-size quantities such as the Casimir amplitudes $\Delta_C^{(\wp)}$ and the scaling functions $\Theta^{(\wp)}$, $\Xi^{(\wp)}$ generally are different, depending on the basin of attraction of the fixed point (κ_1, κ_2) to which they belong. Recall that for $\kappa_j =$ ord, the cumulants (2.7) satisfy the Dirichlet boundary condition $\lim_{x_k \to \mathfrak{B}_j} G^{(N,0)} = 0$. Thus, the universality classes (ord,ord), (ord, κ), and (κ, ord) with $\kappa \neq$ ord can equivalently be labeled as (D, D), (D, κ), and (κ, D), respectively. We shall continue to employ this convention.

E. Renormalization of free energy

The counterterms implied by the reparametrizations (2.8) and (2.9) are sufficient to absorb the uv singularities of the cumulants (2.7). However, the free energy requires additional additive counterterms.[8,12] They can be chosen to be independent of L.[12,14] We therefore add to the Hamiltonian defined by Eqs. (2.1)–(2.5) a contribution

$$\mathcal{A}_{\mathrm{add}} = \int_{\mathfrak{V}} C_{\mathfrak{V}}(\mathring{\tau}, \mathring{u}) dV + \sum_{j=1}^{2} \int_{\mathfrak{B}_j} C_{\partial\mathfrak{V}}(\mathring{\tau}, \mathring{u}, \mathring{c}_j) dA, \quad (2.12)$$

where $C_{\mathfrak{V}}$ is a polynomial in $\mathring{\tau}$ of degree 2, and $C_{\partial\mathfrak{V}}$ is a polynomial of degree 1 in $\mathring{\tau}$ and degree 3 in $\mathring{c}_j$, whose coefficients depend on $\mathring{u}$, but neither on L nor on the position $\boldsymbol{x}$. The coefficients (power series in $\mathring{u}$) are fixed as follows.[32] Let $T_{\mathrm{NP}}^{\leq 4} f(\mathring{\tau})$ denote the Taylor series expansions of the function f to *second* order in $\mathring{\tau}$ (fourth order in $\mathring{\tau}^{1/2}$), and

$$T_{\mathrm{NP}}^{\leq 3} g(\mathring{\tau}, \mathring{c}) = \sum_{\substack{j,k \\ 0 \leq 2j+k \leq 3}} \frac{1}{j!k!} \frac{\partial^{j+k} g}{\partial \mathring{\tau}^j \partial \mathring{c}^k}\bigg|_{\mathrm{NP}} (\mathring{\tau} - \mathring{\tau}_{\mathrm{NP}})^j (\mathring{c} - \mathring{c}_{\mathrm{NP}})^k \quad (2.13)$$

be the corresponding expansion of g in $\mathring{\tau}$ and $\mathring{c}$ to orders j and k, respectively, with $2j + k \leq 3$, about the normalization point $(\mathring{\tau}, \mathring{c}) = (\mathring{\tau}_{\mathrm{NP}}, \mathring{c}_{\mathrm{NP}})$.[33] We choose

$$\mathring{\tau}_{\mathrm{NP}} \equiv \mathring{\tau}|_{\tau=1} = \mathring{\tau}_{c,\infty} + \mu^2 Z_\tau,$$

$$\mathring{c}_{\mathrm{NP}} \equiv \mathring{c}|_{c=1} = \mathring{c}_{\mathrm{sp}} + \mu Z_c, \quad (2.14)$$

and define the dimensionless renormalized bulk free-energy density $f_{b,R}$ by

$$\mu^{-d} f_{b,R}(\tau, u) = f_b(\mathring{\tau}, \mathring{u}) - T_{\mathrm{NP}}^{\leq 4} f_b(\mathring{\tau}, \mathring{u}). \quad (2.15)$$

The excess surface free-energy density $f_s(\mathring{\tau}, \mathring{u}, \mathring{c}_1, \mathring{c}_2)$ of the infinitely thick film is a sum of contributions $f_s(\mathring{\tau}, \mathring{u}, \mathring{c}_1)$ associated with the respective semi-infinite systems bounded on one side by $\mathfrak{B}_j$; i.e.,

$$f_s(\mathring{\tau}, \mathring{u}, \mathring{c}_1, \mathring{c}_2) = f_s(\mathring{\tau}, \mathring{u}, \mathring{c}_1) + f_s(\mathring{\tau}, \mathring{u}, \mathring{c}_2). \quad (2.16)$$

We define the dimensionless renormalized analogs of the latter by

$$\mu^{-(d-1)} f_{s,R}(\tau, u, c) = f_s(\mathring{\tau}, \mathring{u}, \mathring{c}) - T_{\mathrm{NP}}^{\leq 3} f_s(\mathring{\tau}, \mathring{u}, \mathring{c}). \quad (2.17)$$

By construction, these renormalized bulk and surface free-energy densities satisfy the normalization conditions

$$f_{b,R}|_{\mathrm{NP}} \equiv f_{b,R}(1, u) = 0 = \frac{\partial f_{b,R}}{\partial \tau}\bigg|_{\mathrm{NP}} = \frac{\partial^2 f_{b,R}}{\partial \tau^2}\bigg|_{\mathrm{NP}} \quad (2.18)$$

and

$$\frac{\partial^{j+k} f_{s,R}}{\partial \tau^j \partial c^k}\bigg|_{\mathrm{NP}} \equiv \frac{\partial^{j+k} f_{s,R}}{\partial \tau^j \partial c^k}(1, u, 1) = 0, \quad 0 \leq 2j + k \leq 3, \quad (2.19)$$

respectively. The renormalization functions $C_{\mathfrak{V}}$ and $C_{\partial\mathfrak{V}}$ are fixed by these requirements.

The renormalized excess surface free-energy density $f_{s,R}(\tau, u, c_1, c_2)$ one obtains from the action $\mathcal{H} + \mathcal{A}_{\mathrm{add}}$ upon insertion of the reparametrizations is uv finite. Since $C_{\mathfrak{V}}$ and $C_{\partial\mathfrak{V}}$ are independent of L, the subtractions they provide cancel in the residual free energy $f_{\mathrm{res}}(L; \mathring{\tau}, \mathring{u}, \mathring{c}_1, \mathring{c}_2)$ of the film. Accordingly, its dimensionless renormalized counterpart

$$f_{\mathrm{res},R}(\mu L;\tau,u,c_1,c_2) = \mu^{-(d-1)}f_{\mathrm{res}}(L;\mathring{\tau},\mathring{u},\mathring{c}_1,\mathring{c}_2) \quad (2.20)$$

satisfies a *homogeneous* RG equation, whereas both $f_{b,R}$ and $f_{s,R}$ satisfy inhomogeneous ones.

Following the notation conventions of Ref. 12, we introduce the beta function $\beta_u = \mu\partial_\mu|_0 u$, the RG functions $\eta_\kappa = \mu\partial_\mu|_0 \ln Z_\kappa$, $\kappa = \phi, \tau, u, c, 1$, and the operator

$$\mathcal{D}_\mu = \mu\partial_\mu + \beta_u\partial_u - (2+\eta_\tau)\partial_\tau - (1+\eta_c)\sum_{j=1}^{2} c_j\partial_{c_j}. \quad (2.21)$$

Then the RG equation of $f_{\mathrm{res},R}$ can be written as

$$[\mathcal{D}_\mu + (d-1)]f_{\mathrm{res},R}(\mu L;\tau,u,c_1,c_1) = 0. \quad (2.22)$$

Note that the RG functions β_u and η_κ are either bulk quantities [such as $\beta_u(\epsilon,u)$ and $\eta_\tau(u)$] or properties of semi-infinite systems such as $\eta_c(u)$. In accordance with Ref. 12, we have chosen them independent of c_j and τ (fixing them by minimal subtraction of poles in ϵ). Explicit two-loop expressions for these functions can be found in Eqs. (3.75a)–(3.76b) of Ref. 12.

The RG equation (2.22) can be solved in a standard fashion by means of characteristics. Upon setting $\mu = 1$ and choosing the scale parameter ℓ of the transformation $\mu \to \mu\ell$ equal to $1/\xi_\infty$, the inverse bulk correlation length, we see that the residual free-energy density, on sufficiently long length scales, takes the finite-size scaling form

$$f_{\mathrm{res},R}(L;\tau,u,c_1,c_1) \approx L^{-(d-1)}\Theta(L/\xi_\infty;c_1\xi_\infty^\Phi,c_2\xi_\infty^\Phi). \quad (2.23)$$

Here, Φ is the surface crossover exponent of the special transition. The scaling function Θ is universal up to the nonuniversal amplitude of ξ_∞ and the nonuniversal metric factor associated with c_1 and c_2 (Ref. 34); it is given by

$$\Theta(\mathsf{L};\mathsf{c}_1,\mathsf{c}_2) = \mathsf{L}^{d-1}f_{\mathrm{res},R}(\mathsf{L};1,u^*,\mathsf{c}_1,\mathsf{c}_2). \quad (2.24)$$

From it the functions $\Theta^{(\wp)}(\mathsf{L})$ with $\wp = (\mathrm{sp},\mathrm{sp})$, (D,D), and (sp,D) follow by setting $(\mathsf{c}_1,\mathsf{c}_2)$ to the respective fixed-point values $(0,0)$, (∞,∞), and $(0,\infty)$. For example,

$$\Theta^{(\mathrm{sp},\mathrm{sp})}(\mathsf{L}) = \mathsf{L}^{d-1}f_{\mathrm{res},R}(\mathsf{L};1,u^*,0,0). \quad (2.25)$$

For reasons explained in the Introduction, we shall mainly be concerned with the cases of periodic and (sp,sp) boundary conditions.

III. REVISED FIELD-THEORY APPROACH

A. Infrared problems due to zero modes

We now turn to the problem of computing the scaling functions $\Theta^{(\wp)}$ and $\Xi^{(\wp)}$ for $\wp = \mathrm{per}$ and (sp,sp) by means of RG-improved perturbation theory. Only the case $T \geqslant T_{c,\infty}$ will be considered.

The free propagator can be written as

$$G_L^{(\wp)}(\boldsymbol{x};\boldsymbol{x}'|\mathring{\tau}) = \int_p^{(d-1)} \sum_m \frac{\langle z|m\rangle\langle m|z'\rangle}{p^2 + k_m^2 + \mathring{\tau}} e^{i\boldsymbol{p}\cdot(\boldsymbol{y}-\boldsymbol{y}')}, \quad (3.1)$$
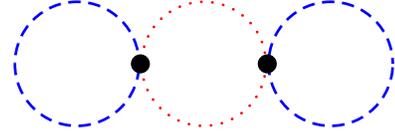
where

FIG. 2. (Color online) Infrared divergent contribution to the free energy. The dashed full blue lines represent the $k_m \neq 0$ part of the free propagator (3.1); the dotted red lines denote its $k_m = 0$ part. The blue subgraphs approach a finite L-dependent limit as $\tau \to 0$; the red dashed subgraphs vary as a negative power of τ and, hence, is infrared singular (Ref. 19).

$$\int_p^{(d-1)} \equiv \int \frac{d^{d-1}p}{(2\pi)^{d-1}} \quad (3.2)$$

is a convenient shorthand for a normalized $(d-1)$-dimensional momentum integral. Further, $|m\rangle = |m\rangle^{(\wp)}$ are eigenstates given by

$$\langle z|m\rangle^{(\mathrm{per})} = \frac{\exp(ik_m z)}{\sqrt{L}}, \quad k_m = \frac{2\pi m}{L}, \quad m \in \mathbb{Z} \quad (3.3)$$

and

$$\langle z|m\rangle^{(\mathrm{sp},\mathrm{sp})} = \frac{1}{\sqrt{L}}\begin{cases} 1 & \text{for } m = 0 \\ \sqrt{2}\cos(k_m z) & \text{for } m \in \mathbb{N}, \end{cases}$$

$$k_m = m\pi/L, \quad m = 0, 1, \ldots, \infty, \quad (3.4)$$

respectively. For either boundary condition, the mode with $m = 0$ and $\boldsymbol{p} = \boldsymbol{0}$ becomes massless at $\tau = 0$.

In their calculation of $\Delta_C^{(\wp)}$ directly at $T_{c,\infty}$, KD therefore subtracted the contribution from the $m = 0$ mode to avoid infrared problems, the rationale being that the subtracted one-loop contribution is formally independent of L so that it does not contribute to the Casimir force. Computing the one- and two-loop graphs at $\tau \geqslant 0$,[8,19] one finds that the contributions from the $k_0 = 0$ modes vary as a positive power of τ and, hence, vanish as $\tau \to 0$. However, at the three-loop level, this is no longer the case because one encounters infrared divergent contributions of the form depicted in Fig. 2. Thus, conventional RG-improved perturbation theory is ill-defined at $T_{c,\infty}$.

The origin of this problem is that Landau theory yields sharp transitions for both the bulk and the film system at the same critical value $\mathring{\tau} = 0$. It is, thus, of a similar kind as encountered in the study of finite-size effects of systems that are finite in all, or in all but one, direction under periodic boundary conditions.[35,36] As discussed in Ref. 19, the remedy is to separate the $k_0 = 0$ mode and construct an effective field theory for the $k_0 = 0$ part of the order parameter.

B. Construction of effective zero-mode action

To this end, we write

$$\boldsymbol{\phi}(\boldsymbol{x}) = \sum_m \boldsymbol{\phi}_m(\boldsymbol{y})\langle z|m\rangle = L^{-1/2}\boldsymbol{\varphi}(\boldsymbol{y}) + \boldsymbol{\psi}(\boldsymbol{y},z), \quad (3.5)$$

decomposing the order parameter into its component along $\boldsymbol{\phi}_0(\boldsymbol{y}) = \boldsymbol{\varphi}(\boldsymbol{y})$ and a remaining $k_m \neq 0$ contribution $\boldsymbol{\psi}(\boldsymbol{y},z)$ with

$$\int_0^L dz\, \boldsymbol{\psi}(\mathbf{y},z) = 0. \tag{3.6}$$

Tracing out $\boldsymbol{\psi}$ defines us a $(d-1)$-dimensional effective field theory with the Hamiltonian

$$\mathcal{H}_{\text{eff}}[\boldsymbol{\varphi}] = -\ln \text{Tr}_{\boldsymbol{\psi}}\, e^{-\mathcal{H}[L^{-1/2}\boldsymbol{\varphi}+\boldsymbol{\psi}]} = \frac{F_{\boldsymbol{\psi}}}{k_B T} + \mathcal{H}[L^{-1/2}\boldsymbol{\varphi}]$$

$$-\ln\langle e^{-\mathcal{H}_{\text{int}}[\boldsymbol{\varphi},\boldsymbol{\psi}]}\rangle_{\boldsymbol{\psi}}. \tag{3.7}$$

Here, $F_{\boldsymbol{\psi}}$, defined by

$$\exp(-F_{\boldsymbol{\psi}}/k_B T) = \text{Tr}_{\boldsymbol{\psi}}\exp(-\mathcal{H}[\boldsymbol{\psi}]), \tag{3.8}$$

is the free energy due to the $k_m \neq 0$ modes. Further,

$$\mathcal{H}_{\text{int}}[\boldsymbol{\varphi},\boldsymbol{\psi}] \equiv \int_{\mathfrak{V}} dV \left[\frac{\mathring{u}}{4L}\varphi^2\psi^2 + \frac{\mathring{u}}{6\sqrt{L}}(\boldsymbol{\varphi}\cdot\boldsymbol{\psi})\psi^2 \right] \tag{3.9}$$

is the interaction part, and

$$\mathcal{H}[L^{-1/2}\boldsymbol{\varphi}] = \int dA \left[\frac{1}{2}\sum_{j=1}^{d-1}\left(\frac{\partial\boldsymbol{\varphi}}{\partial x_j}\right)^2 + \frac{\mathring{\tau}}{2}\varphi^2 + \frac{\mathring{u}}{4!L}\varphi^4 \right]. \tag{3.10}$$

Computing the last term on the right-hand side of Eq. (3.7) in a loop expansion gives

$$\mathcal{H}_{\text{eff}}[\boldsymbol{\varphi}] = \frac{F_{\boldsymbol{\psi}}}{k_B T} + \mathcal{H}[L^{-1/2}\boldsymbol{\varphi}] + \mathcal{H}_{\text{eff}}^{[1]}[\boldsymbol{\varphi}] + \cdots, \tag{3.11}$$

with

$$\mathcal{H}_{\text{eff}}^{[1]}[\boldsymbol{\varphi}] = \frac{1}{2}\text{Tr}\ln\left[\mathbb{1} + \frac{\mathring{u}}{6L}G_{L,\psi}^{(\wp)}\left(\delta_{\alpha\beta}\varphi^2 + 2\varphi_\alpha\varphi_\beta\right)\right]$$

$$= -\varphi \underset{\varphi}{\overset{\frown}{\bullet}} \varphi - \underset{\varphi}{\overset{\varphi}{\times}} \underset{\varphi}{\overset{\varphi}{\times}} + O(\mathring{u}^3), \tag{3.12}$$

where the dashed blue lines (color online) represent free ψ propagators

$$G_{L,\psi}^{(\wp)}(\mathbf{x};\mathbf{x}'|\mathring{\tau}) = \int_{\mathbf{p}}^{(d-1)}\sum_{m\neq 0}\frac{\langle z|m\rangle\langle m|z'\rangle}{p^2 + k_m^2 + \mathring{\tau}}e^{i\mathbf{p}\cdot(\mathbf{y}-\mathbf{y}')} \tag{3.13}$$

and the red bars indicate φ legs.

Writing

$$\delta_{\alpha\beta}\,g_\varphi^{-1}(\mathbf{y}-\mathbf{y}') = \left.\frac{\delta^2\mathcal{H}_{\text{eff}}[\boldsymbol{\varphi}]}{\delta\varphi_\alpha(\mathbf{y})\delta\varphi_\beta(\mathbf{y}')}\right|_{\boldsymbol{\varphi}=0}$$

$$= \delta_{\alpha\beta}\left[(-\partial^2 + \mathring{\tau})\delta(\mathbf{y}-\mathbf{y}') - \sigma_\varphi(\mathbf{y}-\mathbf{y}')\right], \tag{3.14}$$

where ∂^2 means the Laplacian $\sum_{j=1}^{d-1}\partial_j^2$ in $\mathbb{R}^{d-1}$, and

$$\gamma_{\alpha_1,\ldots,\alpha_k}^{(k)}(\mathbf{y}_1,\ldots,\mathbf{y}_k) = \left.\frac{\delta^k\mathcal{H}_{\text{eff}}[\boldsymbol{\varphi}]}{\delta\varphi_{\alpha_1}(\mathbf{y}_1)\cdots\delta\varphi_{\alpha_k}(\mathbf{y}_k)}\right|_{\boldsymbol{\varphi}=0}, \tag{3.15}$$

we introduce the propagator g_φ associated with the φ^2 term of $\mathcal{H}_{\text{eff}}[\boldsymbol{\varphi}]$ and the corresponding self-energy σ_φ as well as
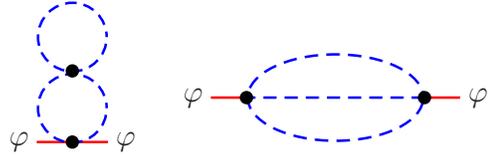

FIG. 3. (Color online) Two-loop contributions to σ_φ. The left graph is local, the one on the right-hand side is nonlocal.

the vertices $\gamma^{(k)}$ of the effective action $\mathcal{H}_{\text{eff}}[\boldsymbol{\varphi}]$. Though not indicated here, all these quantities depend on L and the boundary condition $\wp$.

The first graph in the second line of Eq. (3.12) is the one-loop contribution to σ_φ. It is local in $\mathbf{y}$ space. As can be seen from Fig. 3, both local and nonlocal contributions appear beyond one-loop order. The second graph in the lower line of Eq. (3.12) is the nonlocal one-loop contribution to $\gamma^{(4)}$. Evidently, vertices $\gamma^{(k)}$ of arbitrary even order k are generated through the coupling to the $k_m \neq 0$ modes.

C. Renormalization-group-improved perturbation theory

Now suppose the bulk critical point is approached so that ξ_∞ becomes large. Then the vertices $\gamma^{(k)}$ cannot be computed by perturbation theory below the upper critical dimension $d^* = 4$. However, for arbitrary small $\tau > 0$, we can employ the RG to map to a system with a minimal length scale on the order of ξ_∞, and then employ perturbation theory. The vertex functions $\gamma^{(k)}$ are expected to decay as a function of the relative differences $y_{ij} = |\mathbf{y}_i - \mathbf{y}_j|$ on the scale of ξ_∞.

The renormalized counterparts $\gamma_R^{(k)}$ of these vertices satisfy the RG equations[37]

$$\left(\mathcal{D}_\mu - \frac{N}{2}\eta_\phi\right)\gamma_R^{(k)} = 0. \tag{3.16}$$

Solving them in a standard fashion, one finds that the Fourier transforms $\hat{\gamma}^{(k)}(2\pi)^{d-1}\delta(\Sigma_{j=1}^k \mathbf{p}_j)$ of these functions on sufficiently large length scales take the scaling forms

$$\hat{\gamma}_R^{(2k)}(\{\mathbf{p}_i\}) \approx \mu^{k\eta}L^{1-d+(d-3+\eta)k}X_{2k}^{(\wp)}(\{\mathbf{p}_i\xi_\infty\};L/\xi_\infty), \tag{3.17}$$

where η is a standard bulk critical exponent, while ξ_∞ is the second-moment bulk correlation length. The latter is defined in the conventional manner in terms of the bulk vertex function $\tilde{\Gamma}_b^{(2)}(\mathbf{q}) = 1/\tilde{G}_b^{(2)}(\mathbf{q})$ of the ϕ^4 theory in d-dimensional momentum space or its position-space back transform $G_b^{(2)}(\mathbf{x})$ via

$$\xi_\infty^2 \equiv \left.\left[\frac{\partial}{\partial q^2}\ln\tilde{\Gamma}_b^{(2)}(\mathbf{q})\right]\right|_{q=0} = \frac{1}{2d}\frac{\int d^d x\, x^2 G_b^{(2)}(\mathbf{x})}{\int d^d x\, G_b^{(2)}(\mathbf{x})}. \tag{3.18}$$

Let us verify explicitly to first order in $u^* = O(\epsilon)$ that RG-improved perturbation theory yields such scaling behavior. Consider, for example, $\gamma_R^{(2)} = g_{\varphi,R}^{-1}$. The first graph in the sec-

ond line of Eq. (3.12) is the $O(\mathring{u})$ contribution to $\hat{\sigma}_\varphi(p)$. Introducing

$$I_j^{(\wp)}(L;\mathring{\tau}) \equiv \int_0^L \frac{dz}{L} [G_{L,\psi}^{(\wp)}(\boldsymbol{x};\boldsymbol{x}|\mathring{\tau})]^j, \quad j=1 \text{ and } 2,$$

$$(3.19)$$

we have

$$\hat{\sigma}_\varphi(p) = -\mathring{u}\frac{n+2}{6}I_1^{(\wp)}(L;\mathring{\tau}) + O(\mathring{u}^2). \qquad (3.20)$$

The integrals $I_j^{(\wp)}(L;\mathring{\tau})$ are computed in Appendix A. The results for $I_1^{(\text{per})}$ and $I_1^{(\text{sp,sp})}$ are

$$I_1^{(\text{per})}(L;\mathring{\tau}) = \frac{A_{d-1}}{L}\mathring{\tau}^{(d-3)/2} - A_d \mathring{\tau}^{(d-2)/2} + \frac{2Q_{d,2}(\mathring{\tau}L^2)}{\mathring{\tau}L^d}$$

$$(3.21)$$

and

$$I_1^{(\text{sp,sp})}(L;\mathring{\tau}) = I_1^{(\text{per})}(2L;\mathring{\tau}), \qquad (3.22)$$

where

$$A_d = \frac{2N_d}{4-d} = -(4\pi)^{-d/2}\Gamma\left(1-\frac{d}{2}\right). \qquad (3.23)$$

Here, $Q_{d,2}(r)$ is a special one of the functions defined by

$$Q_{d,\sigma}(r) \equiv \frac{r}{2}\left[\sum_{k\in 2\pi\mathbb{Z}}\int_{\boldsymbol{p}}^{(d-1)} - \int_{\boldsymbol{q}=(\boldsymbol{p},k)}^{(d)}\right]\frac{q^{\sigma-2}}{q^2+r}, \quad (3.24)$$

where $\boldsymbol{p}$ and k are the $(d-1)$-parallel and one-dimensional perpendicular components of the wave vector $\boldsymbol{q}=(\boldsymbol{p},k)$. The properties of these functions are analyzed and discussed in Appendix D, where we compute them for the required parameter values of d and σ. Plots of the functions $Q_{d,2}(r)$ with $d=4$ and 6 are displayed in Fig. 9 (Appendix D).

To facilitate subsequent comparisons with KD's results, let us note how the $Q_{d,2}(r)$ are related to the functions

$$g_{a,b}(z) \equiv \frac{1}{a}\int_1^\infty dt \frac{(t^2-1)^a \ln^b(t^2-1)}{e^{2zt}-1} \qquad (3.25)$$

utilized by these authors. As shown in Appendix C, one has

$$Q_{d,2}(r) = \frac{2^{1-d}\pi^{(1-d)/2}r^{d/2}}{\Gamma[(d-3)/2]} g_{(d-3)/2,0}(\sqrt{r}/2). \qquad (3.26)$$

Using the results (3.21) and (3.22), and expressing $g_{\varphi,R}^{-1} = Z_\phi g_\varphi^{-1}$ in terms of the renormalized variables τ and u, one finds that the pole $\sim\epsilon^{-1}$ cancels. The resulting renormalized expression is easily evaluated at the fixed-point value $u=u^*$. It conforms with the scaling form

$$[\hat{g}_{\varphi,R}^{(\wp)}(p,\tau,L)]^{-1} \approx \mu^\eta L^{\eta-2}X_2^{(\wp)}(p\xi_\infty,L/\xi_\infty) \qquad (3.27)$$

and yields for the scaling functions the ϵ expansions

$$X_2^{(\text{per})}(\mathsf{p},\mathsf{L}) = (\mathsf{p}^2+1)\mathsf{L}^2 + \frac{n+2}{n+8}\epsilon\left[2\pi\mathsf{L} + 16\pi^2\frac{Q_{4,2}(\mathsf{L}^2)}{\mathsf{L}^2}\right]$$

$$+ O(\epsilon^2) \qquad (3.28)$$

and

$$X_2^{(\text{sp,sp})}(\mathsf{p},\mathsf{L}) = (\mathsf{p}^2+1)\mathsf{L}^2 + \frac{n+2}{n+8}\epsilon\left[\pi\mathsf{L} + \pi^2\frac{Q_{4,2}(4\mathsf{L}^2)}{\mathsf{L}^2}\right]$$

$$+ O(\epsilon^2). \qquad (3.29)$$

A few comments are in order here.

(i) The above results imply that $[g_{\varphi,R}^{(\wp)}(0,\tau,L)]^{-1}$ does not vanish at $\tau=0$ when $L<\infty$. Using the fact that $\eta=O(\epsilon^2)$ and the small-r behavior of $Q_{4,2}(r)$ implied by Eq. (A15) yields

$$[g_{\varphi,R}^{(\text{sp,sp})}(0,0,L)^*]^{-1} = [4g_{\varphi,R}^{(\text{per})}(0,0,L)^*]^{-1} + O(\epsilon^2)$$

$$= \epsilon\frac{n+2}{n+8}\frac{\zeta(2)}{L^2} + O(\epsilon^2), \qquad (3.30)$$

where the asterisk indicates evaluation at $u=u^*$.

The physical meaning of this result is obvious. The coupling of the $k_0=0$ mode to the $k_m\neq 0$ modes has produced an L-dependent shift of the temperature at which φ becomes critical, making φ noncritical at $T_{c,\infty}$ when $L<\infty$.

(ii) Verifying the scaling form (3.27) to higher orders in ϵ and the appearance of a nontrivial exponent η by extending RG-improved perturbation theory to $O[(u^*)^2]$ or higher is, in principle, straightforward.

(iii) It is instructive to see what our procedure yields for boundary conditions such as $\wp=(D,D)$, (D,sp), and (ap), where Landau theory does not involve a zero mode at $T_{c,\infty}$. In those cases, we have $\boldsymbol{\varphi}\equiv\boldsymbol{0}$ and $\boldsymbol{\phi}=\boldsymbol{\psi}$. Accordingly, Eq. (3.11) simply yields $F/k_BT\equiv F_\psi/k_BT$ for the reduced free energy. It is, therefore, clear that for those nonzero-mode boundary conditions, conventional expansions in integer powers of ϵ will result for the Casimir force, the scaling functions $\Xi^{(\wp)}$ and $\Theta^{(\wp)}$, and similar quantities for $T\gtrsim T_{c,\infty}$, which must be in accordance with KD's results to $O(\epsilon)$.

(iv) The procedure utilized above for constructing the action of an effective lower-dimensional field theory by integrating out modes via RG-improved perturbation theory that do not become critical for $T=T_{c,\infty}$ at zero-loop order is similar to the one employed in the study of static and dynamic finite-size effects in systems that are finite in all, or in all but one, directions.[35,38–41] In the latter cases, one arrives for small deviations $\epsilon=d^*-d>0$ from the upper critical dimension $d^*=4$ at expansions in powers of $\epsilon^{1/2}$ and $\epsilon^{1/3}$, respectively. The main difference between these cases and ours is that a *sharp transition to a low-temperature phase with long-range order* is ruled out for the former because they involve systems of finite extent along d or $d-1$ Cartesian axes (and the presumed short-range interactions). By contrast, in the case of the slab geometry considered here, such a sharp transition should occur for finite thickness L at a shifted temperature $T_{c,L}<T_{c,\infty}$ whenever $d-1$, the effective dimensionality, is sufficiently large for such a long-range ordered low-temperature phase to occur. [Evidently, $d-1$ must exceed $d_*(n)$, the lower critical dimension, which is $d^*(1)=1$ in the

Ising case $n=1$, and $d_*(n>1)=2$, depending on whether a discrete $\mathbb{Z}_2$ or continuous $O(n)$ symmetry gets spontaneously broken.] When no sharp transition is possible, one expects a rounded one at a shifted pseudocritical temperature (see, e.g., Refs. 42 and 43). The case of $d=3$ and $n=2$, corresponding to an XY model on a slab or liquid ^{4}He film below the bulk λ line T_λ, is exceptional in that a transition of Kosterlitz-Thouless type to a low-temperature phase with quasi-long-range order is expected to occur for finite L.

(v) That the coupling of the $k_0=0$ mode $\boldsymbol{\varphi}$ to the $k\neq 0$ modes $\boldsymbol{\psi}$ produces an L-dependent mass gap for g_φ^{-1} is crucial for making RG-improved perturbation theory well-defined at $T_{c,\infty}$. However, it must be emphasized that such a perturbative approach using $u^*=O(\epsilon)$ as expansion parameter by itself *must not be expected* to give a proper description of the $[(d-1)$ dimensional] critical behavior at $T_{c,L}$. One way to see this is to note that the bare φ^4 coupling constant appearing in $\mathcal{H}_{\mathrm{eff}}[\boldsymbol{\varphi}]$ is $\mathring{u}/L$. To make it dimensionless, we must multiply by the $(5-d)$th power of a length. An appropriate one is ξ_L, the finite-size analog of ξ_∞, defined by

$$\xi_L^2 \equiv \left[\frac{\partial}{\partial p^2} \ln \hat{\Gamma}_{\varphi\varphi}^{(2)}(\boldsymbol{p}) \right]\Bigg|_{\boldsymbol{p}=0}$$

$$= \frac{1}{2(d-1)} \frac{\int d^{d-1}y \, y^2 \langle \boldsymbol{\varphi}(\boldsymbol{y}) \cdot \boldsymbol{\varphi}(\boldsymbol{0}) \rangle^{\mathrm{cum}}}{\int d^{d-1}y \, \langle \boldsymbol{\varphi}(\boldsymbol{y}) \cdot \boldsymbol{\varphi}(\boldsymbol{0}) \rangle^{\mathrm{cum}}}, \quad (3.31)$$

where $\hat{\Gamma}_{\varphi\varphi}(\boldsymbol{p})$ denotes the full $\varphi\varphi$ vertex function in the space of $(d-1)$-dimensional momenta $\boldsymbol{p}$.

The appropriate dimensionless coupling constant, therefore, is $\xi_L^{5-d}\mathring{u}/L$, which diverges as $\xi_L\to\infty$ whenever $d<5$. In accordance with general expectations, we thus see that the appropriate smallness parameter for analyzing the $(d-1)$-dimensional critical behavior at $T_{c,L}$ by means of a dimensionality expansion is $5-d$ rather than ϵ. Constructing a RG approach that is reliable both at $T_{c,\infty}$ and $T_{c,L}$ and capable of describing the crossover from d- to $(d-1)$-dimensional critical behavior is a nontrivial problem, which has so far not been solved in a satisfactory fashion and is beyond the scope of this paper.

IV. CALCULATION OF FREE ENERGIES AND SCALING FUNCTIONS

According to Eq. (3.11), the reduced bare free-energy density per unit area

$$f_L^{(\varphi)} = \lim_{A\to\infty} \frac{F}{Ak_B T} \quad (4.1)$$

is a sum

$$f_L^{(\varphi)}(\mathring{\tau}) = f_\psi^{(\varphi)}(L;\mathring{\tau}) + f_\varphi^{(\varphi)}(L;\mathring{\tau}) \quad (4.2)$$

of a contribution $f_\psi^{(\varphi)}(L;\mathring{\tau})$ from the $k_m\neq 0$ modes and a remainder, which we denote as $f_\varphi^{(\varphi)}$. We first consider the nonzero-mode contribution $f_\psi^{(\varphi)}$.

A. Nonzero-mode contribution to the free energy

A standard loop expansion yields

$$f_\psi^{(\varphi)}(L;\mathring{\tau}) = f_{\psi,[1]}^{(\varphi)}(L;\mathring{\tau}) + f_{\psi,[2]}^{(\varphi)}(L;\mathring{\tau}) + O(\text{three-loops}), \quad (4.3)$$

with

$$f_{\psi,[1]}^{(\varphi)}(L;\mathring{\tau}) = \frac{n}{2} \sum_{k_m\neq 0} \int_p^{(d-1)} \ln(p^2 + k_m^2 + \mathring{\tau}) = f_{\psi,[1]}^{(\varphi)}(L;0)$$

$$+ L\frac{n}{2}J^{(\varphi)}(L;\mathring{\tau}) \quad (4.4)$$

and

$$f_{\psi,[2]}^{(\varphi)}(L;\mathring{\tau}) = \mathring{u}L\frac{n(n+2)}{4!}I_2^{(\varphi)}(L;\mathring{\tau}), \quad (4.5)$$

where

$$J^{(\varphi)}(L;\mathring{\tau}) = \int_0^{\mathring{\tau}} I_1^{(\varphi)}(L;t)dt. \quad (4.6)$$

The $\mathring{\tau}=0$ contributions $f_{\psi,[1]}^{(\varphi)}(L;0)$ are computed in Appendix B. The results are in accordance with those of KD. Expressed in terms of the familiar one-loop values

$$\Delta_{C,[1]}^{(\mathrm{per})} = 2^d \Delta_{C,[1]}^{(\mathrm{sp,sp})} = -n\pi^{-d/2}\Gamma(d/2)\zeta(d) \quad (4.7)$$

of the Casimir amplitudes, they can be written as

$$f_{\psi,[1]}^{(\varphi)}(L;0) = f_{\psi,0}^{(\varphi)} + L^{-(d-1)}\Delta_{C,[1]}^{(\varphi)}. \quad (4.8)$$

Here, $f_{\psi,0}^{(\varphi)}$ are the cutoff and L-dependent quantities defined by Eqs. (B3)–(B5); they vanish in dimensional regularization.

The integrals $I_2^{(\varphi)}$ and $J^{(\varphi)}$ are worked out in Appendix A. The results are given in Eqs. (A4), (A9), (A16), and (A17). Inserting them into Eqs. (4.4) and (4.5) gives

$$f_{\psi,[1]}^{(\mathrm{per})}(L;\mathring{\tau}) = f_{\psi,0}^{(\mathrm{per})} + n\left[\frac{A_{d-1}}{d-1}\mathring{\tau}^{(d-1)/2} - L\frac{A_d}{d}\mathring{\tau}^{d/2} - \frac{4\pi Q_{d+2,2}(\mathring{\tau}L^2)}{\mathring{\tau}L^{d+1}} \right], \quad (4.9)$$

$$f_{\psi,[2]}^{(\mathrm{per})}(L;\mathring{\tau}) = \mathring{u}L\frac{n(n+2)}{4!}\left[\frac{A_{d-1}}{L}\mathring{\tau}^{(d-3)/2} - A_d\mathring{\tau}^{(d-2)/2} + \frac{2Q_{d,2}(\mathring{\tau}L^2)}{\mathring{\tau}L^d} \right]^2, \quad (4.10)$$

and

$$f_{\psi,[1]}^{(\mathrm{sp,sp})}(L;\mathring{\tau}) = f_{\psi,0}^{(\mathrm{sp,sp})} + n\left[\frac{1}{2}\frac{A_{d-1}}{d-1}\mathring{\tau}^{(d-1)/2} - L\frac{A_d}{d}\mathring{\tau}^{d/2} - \frac{\pi Q_{d+2,2}(4\mathring{\tau}L^2)}{2^d\mathring{\tau}L^{d+1}} \right], \quad (4.11)$$

$$f_{\psi,[2]}^{(\mathrm{sp,sp})}(L;\mathring{\tau}) = \mathring{u}L\frac{n(n+2)}{4!}\left\{\left[\frac{A_{d-1}}{2L}\mathring{\tau}^{(d-3)/2} - A_d\mathring{\tau}^{(d-2)/2}\right.\right.$$
$$\left.+\frac{Q_{d,2}(4\mathring{\tau}L^2)}{2^{d-1}\mathring{\tau}L^d}\right]^2 + \frac{B_d}{L}\left[\frac{A_{2d-4}}{2L}\mathring{\tau}^{d-3} - A_{2d-3}\mathring{\tau}^{d-5/2}\right.$$
$$\left.\left.+\frac{Q_{2d-3,2}(4\mathring{\tau}L^2)}{2^{2d-4}\mathring{\tau}L^{2d-3}}\right]\right\}, \qquad (4.12)$$

respectively, where $f_{\psi,0}^{(\wp)}$ and B_d are constants defined in Eqs. (B3) and (A10).

The contributions $-nLA_d\tau^{d/2}/d$ to $f_{\psi,[1]}^{(\wp)}$ have simple poles at $d=4$, which get cancelled upon renormalization by the additive bulk counterterm $\propto\tau^2$ implied by the subtraction (2.15). The two-loop terms $f_{\psi,[2]}^{(\wp)}$ involve uv singular bulk terms linear in A_d, whose poles at $\epsilon=0$ get cancelled by the $O(u)$ contribution to the counterterm $(Z_\phi Z_\tau-1)\mu^2\tau\int_\mathfrak{V}\phi_R^2/2$. That no pole-term singularities located at the boundary planes $\mathfrak{B}_1$ and $\mathfrak{B}_2$ appear at $\epsilon=0$ in $f_{\psi,[1]}^{(\mathrm{sp,sp})}$ and $f_{\psi,[2]}^{(\mathrm{sp,sp})}$ is because both renormalized enhancement variables c_1 and c_2 are zero.

Since our main interest is in the renormalized residual free energy $f_{\mathrm{res},R}^{(\wp)}$, we can avoid dealing with additive counterterms by focusing directly on its calculation. To determine its nonzero-mode contributions $f_{\psi,\mathrm{res},R}^{(\wp)}$, we must subtract from the sums of the above one- and two-loop terms the bulk and surface contributions and express the difference in terms of the renormalized variables τ and u:

$$f_{\psi,\mathrm{res},R}^{(\wp)}(L;\tau,u,\mu) = f_\psi^{(\wp)}(L;\mathring{\tau},\mathring{u}) - Lf_b^{(\wp)}(\mathring{\tau},\mathring{u}) - f_{\psi,s}^{(\wp)}(\mathring{\tau},\mathring{u}). \qquad (4.13)$$

From the results (4.9)–(4.12), one easily reads off the ($\wp$-independent) bulk terms

$$f_b = f_{b,0} - \frac{nA_d}{d}\mathring{\tau}^{d/2} + \mathring{u}\frac{n(n+2)}{4!}A_d^2\mathring{\tau}^{d-2} + O(\mathring{u}^2) \quad (4.14)$$

as well as the $\wp$-dependent surface terms

$$f_{\psi,s}^{(\mathrm{per})} = f_{\psi,s,0}^{(\mathrm{per})} + \frac{nA_{d-1}}{d-1}\mathring{\tau}^{(d-1)/2} - \mathring{u}\frac{n(n+2)}{12}A_dA_{d-1}\mathring{\tau}^{d-5/2} + O(\mathring{u}^2) \qquad (4.15)$$

and

$$f_{\psi,s}^{(\mathrm{sp,sp})} = \frac{1}{2}f_{\psi,s}^{(\mathrm{per})} - \mathring{u}\frac{n(n+2)}{4!}B_dA_{2d-3}\mathring{\tau}^{d-5/2} + O(\mathring{u}^2). \qquad (4.16)$$

No confusion should arise from the fact that $f_{\psi,s}^{(\mathrm{per})}$ does not vanish. As is easily checked, and our results for $f_\varphi^{(\mathrm{per})}$ to be given below will show, this term cancels exactly with the surface contribution to $f_\varphi^{(\mathrm{per})}$, as it must. Of course, such cancellations are neither expected nor occur for $\wp=(\mathrm{sp,sp})$ and other boundary conditions.

With the aid of the property

$$\frac{d}{dr}\left[\frac{Q_{d+2,2}(r)}{r}\right] = -\frac{Q_{d,2}(r)}{4\pi r} \qquad (4.17)$$

derived in Appendix B of Ref. 21, the calculation of $f_{\psi,\mathrm{res},R}^{(\wp)}$ becomes straightforward, giving

$$\frac{f_{\psi,\mathrm{res},R}^{(\mathrm{per})}}{\mu^{d-1}n} = -\frac{4\pi\,Q_{d+2,2}(\mu^2\tau L^2)}{\tau(\mu L)^{d+1}} + \frac{u}{\mu L}\frac{n+2}{4!}\left\{\frac{1}{N_d}\left[A_{d-1}\tau^{(d-3)/2}\right.\right.$$
$$\left.+\frac{2Q_{d,2}(\mu^2\tau L^2)}{\tau(\mu L)^{d-1}}\right]^2 - \frac{\tau^{-\epsilon/2}-1}{\epsilon}\frac{8Q_{d,2}(\mu^2\tau L^2)}{(\mu L)^{d-1}}\Bigg\}$$
$$+ O(u^2) \qquad (4.18)$$

and

$$\frac{f_{\psi,\mathrm{res},R}^{(\mathrm{sp,sp})}}{\mu^{d-1}n} = -\frac{2\pi\,Q_{d+2,2}(4\mu^2\tau L^2)}{\tau(2\mu L)^{d+1}} + \frac{u}{\mu L}\frac{n+2}{4!}\left\{\frac{1}{N_d}\left[\frac{A_{d-1}}{2}\tau^{(d-3)/2}\right.\right.$$
$$+\left.\frac{Q_{d,2}(4\mu^2\tau L^2)}{\tau(2\mu L)^{d-1}}\right]^2 + \frac{B_d}{N_d}\left[\frac{A_{2d-4}}{2}\tau^{d-3}\right.$$
$$\left.+\frac{Q_{2d-3,2}(4\mu^2\tau L^2)}{\tau(2\mu L)^{2d-4}}\right] - \frac{\tau^{-\epsilon/2}-1}{\epsilon}\frac{2Q_{d,2}(4\mu^2\tau L^2)}{(2\mu L)^{d-2}}\Bigg\}$$
$$+ O(u^2). \qquad (4.19)$$

B. Remaining free-energy terms

We next turn to the computation of $f_\varphi^{(\wp)}$. For $\mathring{u}=0$, the Hamiltonian $\mathcal{H}_{\mathrm{eff}}[\boldsymbol{\varphi}]$ describes a free field theory whose two-point function is the familiar Gaussian bulk propagator

$$G_\infty^{(d-1)}(\mathbf{y}|\mathring{\tau}) = \int_p (p^2+\mathring{\tau})^{-1}e^{i\mathbf{p}\cdot\mathbf{y}} = \frac{(\mathring{\tau}/y^2)^{(d-3)/4}}{(2\pi)^{(d-1)/2}}K_{(d-3)/2}(y\sqrt{\mathring{\tau}}) \qquad (4.20)$$

in $d-1$ dimensions. As we have seen, using this as free propagator in a Feynman graph expansion would lead to Feynman integrals that are infrared divergent at $T_{c,\infty}$ and make the expansion ill-defined beyond two-loop order. This suggests working with a free propagator whose mass parameter, first, remains positive for $T\geqslant T_{c,\infty}$ when $L<\infty$, and second, has a well-defined physical meaning beyond perturbation theory. A natural candidate that has these properties is the inverse finite-size susceptibility $r_L^{(\wp)}\equiv r_L$, defined by

$$(r_L)^{-1}\delta_{\alpha\beta} = \chi_L\delta_{\alpha\beta} = \int d^{d-1}y\,\langle\varphi_\alpha(\mathbf{y})\varphi_\beta(\mathbf{0})\rangle^{\mathrm{cum}}. \qquad (4.21)$$

We therefore use

$$G_\varphi(\mathbf{y}) \equiv G_\infty^{(d-1)}(\mathbf{y}|\mathring{r}_L) \qquad (4.22)$$

as free propagator. A tacit assumption underlying our calculation is that the disordered phase is the correct reference state to expand about for the parameter values of L and $\tau\geqslant 0$ considered. Since the transition temperature $T_{c,L}$ for finite L is expected to be lower than the bulk critical temperature $T_{c,\infty}$ (in those cases of d and n for which a sharp transi-

tion occurs when $L<\infty$), this is physically reasonable. However, there is no *a priori* guarantee that extrapolations to $d=3$ of results based on RG-improved perturbation theory will fulfill all necessary requirements. In particular, we should check whether the so-obtained approximate inverse finite-size susceptibilities $r_L^{(\wp)}$ remain positive when $L<\infty$. This issue may be expected to be more delicate for $\wp=(\mathrm{sp,sp})$ than for periodic boundary conditions. The reason is that sp-sp boundary conditions are associated with a multicritical point of the surface phase diagram (located at $c=\tau=0$) at which the line of surface transition $T_{c,s}(c)$ meets the bulk critical line (whose sections with $c>0$ and $c<0$ form the lines of ordinary and extraordinary transitions, respectively).[12,44] For finite L, one expects shifts of this multicritical point and the phase boundaries. To account for these shifts, one would have to vary the surface enhancement variables c_j as well, giving up the restriction $c_1=c_2=0$. This is a difficult problem and is beyond the scope of the present investigation.

Let us represent the propagator (4.22) by a red line, the effective two-point vertex $\mathring{\tau}-\mathring{r}_L-\sigma_\varphi$ by a red dot with two legs, and the effective k-point vertices $\gamma^{(k)}$ with $k>2$ by red dots with k legs. Then the Feynman graph expansion of $f_\varphi^{(\wp)}(L)$ becomes

$$-f_\varphi^{(\wp)}(L) = \bigcirc + \varodot + \text{⊗} + \cdots . \tag{4.23}$$

The first graph on the right-hand side is given by

$$-\bigcirc = n\,f_{\varphi,0} + \frac{n}{2}\int_0^{\mathring{r}_L} G_\infty^{(d-1)}(\mathbf{0}|t)\,dt \tag{4.24}$$

with

$$f_{\varphi,0} = \frac{n}{2}\int_p^{(d-1)} \ln p^2. \tag{4.25}$$

Our results (3.14) and (3.20) for g_φ^{-1} and σ_φ imply that

$$\mathring{\tau}-\mathring{r}_L-\sigma_\varphi = \frac{n+2}{6}\frac{\mathring{u}}{L}G_\infty^{(d-1)}(\mathbf{0}|\mathring{r}_L) + O(\mathring{u}^2)$$

$$= \frac{n+2}{6}\frac{A_{d-1}\mathring{u}}{L}\mathring{r}_L^{(d-3)/2} + O(\mathring{u}^2). \tag{4.26}$$

Using this in conjunction with the fact that the effective four-point vertex, to first order in u^*, is a local φ^4 coupling with interaction constant u^*/L, one finds that the contributions from the other two graphs can be written as

$$\text{⊗} = -\frac{\mathring{u}}{L}\frac{n(n+2)}{4!}\left[G_\infty^{(d-1)}(\mathbf{0}|\mathring{r}_L)\right]^2 + O(\mathring{u}^2)$$

$$= -\frac{1}{2}\varodot + O(\mathring{u}^2). \tag{4.27}$$

Upon inserting the $y\to 0$ limit of the free Gaussian propagator (4.20) into Eqs. (4.24) and (4.27), the required integrals can be performed to obtain

$$f_\varphi^{(\wp)} = f_{\varphi,0} - n\frac{A_{d-1}}{d-1}\mathring{r}_L^{(d-1)/2} - \frac{\mathring{u}}{L}\frac{n(n+2)}{4!}A_{d-1}^2\mathring{r}_L^{d-3} + \cdots . \tag{4.28}$$

Just as the constants $f_{\psi,0}^{(\wp)}$ introduced in Appendix B, $f_{\varphi,0}$ involves uv divergent contributions which are eliminated in the renormalized theory by the additive renormalization of the free energy. Furthermore, it should be remembered that $\mathring{r}_L=\mathring{r}_L^{(\wp)}$ depends on the boundary condition $\wp$. We have

$$\mathring{r}_L^{(\mathrm{per})} = \mathring{\tau} - \frac{n+2}{6}\mathring{u}\left\{A_d\mathring{\tau}^{(d-2)/2} - \frac{2Q_{d,2}(L^2\mathring{\tau})}{\mathring{\tau}L^d}\right\} + O(\mathring{u}^2) \tag{4.29}$$

and

$$\mathring{r}_L^{(\mathrm{sp,sp})} = \mathring{\tau} - \frac{n+2}{6}\mathring{u}\left\{A_d\mathring{\tau}^{(d-2)/2} - \frac{2Q_{d,2}(4L^2\mathring{\tau})}{\mathring{\tau}(2L)^d} + \frac{A_{d-1}}{2L}\mathring{\tau}^{(d-3)/2}\right\}$$

$$+ O(\mathring{u}^2), \tag{4.30}$$

respectively.

The $O(u)$ contributions $\propto A_d=N_d/\epsilon$ of $\mathring{r}_L^{(\wp)}$ have uv poles at $\epsilon=0$. These are cured by the bulk counterterm $(Z_\phi Z_\tau-1)\mu^2\tau\int_{\mathfrak{V}}\phi_R^2/2$. For the resulting renormalized dimensionless inverse susceptibilities $r_L^{(\wp)}=Z_\phi\mathring{r}_L^{(\wp)}/\mu^2$, one obtains

$$r_L^{(\mathrm{per})} = \tau + \tau\frac{n+2}{6}\frac{u}{\tau^{\epsilon/2}}\left[\frac{\tau^{\epsilon/2}-1}{\epsilon/2} + \frac{2Q_{d,2}(\mu^2\tau L^2)}{(\mu^2L^2\tau)^{d/2}N_d}\right] + O(u^2) \tag{4.31}$$

and

$$r_L^{(\mathrm{sp,sp})} = \tau + \tau\frac{n+2}{6}\frac{u}{\tau^{\epsilon/2}}\left[\frac{\tau^{\epsilon/2}-1}{\epsilon/2} - \frac{A_{d-1}}{2\mu L\tau^{1/2}N_d}\right.$$

$$\left. + \frac{2Q_{d,2}(4\mu^2\tau L^2)}{(4\mu^2L^2\tau)^{d/2}N_d}\right] + O(u^2). \tag{4.32}$$

In Sec. IV D, we will verify that these results comply with the scaling form

$$r_L^{(\wp)} = r_\infty \mathsf{R}^{(\wp)}(L/\xi_\infty), \tag{4.33}$$

where

$$r_\infty = \chi_{\mathrm{b}+}^{-1}\tau^\gamma \tag{4.34}$$

is the inverse bulk susceptibility, and try to employ them to determine the scaling functions $\mathsf{R}^{(\wp)}$ by means of the ϵ expansion.

Returning to the calculation of free energies, we now subtract from $f_\varphi^{(\wp)}$ in Eq. (4.28) the surface contribution $f_\varphi^{(\wp)}|_{L=\infty,r_L=r_\infty}$ to obtain the associated contributions $f_{\varphi,\mathrm{res}}^{(\wp)}$ to the residual free energies. Expressing the result in terms of renormalized quantities then yields

$$\frac{f_{\varphi,\mathrm{res},R}^{(\wp)}}{\mu^{d-1}n} = -\frac{A_{d-1}}{d-1}[r_L^{(d-1)/2}-r_\infty^{(d-1)/2}] - \frac{u}{\mu L}\frac{n+2}{4!}\frac{A_{d-1}^2}{N_d}r_L^{d-3}$$

$$+ O(u^2) \tag{4.35}$$

for their renormalized analogs.

C. General properties of the scaling functions

Before we embark on the calculation of the scaling functions $R^{(\wp)}(L)$ and $\Theta^{(\wp)}(L)$ of the inverse finite-size susceptibility and the residual free energy, it will be helpful to discuss some general properties they should have.

In the limits $L \to \infty$ and $L \to 0$, Eq. (4.33) must yield the correct bulk behavior and finite positive finite-size susceptibility, respectively. This implies

$$R^{(\wp)}(L) \approx \begin{cases} 1 & \text{for } L \to \infty \\ \rho_{0+}^{(\wp)} L^{\eta-2} & \text{with } \rho_{0+}^{(\wp)} > 0, \text{ for } L \to 0. \end{cases}$$
(4.36)

Turning to the free-energy scaling functions $\Theta^{(\wp)}(L)$, let us first consider their limiting behavior as $L \to 0$. This must comply with the requirement that the finite-size free energy be analytic in T at the bulk critical temperature when $L < \infty$. As explained by KD, this translates into the limiting form

$$\Theta^{(\wp)}(L) \underset{L \to 0}{\approx} \frac{a_{b+} L^d}{\alpha(1-\alpha)(2-\alpha)} + \frac{a_{s+}^{(\wp)} L^{d-1}}{\alpha_s(1-\alpha_s)(2-\alpha_s)} + \Delta_C^{(\wp)}$$
$$+ \sum_{k=1}^{\infty} \Delta_{k+}^{(\wp)} L^{k/\nu},$$
(4.37)

where $\alpha_s = \alpha + \nu$ is a familiar surface critical index (of the surface excess specific heat[12,44]). Further, a_{b+} is a universal number whose ϵ expansion

$$a_{b+} = \frac{n}{32\pi^2} \left\{ 1 + \frac{\epsilon}{2} \left[\ln(4\pi) - C_E + 3\frac{n+2}{n+8} \right] + O(\epsilon^2) \right\}$$
(4.38)

may be gleaned from Eq. (8.12) of Ref. 8. The plus signs at a_{b+}, a_{s+}, and $\Delta_{k+}^{(\wp)}$, as usual, indicate that these numbers pertain to the limit $\tau \to 0+$.

The first two terms on the right-hand side of Eq. (4.37) remove the singularities of the subtracted bulk and surface contributions to $f_{\mathrm{res},R}^{(\wp)}$; the remaining power series involves integer powers of $\tau \propto (T - T_{c,\infty})/T_{c,\infty}$. Note that neither nonlinear contributions to the temperature scaling field have been taken into account nor those of irrelevant bulk and surface scaling fields. Both sources would entail corrections to the leading thermal singularities of the bulk and surface free energies. The implied additional terms nonanalytic in temperature would have to be removed as well in the finite-size free energy and, hence, entail further nonanalytic contributions to the limiting small-L form (4.37).

The absence of boundaries in the case of periodic boundary conditions implies that the surface amplitudes $a_{s+}^{(\mathrm{per})}$ are exactly zero. For the other case of interest, $\wp = (\mathrm{sp}, \mathrm{sp})$, one has

$$a_{s+}^{(\mathrm{sp},\mathrm{sp})} = \frac{n}{128\pi} \left\{ 1 + \epsilon \left[2 + \ln \pi - C_E + \frac{n+2}{n+8} \right] + O(\epsilon^2) \right\}$$
(4.39)

according to KD's equations (E6) and (E9).

We next turn to a discussion of the limiting forms of the functions $\Theta^{(\wp)}(L)$ as $L \to \infty$. Since we have chosen periodic boundary conditions along all $(d-1)$-parallel directions y_j, no edge contributions $\sim L^{d-2}$ to the total free energy are expected. Accordingly, the residual free energy should decay exponentially as $L \equiv L/\xi_\infty \to \infty$. The asymptotic behavior should simply follow from perturbation theory.

To become more precise, it is useful to recall the representations [see, e.g., Eqs. (4.2) and (4.12) of Ref. 12]

$$G_L^{(\mathrm{per})}(\mathbf{x}_{12}|\overset{\circ}{\tau}) = \sum_{j=-\infty}^{\infty} G_\infty^{(d)}(\mathbf{x}_{12} + jL\mathbf{e}_z|\overset{\circ}{\tau})$$
(4.40)

and

$$G_L^{(\mathrm{sp},\mathrm{sp})}(\mathbf{x}_1, \mathbf{x}_2|\overset{\circ}{\tau}) = \sum_{j=-\infty}^{\infty} [G_\infty^{(d)}(\mathbf{x}_{12} + 2jL\mathbf{e}_z|\overset{\circ}{\tau})$$
$$+ G_\infty^{(d)}(\mathbf{x}_{12} + 2(jL + z_2)\mathbf{e}_z|\overset{\circ}{\tau})]$$
(4.41)

of the free propagators in terms of the bulk propagator $G_\infty^{(d)}$, where $\mathbf{x}_{12} = \mathbf{x}_1 - \mathbf{x}_2 = (\mathbf{y}_1, z_1) - (\mathbf{y}_2, z_2)$.

The $j = 0$ terms $G_\infty^{(d)}(\mathbf{x}_{12}|\overset{\circ}{\tau})$ yield the bulk contributions of $G_L^{(\wp)}$. The $j = 0$ term $G_\infty^{(d)}(\mathbf{x}_{12} + 2z_2|\overset{\circ}{\tau})$ and the $j = -1$ term $G_\infty^{(d)}[\mathbf{x}_{12} + 2(z_2 - L)|\overset{\circ}{\tau}]$ in Eq. (4.41) represent surface contributions. Since $G_\infty^{(d)}(\mathbf{x}|\overset{\circ}{\tau})$ decays exponentially as $|\mathbf{x}| \to \infty$, it is clear that of the remaining terms, those involving spatial differences that are constrained by the smallest lower bounds will govern the limiting large-L behavior of the functions $\Theta^{(\wp)}$. In the case of periodic boundary conditions, this applies to the $j = \pm 1$ terms, which involve position vectors of lengths $\geqslant L$. Hence, $\Theta^{(\mathrm{per})}(L)$ must vary as $\sim e^{-L}$ in the limit $L \to \infty$, up to powers of L.

On the other hand, for $\wp = (\mathrm{sp}, \mathrm{sp})$, there are four contributions involving position vectors constrained by the lower-distance bound $2L$ which govern the large-L behavior. Thus, $\Theta^{(\mathrm{sp},\mathrm{sp})}(L)$ must decay $\sim e^{-2L}$ up to powers of L.

To elaborate on these arguments, one can employ the above expressions (4.40) and (4.41) for the free propagators in perturbation theory, dropping all of their summands that do not contribute to the leading large-L behavior. In the case of the one-loop integrals, it is again convenient to first determine the large-L forms of their $\overset{\circ}{\tau}$ derivatives and then integrate with respect to $\overset{\circ}{\tau}$. However, from our perturbative results gathered in Eqs. (4.9)–(4.12), (4.24), (4.27), and (4.35), the one- and two-loop Feynman integrals with *all* contributions to the free propagators included can be inferred. Thus, no renewed calculation is necessary. To determine the large-L behavior of the $\Theta^{(\wp)}$, we must merely replace the functions $Q_{d,2}$ and $Q_{d+2,2}$ by their asymptotic forms (D4) given in Appendix D. This yields

$$\Theta^{(\mathrm{per})}(L) \underset{L \to \infty}{\approx} -\frac{n}{(2\pi)^{(d-1)/2}} L^{(d-1)/2} e^{-L} [1 + O(u^*)]$$
(4.42)

and

$$\Theta^{(\mathrm{sp,sp})}(\mathsf{L}) \underset{\mathsf{L}\to\infty}{\approx} -\frac{n}{2^d \pi^{(d-1)/2}} \mathsf{L}^{(d-1)/2} e^{-2\mathsf{L}} [1 + O(u^*)]. \tag{4.43}$$

Finally, let us briefly recall what can be said about the behavior of the $\tau < 0$ analogs of the scaling functions $\Theta^{(\wp)}$, which we denote as $\Theta_-^{(\wp)}(\mathsf{L})$, at the transition temperature $T_{c,L}$ of the film in those cases where a sharp transition to a long-range ordered phase is possible for finite L, such as in the Ising case $n=1$ for bulk dimension $d=3$. As a function of the temperature deviation $t_L = (T - T_{c,L})/T_{c,L}$, the excess free energy per cross-sectional area A must have a contribution that behaves as $\sim t_L^{2-\alpha_{d-1}}$ as $t_L \to 0$, where α_{d-1} is the specific heat exponent for bulk dimension $d-1$. The transition point translates into a nonzero value L_0 at which the functions $\Theta_-^{(\wp)}(\mathsf{L})$ behave in a nonanalytic fashion. Standard matching of the temperature singularities then yields the behavior

$$\Theta_-^{(\wp)}(\mathsf{L}) \sim |\mathsf{L}^{1/\nu} - \mathsf{L}_0^{1/\nu}|^{2-\alpha_{d-1}}, \tag{4.44}$$

where $\nu \equiv \nu_d$, as before, is the correlation-length exponent of the d-dimensional bulk system.

A well-known consequence is that the critical-temperature shift varies as[42,43]

$$(T_{c,\infty} - T_{c,L})/T_{c,\infty} \sim L^{-1/\nu}. \tag{4.45}$$

This conclusion that the shift exponent is given by $1/\nu$ is more or less automatic when the finite-size scaling form (1.5) of the residual free energy applies and, hence, is in complete accordance with our theory.

D. Scaling functions of inverse finite-size susceptibilities

We proceed by combining our perturbative results of Secs. IV A and IV B with the RG to compute the desired scaling functions, beginning with those of the inverse finite-size susceptibilities $r_L^{(\wp)}$. To this end, we use the RG flow to map the original renormalized theory to one corresponding to the choice $\ell = (\mu \xi_\infty)^{-1}$ of the scale parameter. The running coupling constant $\bar{u}(\ell)$ can be replaced by the fixed-point value $u^* = 3\epsilon/(n+8) + O(\epsilon^2)$ at the expense of neglecting corrections to scaling $\sim \bar{u}(\ell) - u^*$. The running temperature variable $\bar{\tau}(1/\mu \xi_\infty)$ is exactly unity (at the required first order in u^*, when $\tau > 0$).

As straightforward consequences of Eqs. (4.31) and (4.32), we thus obtain

$$\mathsf{R}^{(\mathrm{per})}(\mathsf{L}) = 1 + \epsilon \frac{n+2}{n+8} \frac{16\pi^2 Q_{4,2}(\mathsf{L}^2)}{\mathsf{L}^4} + o(\epsilon) \tag{4.46}$$

and

$$\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L}) = 1 + \epsilon \frac{n+2}{n+8} \frac{\pi^2 Q_{4,2}(4\mathsf{L}^2) - \pi \mathsf{L}^3}{\mathsf{L}^4} + o(\epsilon). \tag{4.47}$$

Using the asymptotic forms (D1) and (D5) of $Q_{4,2}(4\mathsf{L}^2)$ for small and large L, one sees that these results are in conformity with the limiting behavior (4.36). The amplitudes $\rho_{0+}^{(\wp)}$ are found to be

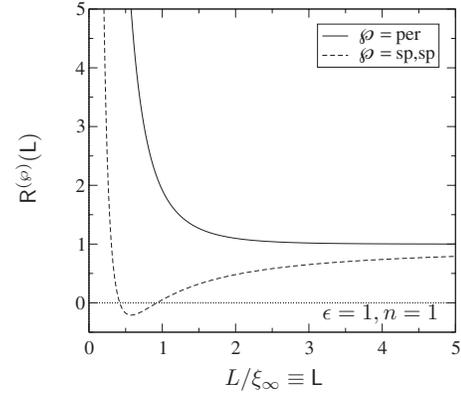FIG. 4. Plots of the scaling functions $\mathsf{R}^{(\mathrm{per})}(\mathsf{L})$ and $\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L})$ for $n=1$ and $d=3$, as obtained from Eqs. (4.46) and (4.47) by setting $\epsilon = n = 1$.

$$\rho_{0+}^{(\mathrm{per})} = 4\rho_{0+}^{(\mathrm{sp,sp})} + o(\epsilon) = \epsilon \frac{n+2}{n+8} \frac{2\pi^2}{3} + o(\epsilon). \tag{4.48}$$

The approach to the large-L limit $\mathsf{R}^{(\wp)}(\infty) = 1$ is qualitatively different for periodic and sp-sp boundary conditions: it is of an exponential and algebraic form in the first and latter cases, respectively.

In Fig. 4, we have plotted the extrapolations to $d=3$ of the $O(\epsilon)$ results (4.46) and (4.47), obtained by setting $\epsilon = 1$, for the one-component case $n=1$. It reveals another important difference: The extrapolation $\mathsf{R}^{(\mathrm{per})}(\mathsf{L})|_{\epsilon=n=1}$ remains positive for all $\mathsf{L} > 0$, reassuring us, thus, that the theory is consistent in that the disordered state about which we expanded satisfies this necessary stability condition. By contrast, the extrapolation $\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L})|_{\epsilon=n=1}$ *becomes negative* for $0.42 \lesssim \mathsf{L} \lesssim 0.93$. When extrapolated to $d=3$ in this naïve manner, the theory, thus, yields a violation of stability of the disordered state in this range of parameters.

It is to be emphasized that this is a problem already for KD's original extrapolations of their ϵ-expansion results for the Casimir effect. As we shall see below, in our reformulated field theory, it will show up in an even more exposed fashion. Note, however, that negative values of the $O(\epsilon)$ result for $\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L})$ are encountered only for values of $\epsilon \gtrsim 0.8265$. This is illustrated in Fig. 5, where $\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L})|_{n=1}$ is plotted for several different values of ϵ. It is conceivable, although not at all guaranteed, that extrapolations based on perturbative calculations to higher orders will yield positive definite functions $\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L})$. As already remarked above, we believe that in systematic studies of the stability of the disordered phase, besides temperature, the surface enhancement variables c_1 and c_2 should be allowed to vary—a difficult task which is beyond the scope of our present analysis.

E. Scaling functions of the residual free energies

To determine the free-energy scaling functions $\Theta^{(\wp)}(\mathsf{L})$, we start with the decompositions

$$f_{\mathrm{res},R}^{(\wp)}(L; \tau, u, \mu) = f_{\psi,\mathrm{res},R}^{(\wp)} + f_{\varphi,\mathrm{res},R}^{(\wp)} \tag{4.49}$$
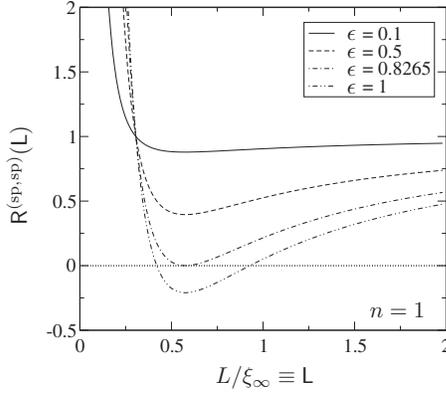
and

FIG. 5. Plots of $O(\epsilon)$ result for the scaling function $\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L})$ for $n=1$ and the indicated values $\epsilon=0.1$, 0.5, 0.8265, and 1.

$$\Theta^{(\wp)}(\mathsf{L}) = \Theta^{(\wp)}_{\psi}(\mathsf{L}) + \Theta^{(\wp)}_{\varphi}(\mathsf{L}), \qquad (4.50)$$

analogous to Eq. (4.2). We now substitute the perturbative expressions (4.18), (4.19), and (4.35) for $f^{(\wp)}_{\psi,\mathrm{res},R}$ and $f^{(\wp)}_{\varphi,\mathrm{res},R}$, and insert Eqs. (4.31) and (4.32) for $r_L^{(\mathrm{per})}$ and $r_L^{(\mathrm{sp,sp})}$, together with their common large-L limit

$$r_{\infty} = \tau + \tau \frac{n+2}{6} \frac{u}{\tau^{\epsilon/2}} \frac{\tau^{\epsilon/2}-1}{\epsilon/2} + O(u^2) \qquad (4.51)$$

for the inverse bulk susceptibility r_{∞}. This yields the (truncated) series-expansion results for $f^{(\wp)}_{\mathrm{res},R}(L;\tau,u,\mu)$ on which our subsequent analysis is based. We now combine them with the RG, proceeding along the lines explained and followed above.

The functions $\Theta^{(\wp)}_{\psi}$ have conventional expansions in integer powers of ϵ, which to first order in ϵ follow directly from Eqs. (4.18) and (4.19). Our results are

$$\Theta^{(\mathrm{per})}_{\psi}(\mathsf{L}) = -n\frac{4\pi[Q_{6,2}(\mathsf{L}^2) - \epsilon R_{6,2}(\mathsf{L}^2)]}{\mathsf{L}^2}$$
$$+ n\epsilon \frac{n+2}{n+8} \frac{[\mathsf{L}^3 + 8\pi Q_{4,2}(\mathsf{L}^2)]^2}{8\mathsf{L}^4} + O(\epsilon^2) \qquad (4.52)$$

and

$$\Theta^{(\mathrm{sp,sp})}_{\psi}(\mathsf{L}) = -n\pi \frac{(1+\epsilon \ln 2)Q_{6,2}(4\mathsf{L}^2) - \epsilon R_{6,2}(4\mathsf{L}^2)}{16\mathsf{L}^2}$$
$$+ n\epsilon \frac{n+2}{n+8} \frac{\pi Q_{4,2}(4\mathsf{L}^2)[2\mathsf{L}^3 + \pi Q_{4,2}(4\mathsf{L}^2)]}{32\mathsf{L}^4}$$
$$+ O(\epsilon^2), \qquad (4.53)$$

where $R_{6,2}$ is defined by

$$R_{d,\sigma}(r) \equiv \frac{\partial Q_{d,\sigma}(r)}{\partial d}. \qquad (4.54)$$

Inspection of KD's work reveals that the nonzero-mode part of their $O(\epsilon)$ expression for $\Theta^{(\mathrm{sp,sp})}$ coincides with their result for $\Theta^{(D,D)}$. By consistency, the latter should agree with

our result (4.53) for $\Theta^{(\mathrm{sp,sp})}_{\psi}$. This is, indeed, the case, as can easily be verified by comparison, using the relation

$$R_{6,2}(r) = \frac{r^3}{32\pi^3} \left[\left(C_E - \frac{8}{3} + \ln\frac{r}{\pi} \right) g_{3/2,0}\left(\frac{\sqrt{r}}{2}\right) + g_{3/2,1}\left(\frac{\sqrt{r}}{2}\right) \right] \qquad (4.55)$$

implied by Eq. (3.26).

A consistency check can also be made for $\Theta^{(\mathrm{per})}_{\psi}$ by noting that the contribution produced by the L^3 term in $[\dots]^2$ of Eq. (4.52) corresponds to the subtracted $k_0=0$ part. Thus, by dropping it, we should recover KD's result for $\Theta^{(\mathrm{per})}$ given in the third line of their equations (6.13). Confirming this is, again, straightforward by virtue of Eq. (4.55).

We stress that unlike the full scaling functions $\Theta^{(\wp)}(\mathsf{L})$, their nonzero-mode parts $\Theta^{(\wp)}_{\psi}(\mathsf{L})$ *do not, in general, decay exponentially* as $\mathsf{L}\to\infty$ and *should not be expected* to have this property. This is because the zero-mode pieces projected out involve contributions to the residual free-energy density $f_{\mathrm{res},R}$ that decay as $1/L$. These imply contributions to $\Theta^{(\wp)}_{\psi}(\mathsf{L})$ that vary as L^{d-2} in the large-L limit. Inspection of our result (4.52) shows that the $O(\epsilon)$ term of $\Theta^{(\mathrm{per})}_{\psi}$, indeed, grows as L^2. By contrast, our $O(\epsilon)$ result (4.53) for $\Theta^{(\mathrm{sp,sp})}_{\psi}$ is seen to decay exponentially for large L because both the functions $Q_{d,2}$ and $R_{d,2}$ do so [cf. Eq. (D4)]. The absence of an analogous $O(\epsilon)$ contribution $\sim\mathsf{L}^2$ to $\Theta^{(\mathrm{sp,sp})}_{\psi}$ is due to the cancellation of the two terms of $f_{\psi,[2]}$ in Eq. (4.12) proportional to A_{d-1}^2/L and B_d/L, respectively. Of course, if such cancellation did not occur, then the above-mentioned equality of $\Theta^{(\mathrm{sp,sp})}_{\psi}$ with $\Theta^{(D,D)}_{\psi}$ to first order in ϵ would be impossible.

We next turn to the computation of the functions $\Theta^{(\wp)}_{\varphi}$. This is a considerably more subtle problem, which requires care. It should be clear that we must not simply expand in powers of ϵ. The small-L behavior of the scaling functions $\Theta^{(\wp)}$ should be compatible with the behavior found for $\tau=0$ in Ref. 19 and, hence, yield the contributions $\sim\epsilon^{3/2}$ to the Casimir amplitudes. The mechanism by which this happens is that the inverse susceptibilities $r_L^{(\wp)}(\tau,u^*)$ approach nonzero limits $r_L^*(0,u^*)=O(u^*)$ as $\tau\to 0$ when $L<\infty$. The $O(\epsilon^{3/2})$ terms then result from the contributions $\sim r_L^{(d-1)/2} = r_L^{3/2+O(\epsilon)}$ to $f^{(\wp)}_{\varphi,\mathrm{res},R}$ in Eq. (4.35).

On the other hand, if we expand in powers of ϵ, taking L (i.e., τ) to be positive, then KD's series-expansion results to order ϵ still ought to be recovered.

Substitution of the respective one-loop results (4.31) and (4.32) for $r_L^{(\wp)}$ in the zero-mode free-energy contribution (4.35), in conjunction with Eq. (2.24), yields

$$\Theta^{(\wp)}_{\varphi}(\mathsf{L}) = \frac{n\mathsf{L}^3}{12\pi} \left\{ 1 - \frac{3\pi}{2\mathsf{L}}\frac{n+2}{n+8}\epsilon - [\mathsf{R}^{(\wp)}(\mathsf{L})]^{3/2} \right\}, \qquad (4.56)$$

where $\mathsf{R}^{(\wp)}(\mathsf{L})$ represents the respective $O(\epsilon)$ expression for these scaling functions given in Eqs. (4.46) and (4.47).

In the case of periodic boundary conditions, which we consider first, the combination of Eqs. (4.46), (4.50), (4.52), and (4.56) leads to

$$\Theta^{(\mathrm{per})}(\mathsf{L}) = - n \frac{4\pi[Q_{6,2}(\mathsf{L}^2) - \epsilon R_{6,2}(\mathsf{L}^2)]}{\mathsf{L}^2} + n\epsilon \frac{n+2}{n+8}$$

$$\times \frac{[\mathsf{L}^3 + 8\pi Q_{4,2}(\mathsf{L}^2)]^2 - \mathsf{L}^6}{8\mathsf{L}^4} + \frac{n\mathsf{L}^3}{12\pi}$$

$$\times \left[1 - \left(1 + \epsilon \frac{n+2}{n+8} \frac{16\pi^2 Q_{4,2}(\mathsf{L}^2)}{\mathsf{L}^4} \right)^{3/2} \right] + o(\epsilon^{3/2}).$$

$$(4.57)$$

This result has the following properties:

(i) Upon expanding it to first order in ϵ [i.e., the term $[\dots]^{3/2}$ in Eq. (4.57)] when $\mathsf{L}=0$, one recovers KD's result.

(ii) The limiting value $\Theta^{(\mathrm{per})}(0)$ agrees with our $O(\epsilon^{3/2})$ result for

$$\Delta_C^{(\mathrm{per})} = -\frac{n\pi^2}{90} + \frac{n\pi^2\epsilon}{180} \left[1 - C_E - \ln\pi + \frac{2\zeta'(4)}{\zeta(4)} + \frac{5\,n+2}{2\,n+8} \right]$$

$$- \frac{n\pi^2}{9\sqrt{6}} \left(\frac{n+2}{n+8} \right)^{3/2} \epsilon^{3/2} + O(\epsilon^2) \qquad (4.58)$$

in Ref. 19.

(iii) The small-L behavior of $\Theta^{(\mathrm{per})}(\mathsf{L})$ differs from the requested one specified in Eq. (4.37) by terms $\propto \epsilon^{3/2}\mathsf{L}$; we have

$$\Theta^{(\mathrm{per})}(\mathsf{L}) \underset{\mathsf{L}\to 0}{\approx} \Delta_C^{(\mathrm{per})} + \frac{n\pi}{2\sqrt{6}} \left(\frac{n+2}{n+8} \right)^{3/2} \epsilon^{3/2}\mathsf{L} + O(\mathsf{L}^2).$$

$$(4.59)$$

In KD's result, the term linear in L that is at variance with the limiting form (4.37) is of first order in ϵ. Here, it is of the same order $\epsilon^{3/2}$ to which we determined $\Delta_C^{(\mathrm{per})}$.

(iv) The large-L asymptotic behavior of $\Theta^{(\mathrm{per})}(\mathsf{L})$ is in conformity with Eq. (4.42), just as KD's result is.

It is gratifying that our result has the properties (i), (ii), and (iv). On the other hand, it still does not fully comply with the small-L form (4.37) dictated by the analyticity of the total finite-size free energy at $T_{c,\infty}$, though the violations now occur at the corresponding higher order $\epsilon^{3/2}$.

In Fig. 6, our result for the scaling function $\Theta^{(\mathrm{per})}(\mathsf{L})$ with $n=1$ and $d=3$, obtained by setting $\epsilon=1$ in Eq. (4.57), is plotted and compared with its analog for KD's ϵ-expansion result. The minimum in KD's extrapolation result appears to be due to the inadequate handling of the zero-mode contributions. Our extrapolation gives a monotonic behavior at small L, which agrees better both with the Monte Carlo data of Ref. 23 as well as with improved, more recent ones.[25,26]

In Fig. 7, analogous extrapolations to $d=3$ of the scaling functions for $n=2$, $n=3$, and $n=\infty$ are displayed, along with the exact spherical-model result for $d=3$. The comparison with the extrapolations based on KD's $O(\epsilon)$ results displayed in Fig. 1 indicates, on the one hand, that the extrapolations for given n oscillate as the order of the series expansion is increased and, on the other hand, that the variations with order are bigger the larger n is.

Next, we consider the case of sp-sp boundary conditions. In discussing extrapolations to $d=3$ dimensions, we shall restrict ourselves to the $n=1$ component case. The reason
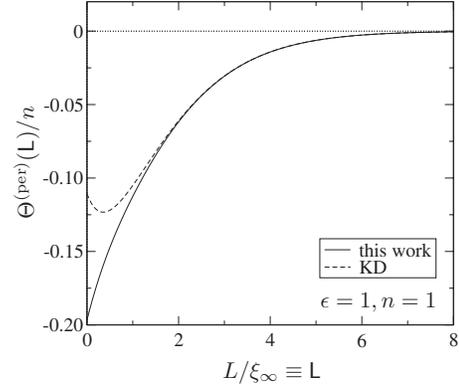

FIG. 6. Extrapolations to $d=3$ of the scaling function $\Theta^{(\mathrm{per})}(\mathsf{L})$ for $n=1$, obtained by setting $\epsilon=1$ in Eq. (4.57) and KD's original $O(\epsilon)$ result, respectively.

should be clear: Only when $n=1$ is a multicritical point expected to occur at $T_{c,\infty}$ and a finite enhancement of the surface interaction constants.[45–47]

A first problem was encountered in our investigation of the inverse finite-size susceptibility $r_L^{(\mathrm{sp,sp})}$: Our one-loop result for the scaling function $R^{(\mathrm{sp,sp})}(\mathsf{L},n=1,\epsilon=1)$ becomes negative for $0.42 \lesssim \mathsf{L} \lesssim 0.93$. Clearly, convincing predictions for the scaling functions $\Theta^{(\mathrm{sp,sp})}(\mathsf{L})$ in $d=3$ dimensions must also fulfill necessary stability conditions such as the positive definiteness of r_L. Thus, the violation of this stability criterion of the disordered state is a problem even for extrapolations to $d=3$ of KD's original $O(\epsilon)$ results. In our result given by the combination of Eqs. (4.47), (4.50), (4.53), and (4.56), it manifests itself in an obvious, striking manner: For values of the scaling variable L in the mentioned interval, the extrapolation to $d=3$ would yield complex numbers for $\Theta^{(\mathrm{sp,sp})}(\mathsf{L})$.

A further problem occurs for large L: The contribution to $\Theta^{(\mathrm{sp,sp})}(\mathsf{L})$ originating from the term $\propto 1/\mathsf{L}$ in curly brackets in Eq. (4.56) in conjunction with the part $\propto 1/\mathsf{L}$ of $R^{(\mathrm{sp,sp})}$ produces a large-L behavior of the form $O(\epsilon^2)\mathsf{L} + O(\epsilon^3)\mathsf{L}^0$. Thus, unless we subtract these asymptotic terms $\propto \epsilon^2\mathsf{L}$ and $\propto \epsilon^3\mathsf{L}^0$, our approximation for $\Theta^{(\mathrm{sp,sp})}(\mathsf{L})$ will not have a finite
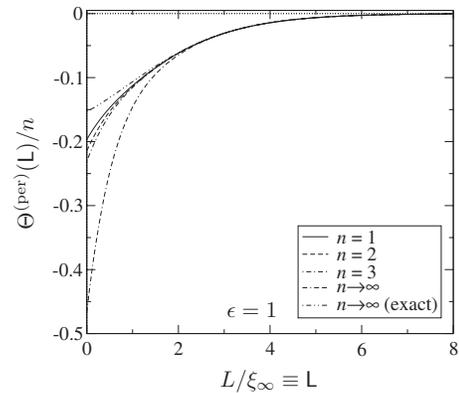

FIG. 7. Extrapolations to $d=3$ of the scaling function $\Theta^{(\mathrm{per})}(\mathsf{L})$ for $n=2$, $n=3$, and $n=\infty$, obtained by setting $\epsilon=1$ in Eq. (4.57). For comparison, the spherical-model result for $d=3$ (Refs. 5 and 20), which is exact for $n=\infty$, is also shown.
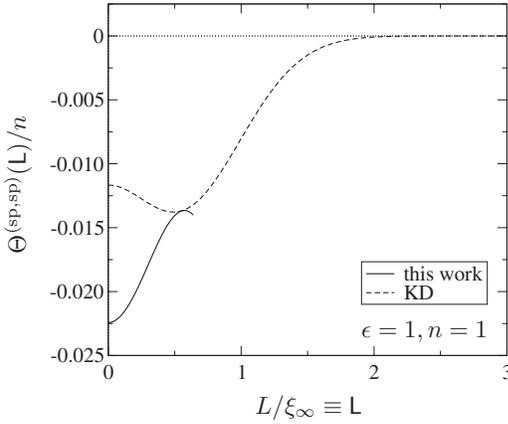
FIG. 8. Extrapolations to $d=3$ of the scaling function $\Theta^{(\mathrm{sp,sp})}$ for $n=1$. The curve labeled "KD" corresponds to the $O(\epsilon)$ results of Ref. 8 evaluated at $\epsilon=1$; the other one is our result, given by Eqs. (4.47), (4.50), (4.53), and (4.56), with ϵ set to 1. For further explanations, see main text.

limit as $\mathsf{L}\to\infty$, and, hence, yield unacceptable results at $d=3$ even in the regime $\mathsf{L}\gtrsim 0.92$, where the positivity condition $\mathsf{R}^{(\mathrm{sp,sp})}>0$ is satisfied.

The combination of these two problems puts us in a bad position to suggest convincing extrapolations to $d=3$. Let us, however, note some appealing properties the result given by Eqs. (4.47), (4.50), (4.53), and (4.56) has. All above properties (i)–(iii) of the small-L behavior hold just as in the case of periodic boundary conditions. That is, KD's $O(\epsilon)$ results are recovered when the term $[\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L})]^{3/2}$ in Eq. (4.56) is expanded in powers of ϵ. Second, the limiting value $\Theta^{(\mathrm{sp,sp})}(0)$ reproduces the expansion of the Casimir amplitude to order $\epsilon^{3/2}$,

$$\Delta_C^{(\mathrm{sp,sp})} = -\frac{n\pi^2}{1440} + \frac{n\pi^2\epsilon}{2880}\left[1 - C_E - \ln(4\pi) + \frac{2\zeta'(4)}{\zeta(4)}\right.$$
$$\left. + \frac{5}{2}\frac{n+2}{n+8}\right] - \frac{n\pi^2}{72\sqrt{6}}\left(\frac{n+2}{n+8}\right)^{3/2}\epsilon^{3/2} + O(\epsilon^2).$$

$$(4.60)$$

Third, the term linear in L that violates the limiting form (4.37) is of order $\epsilon^{3/2}$ rather than linear in ϵ. We have

$$\Theta^{(\mathrm{sp,sp})}(\mathsf{L}) \underset{\mathsf{L}\to 0}{\approx} \Delta_C^{(\mathrm{sp,sp})} + \frac{n\pi}{4\sqrt{6}}\left(\frac{n+2}{n+8}\right)^{3/2}\epsilon^{3/2}\mathsf{L} + O(\mathsf{L}^2).$$

$$(4.61)$$

Furthermore, the large-L behavior still is in accordance with Eq. (4.43) in the sense that the differences are of higher than first order in ϵ. However, as already mentioned, it would lead to extrapolations to $d=3$ that grow $\sim\mathsf{L}$ in the limit $\mathsf{L}\to\infty$ unless contributions of the form $\sim O(\epsilon^2)\mathsf{L}+O(\epsilon^3)\mathsf{L}^0$ are subtracted.

In Fig. 8, we have plotted the extrapolated scaling function $\Theta^{(\mathrm{sp,sp})}(\mathsf{L})$ one obtains from Eqs. (4.47), (4.50), (4.53), and (4.56) upon setting $\epsilon=1$, together with its analog (labeled KD) implied by the ϵ-expansion result. The former function is depicted only for values L below the lower

threshold $\simeq 0.42$ beyond which the extrapolated scaling function $\mathsf{R}^{(\mathrm{sp,sp})}$ of the inverse susceptibility becomes negative. We have refrained from displaying it (or appropriate modifications of it) for values larger than the upper positivity threshold $\simeq 0.93$. In view of the $O(\epsilon^2)$ corrections the result would require for large L to ensure its decay for $\mathsf{L}\to\infty$, we have no convincing reasons to expect such *ad hoc* modifications to yield much better results in this regime of L than the extrapolated ϵ expansion.

One might wonder whether the above problems could be avoided by a different choice of the free propagator G_φ in Eq. (4.22). For example, one might want to use one whose mass parameter is simply the sum of the free contribution $\mathring{\tau}$ and the first-order perturbative correction (3.20). We have, in fact, explored this possibility. It yields a modified scaling function $\widetilde{\Theta}^{(\mathrm{sp,sp})}(\mathsf{L})$, whose large-$\mathsf{L}$ behavior must be corrected by $O(\epsilon^2)$ contributions to avoid unacceptable divergences. Once this is done, its extrapolation to $\epsilon=1$ gives real values for all L. We refrain from displaying the results because we consider them unsatisfactory for two reasons. First of all, as explained before Eq. (4.22), we believe that the use of the inverse finite-size susceptibility r_L^{-1} as mass parameter is the more natural choice. Second, the fact that one is able to produce a well-defined extrapolated scaling function $\widetilde{\Theta}^{(\mathrm{sp,sp})}(\mathsf{L})$ does not cure the problem that the $O(\epsilon)$ result for the scaling function $\mathsf{R}^{(\mathrm{sp,sp})}(\mathsf{L})$ of r_L becomes negative when extrapolated to $\epsilon=1$. Convincing improvements should yield meaningful extrapolation results for both the scaling function $\Theta^{(\mathrm{sp,sp})}(\mathsf{L})$ and r_L within one and the same consistent approximation scheme. Evidently, further work is necessary to improve on the present unsatisfactory state of these results for sp-sp boundary conditions.

On the other hand, the behavior of our results at small L may be expected to be superior to those based on the ϵ expansion. One indication is that, in the case of periodic boundary conditions, our results are in conformity with the exact solution in the large-n limit (see Sec. V).

V. COMPARISON WITH SPHERICAL-MODEL RESULTS FOR PERIODIC BOUNDARY CONDITIONS

As is well known, for translation invariant systems, results that are exact in the limit $n\to\infty$ can be obtained from the exact solution of spherical models.[48] The self-consistent equations from which the scaling function $\Theta_{\mathrm{SM}}^{(\mathrm{per})}(\mathsf{L})$ for the spherical model with periodic boundary conditions must be determined can be found in the literature.[5,20–22] Our aim here is to verify the consistency of our results for periodic boundary conditions with the exact solution of the spherical model for $2<d=4-\epsilon<4$. Making an analogous check for $\wp=(\mathrm{sp,sp})$ is a much harder challenge and will not be attempted here. The reason is that the presence of surfaces, in general, destroys translation invariance perpendicular to the boundary planes. The large-n limit of n-vector models on slabs with two parallel boundary planes $\mathfrak{B}_1$ and $\mathfrak{B}_2$ is known to correspond to a modified spherical model involving separate constraints on the sums $\Sigma_{j\in\mathrm{layer}\ z}S_j^2$ of the squares of the spin variables for each layer z.[49] The resulting self-consistent

equations, while not difficult to determine, involve a z-dependent self-consistent pair interaction and so far have not been solved analytically.

The exact solution for the spherical-model scaling function $\Theta_{SM}^{(per)}(L) = \lim_{n \to \infty} \Theta^{(per)}(L)/n$ may be gleaned from Ref. 21, where this function was denoted as Y_0. It is given by

$$\Theta_{SM}^{(per)}(L) = \frac{A_d}{2} L^{d-2}(R_0 - L^2) - \frac{A_d}{d}(R_0^{d/2} - L^d) - \frac{4\pi Q_{d+2,2}(R_0)}{R_0},$$

(5.1)

where $R_0 = L^2 R_{SM}^{(per)}(L)$ is a solution to

$$\frac{2Q_{d,2}(R_0)}{R_0} = A_d(R_0^{(d-2)/2} - L^{d-2}).$$

(5.2)

The latter equation is easily solved for small ϵ. Since A_d has a pole $\propto \epsilon^{-1}$, the left-hand side starts to contribute at $O(\epsilon)$. One obtains

$$R_0(L) = L^2 + \epsilon \frac{16\pi^2 Q_{4,2}(L^2)}{L^2} + o(\epsilon),$$

(5.3)

which becomes

$$R_0(0) = \epsilon \frac{2}{3}\pi^2 + o(\epsilon)$$

(5.4)

at the bulk critical point. Comparison of these results with ours for $L^2 R_{SM}^{(per)}(L)$ contained in Eqs. (4.46) and (4.48) shows that the latter reduce to them in the limit $n \to \infty$.

Turning to $\Theta_{SM}^{(per)}(L)$, we note that according to the representation (C9) of $Q_{d+2,2}$, two contributions in Eq. (5.1) can be combined as

$$\frac{-A_d}{d} R_0^{d/2} - \frac{4\pi Q_{d+2,2}(R_0)}{R_0}$$

$$= \frac{-A_{d-1}}{d-1} R_0^{(d-1)/2} - \sum_{k=0}^{\infty} \frac{a_k(d)}{k!}(-R_0)^k,$$

(5.5)

where

$$a_k(d) = \frac{\pi^{(d-1)/2}}{(2\pi)^{2k}} \Gamma\left[k + \frac{1-d}{2}\right] \zeta(1 - d + 2k).$$

(5.6)

Except for $a_2(d)$, which has a simple pole at $d=4$, the coefficients $a_k(d)$ are regular at $d=4$. We, therefore, separate the contribution from the first term in the second line of Eq. (5.5)

$$\frac{-A_{d-1}}{d-1} R_0^{(d-1)/2} = \frac{-1}{12\pi}\left[L^2 + \epsilon \frac{16\pi^2 Q_{4,2}(L^2)}{L^2}\right]^{3/2} + o(\epsilon^{3/2}),$$

(5.7)

where we substituted R_0 by its expansion (5.3), and then expand the remaining contributions to $\Theta_{SM}^{(per)}(L)$ in powers of ϵ. This gives

$$\Theta_{SM}^{(per)}(L) = \frac{-1}{12\pi}\left[L^2 + \epsilon \frac{16\pi^2 Q_{4,2}(L^2)}{L^2}\right]^{3/2} + \frac{L^3}{12\pi}$$

$$- \frac{4\pi[Q_{6,2}(L^2) - \epsilon R_{6,2}(L^2)]}{L^2} + \epsilon \frac{8\pi^2 Q_{4,2}(L^2)}{L^2}$$

$$\times \left[\frac{L}{4\pi} + \frac{Q_{4,2}(L^2)}{L^2}\right] + o(\epsilon^{3/2}).$$

(5.8)

The result agrees with the one for $\Theta^{(per)}(L)/n$ given in Eq. (4.57) if the factor $(n+2)/(n+8)$ is replaced by its large-n limit (=1). In particular, its value at $L=0$,

$$\Theta_{SM}^{(per)}(0) = -\frac{\pi^2}{90} + \frac{\pi^2}{180}\left[\frac{7}{2} - C_E - \ln \pi + \frac{2\zeta'(4)}{\zeta(4)}\right]\epsilon - \frac{\pi^2}{9\sqrt{6}}\epsilon^{3/2}$$

$$+ O(\epsilon^2),$$

(5.9)

coincides with the limit $\lim_{n \to \infty} \Delta_C^{(per)}/n$ of the expansion (4.58). The same holds for the coefficient of the term linear in L, for which we find

$$\left.\frac{d\Theta_{SM}^{(per)}(L)}{dL}\right|_{L=0} = \frac{\pi}{2\sqrt{6}}\epsilon^{3/2} + o(\epsilon^{3/2}),$$

(5.10)

which is consistent with Eq. (4.59).

VI. SUMMARY AND CONCLUDING REMARKS

In this paper, we have reconsidered the use of renormalized field theory near the upper critical bulk dimension $d^* = 4$ to the study of finite-size scaling in slabs of finite thickness and the thermodynamic Casimir effect. In a previous work,[19] it had become clear that in those cases where the boundary conditions involve zero modes in Landau theory at the bulk critical point, the conventional RG-improved perturbation theory based on the ϵ expansion becomes ill-defined at $T_{c,\infty}$ due to infrared singularities. This could be remedied by means of a reorganization of field theory, which revealed that noninteger powers such as $\epsilon^{3/2}$ appear in the small-ϵ expansion.

Our main aim here was to examine how the calculation of scaling functions describing the large length-scale behavior of the residual free energy and the Casimir force near the bulk critical point can be reconciled with these findings, so that the results of Ref. 19 for $T = T_{c,\infty}$ are recovered in the appropriate limit.

We were able to show that consistent scaling functions can, indeed, be obtained both for the case of periodic and sp-sp boundary conditions. It became clear that the ill-definedness of the conventional ϵ-expansion theory due to zero modes manifests itself already at two-loop order inasmuch as contributions found at this order were found to have no power-series expansion in ϵ at $T_{c,\infty}$ since they vary $\sim \epsilon^{3/2}$.

In calculations of crossover scaling functions by means of RG-improved perturbation theory near an upper critical dimension, one usually is faced with the following problem. The RG commonly achieves the proper exponentiation of the infrared singularities only at the unstable fixed point. However, it does not normally do this—at least, not

automatically—for the modified singularities that occur as the scaled crossover variable becomes large. Knowledge about the corresponding asymptotic behavior frequently is obtained from other sources, such as RG analyses of a different model or fixed point, or short-distance expansion. Representative examples are the calculation of the two-point correlation function,[50] the crossover at a bicritical point,[51,52] and the crossover from critical to Goldstone-mode behavior in isotropic ferromagnets.[53,54] To obtain and verify the correct singularities of the behavior to which the crossover occurs by means of the ϵ expansion, it must be supplemented by appropriate assumptions, or preferably knowledge, about the respective asymptotic forms. In some cases, it has even been possible to design RG procedures that yield the correct asymptotic behaviors at both the unstable fixed point as well as the stable one to which the crossover occurs,[52,54] albeit with somewhat limited range of applicability and success.

Similar problems evidently had to be expected in the study of the problems considered here—finite-size effects and thermodynamic Casimir forces. However, the challenges are actually greater and the difficulties more severe. Ideally, one would like to have a theory that has the power to correctly treat the infrared singularities at both the bulk critical point as well as the film critical point and, moreover, is capable of handling the corresponding dimensional crossover. For reasons discussed at the end of Sec. III, such ambitious goals would be unrealistic for a theory based on an expansion about the upper critical dimension. We, therefore, set out to reach more modest goals, namely, to modify and correct the previous theory by an appropriate treatment of the zero mode in such a way that (i) RG-improved perturbation theory becomes well defined for temperatures $T \gtrsim T_{c,\infty}$, (ii) reasonable scaling functions result, whose limiting behavior complies with the theory's predictions directly at $T_{c,\infty}$ and can be extrapolated to $d=3$ dimensions, and (iii) hence, bring it into a state comparable to the one it has for the nonzero-mode boundary conditions $\wp=$ap, (D,D), and (D,sp).

We feel that, on the whole, our results are encouraging, in particular, for the case of periodic boundary conditions, where besides achieving (i)–(iii), we were able to demonstrate consistency with the exact large-n solution. Moreover, the scaling function obtained by extrapolation to $d=3$, at least in the one-component case, appears to agree reasonably well with Monte Carlo results.[25,26]

The case of sp-sp boundary conditions turned out to be more delicate. First of all, we found that the one-loop expression for the scaling function $\mathsf{R}^{(\mathrm{sp},\mathrm{sp})}(\mathsf{L})$ of the inverse finite-size susceptibility becomes negative in a small regime of $\mathsf{L} = L/\xi_\infty$ when ϵ exceeds the value $\simeq 0.8265$ (see Figs. 4 and 5). This tells us that all extrapolations of free-energy scaling functions and Casimir forces to $d=3$ based on approximations which yield the same one-loop scaling function $\mathsf{R}^{(\mathrm{sp},\mathrm{sp})}(\mathsf{L})$ are questionable, at least in the regime where the positivity condition $\mathsf{R}^{(\mathrm{sp},\mathrm{sp})}(\mathsf{L}) \geq 0$ is violated. This applies both to KD's original extrapolation and ours (see Fig. 8).

Our investigation of this case also revealed another problem: Perturbative RG calculations do not necessarily yield the correct asymptotic large-L behavior, at least not automatically. This applies even for the conventional ϵ expansion in cases where no zero mode is present inasmuch as the

algebraic prefactors $\sim \mathsf{L}^{(d-1)/2}$ appearing in the asymptotic exponential behaviors of $\Theta^{(\mathrm{per})}(\mathsf{L})$ and $\Theta^{(\mathrm{sp},\mathrm{sp})}(\mathsf{L})$ given in Eqs. (4.42) and (4.43), respectively, are obtained only in ϵ-expanded form. However, it is more troublesome in the cases studied here, especially, for $\wp = (\mathrm{sp},\mathrm{sp})$. The reason may be understood as follows. On the one hand, we encountered powers of inverse finite-size susceptibilities we had to retain to ensure consistency with the behavior at $T_{c,\infty}$. On the other hand, by expanding other contributions in ϵ, L-dependent terms of order ϵ^2 and higher are dropped, which may be needed to cancel similar L-dependent contributions originating from the unexpanded powers of R in order to avoid incorrect or even divergent large-L behavior of the scaling functions.

A qualitative difference between periodic and sp-sp boundary conditions is that the latter involve, even in the semi-infinite case $L=\infty$, both d- and $(d-1)$-dimensional critical behaviors, rather than just a dimensional crossover. With hindsight, it is, therefore, perhaps not too surprising that the latter turned out to be the more difficult case.

As remarked earlier, special surface transitions are expected to occur in three bulk dimensions only in the $n=1$ case. When $n>1$, anisotropic special transitions should be possible if the continuous $O(n)$ symmetry is broken by an appropriate easy-axis spin anisotropy at the surface.[45–47] This is because surface phases with long-range order should not be thermodynamically stable at temperatures $T>T_{c,\infty}$, by analogy with the Mermin-Wagner theorem.[55] However, the $O(2)$ case is exceptional in that a surface phase with quasi-long-range order should be possible. In fact, recent Monte Carlo work[56,57] indicated that the surface phase transition is of Kosterlitz-Thouless type. Thus, a multicritical surface-bulk point at which the line of these surface transitions reaches $T_{c,\infty}$ should exist as well,[12] and was reported to be found in the cited Monte Carlo analyses.

Since the lambda transition of helium involves a (real-valued) two-component order parameter, this $O(2)$ case is of potential relevance for Casimir forces in confined liquid He. In the case of ^{3}He-^{4}He mixtures in contact with a substrate (see, e.g., Refs. 58 and 59), ^{4}He usually gets enriched near the wall and a superfluid surface film may form there. Since order-parameter correlations decay algebraically in it, the bulk transition in the presence of such a critical surface phase is reminiscent of the special transition. Whether the central issue we were concerned with in this work—the presence of zero modes in Landau theory—arises also in the study of the thermodynamic Casimir effect in such systems and what its consequences are remain to be seen. A proper analysis of this question requires generalizations of our model. To describe mixtures, a second density besides the order parameter is needed. In addition, care must be taken to ensure a proper description of the Kosterlitz-Thouless-type surface transition.

The present work suggests extensions and complementary work along several lines. The situation in the case of sp-sp boundary conditions is rather unsatisfactory. To improve it, it would be desirable to extend our analysis by allowing the surface enhancement variables c_j to vary. In fact, in order to clarify the effects of finite size on the phase diagram, and, in

turn, resolve the issue in which range of parameters the disordered state is thermodynamically stable, such a generalization appears to be unavoidable. Another appealing aspect of it would be that by varying the c_j, one could smoothly interpolate between the boundary conditions $\wp = (D,D)$, (D,sp), and $(\mathrm{sp},\mathrm{sp})$.

In view of the great technical and conceptual difficulties one is faced with in such analytical approaches, we believe that careful checks of their predictions by alternative means such as Monte Carlo simulations are absolutely necessary. For a long time, detailed studies of the thermodynamic Casimir effect by this method existed only for the case of periodic boundary conditions.[3,23,60] However, recently, new simulation strategies for investigating this effect in lattice spin systems with free boundary conditions have been developed.[24–26] As a result, systematic numerical studies of the thermodynamic Casimir effect under all sorts of interesting boundary conditions have become possible.

On the side of analytical theories, it would be interesting to explore whether the present approach can be combined with existing RG approaches at fixed dimension d for the study of bulk and surface critical phenomena.[28–30,61] Another important challenge is to develop reliable analytical approaches by which the Casimir effect can be investigated below the bulk and film critical temperatures. Recent investigations of the ordered phase based on Landau theory or RG-improved Landau theory[62,63] certainly should not remain the final word since they fail to give correct descriptions of the critical behavior at both the bulk critical point as well as at eventual film critical points. In addition, they are known to be sometimes even qualitatively wrong inasmuch as they may predict phases with long-range order that can be shown to be destroyed by thermal fluctuations.

APPENDIX A: COMPUTATION OF REQUIRED INTEGRALS

The one- and two-loop Feynman integrals for $f_\psi^{(\wp)}$ involve the free ψ propagator (3.13) at coincident points $\boldsymbol{x} = \boldsymbol{x}'$. Substitution of the eigenfunctions (3.3) and (3.4) into Eq. (3.13) yields

$$G_{L,\psi}^{(\mathrm{per})}(\boldsymbol{x};\boldsymbol{x}|\mathring{\tau}) = \frac{2}{L}\int_{\boldsymbol{p}}^{(d-1)}\sum_{m=1}^{\infty}\frac{1}{p^2 + (2\pi m/L)^2 + \mathring{\tau}} \quad (\text{A1})$$

and

$$G_{L,\psi}^{(\mathrm{sp,sp})}(\boldsymbol{x};\boldsymbol{x}|\mathring{\tau}) = \frac{2}{L}\int_{\boldsymbol{p}}^{(d-1)}\sum_{m=1}^{\infty}\frac{\cos^2(\pi m z/L)}{p^2 + (\pi m/L)^2 + \mathring{\tau}}. \quad (\text{A2})$$

In order to compute the integrals $I_1^{(\wp)}(L;\mathring{\tau})$ introduced in Eq. (3.19), we add and subtract a summand with $m=0$ and then use Poisson's summation formula [see, e.g., Eq. (4.8.28) in Ref. 64]

$$\sum_{m=-\infty}^{\infty}f(am) = \sum_{j=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dt}{a}\,f(t)\,e^{2\pi i jt/a}. \quad (\text{A3})$$

Recalling the definition (3.24) of the functions $Q_{d,\sigma}$ and performing the required momentum integrals, one arrives at the results for $I_1^{(\mathrm{per})}(L;\mathring{\tau})$ and $I_1^{(\mathrm{sp,sp})}(L;\mathring{\tau})$ given in Eqs. (3.21) and (3.22).

Turning to the calculation of $I_2^{(\wp)}(L;\mathring{\tau})$, we note that for $\wp = \mathrm{per}$ we have

$$I_2^{(\mathrm{per})}(L;\mathring{\tau}) = [I_1^{(\mathrm{per})}(L;\mathring{\tau})]^2 \quad (\text{A4})$$

as a consequence of translation invariance along the z direction.

To compute $I_2^{(\mathrm{sp,sp})}$, we use the representation

$$\begin{aligned}I_2^{(\mathrm{sp,sp})}(L;\mathring{\tau}) &= \int_0^L\frac{dz}{L}[G_{L,\psi}^{(\mathrm{sp,sp})}(\boldsymbol{x};\boldsymbol{x}|\mathring{\tau})]^2 \\ &= \sum_{m,m'=1}^{\infty}\int_{\boldsymbol{p}_1}^{(d-1)}\int_{\boldsymbol{p}_2}^{(d-1)}\frac{4}{L^2}\int_0^L\frac{dz}{L} \\ &\quad \times \frac{\cos^2(k_m z)\cos^2(k_{m'}z)}{(p_1^2 + k_m^2 + \mathring{\tau})(p_2^2 + k_{m'}^2 + \mathring{\tau})}\end{aligned} \quad (\text{A5})$$

and the fact that

$$4\int_0^L\frac{dz}{L}\cos^2(k_m z)\cos^2(k_{m'}z) = 1 + \frac{1}{2}\delta_{mm'}, \quad (\text{A6})$$

for $k_m = m\pi/L$ and $m,m' \neq 0$. Upon inserting the latter result into Eq. (A5), one arrives at

$$I_2^{(\mathrm{sp,sp})}(L;\mathring{\tau}) = [I_1^{(\mathrm{sp,sp})}(L;\mathring{\tau})]^2 + \frac{1}{2L^2}A_{d-1}^2\sum_{m=1}^{\infty}(k_m^2 + \mathring{\tau})^{d-3}, \quad (\text{A7})$$

where A_d was defined in Eq. (3.23).

In order to evaluate the second term on the right-hand side of this equation, we employ the analytical continuation of the Epstein-Hurwitz zeta function discussed in Appendix A of Ref. 65, namely,

$$\sum_{j=1}^{\infty} (j^2 + \alpha^2)^{-s} = -\frac{1}{2\alpha^{2s}} + \frac{\sqrt{\pi}}{2\alpha^{2s-1}\Gamma(s)} \Bigg[\Gamma(s-1/2)$$

$$+ \frac{4}{(\pi\alpha)^{(1-2s)/2}} \sum_{m=1}^{\infty} m^{s-1/2} K_{(1-2s)/2}(2\pi m \alpha) \Bigg],$$

$$s \neq \frac{1}{2}. \tag{A8}$$

A straightforward calculation then yields

$$I_2^{(\mathrm{sp,sp})}(L;\mathring{\tau}) = [I_1^{(\mathrm{sp,sp})}(L;\mathring{\tau})]^2 + \frac{B_d}{L}\Bigg[\frac{A_{2d-4}}{2L}\mathring{\tau}^{d-3} - A_{2d-3}\mathring{\tau}^{d-5/2}$$

$$+ \frac{Q_{2d-3,2}(4\mathring{\tau}L^2)}{2^{2d-4}\mathring{\tau}L^{2d-3}} \Bigg], \tag{A9}$$

with

$$B_d = \frac{\pi}{8\Gamma(3-d)\Gamma^2[(d-1)/2]\cos^2(d\pi/2)}. \tag{A10}$$

Aside from $I_j^{(\wp)}(L;\mathring{\tau})$ ($j=1$ and 2), we also need to calculate the integrals $J^{(\wp)}(L;\mathring{\tau})$ introduced in Eq. (4.6) for $\wp$ = per and $\wp = (\mathrm{sp,sp})$. To this end, we insert our above results for $I_1^{(\wp)}$ into Eq. (4.6) and use the property (4.17), obtaining

$$J^{(\mathrm{per})}(L;\mathring{\tau}) = \frac{2}{L}\frac{A_{d-1}}{d-1}\mathring{\tau}^{(d-1)/2} - \frac{2A_d}{d}\mathring{\tau}^{d/2}$$

$$- \left(1 - \lim_{\mathring{\tau}\to 0}\right)\frac{8\pi Q_{d+2,2}(\mathring{\tau}L^2)}{\mathring{\tau}L^{d+2}} \tag{A11}$$

and

$$J^{(\mathrm{sp,sp})}(L;\mathring{\tau}) = J^{(\mathrm{per})}(2L;\mathring{\tau}). \tag{A12}$$

The $\mathring{\tau}\to 0$ limit on the right-hand side can be evaluated in a straightforward fashion with the aid of the representation

$$Q_{d,2}(r) = \frac{r^{(d+2)/4}}{(2\pi)^{d/2}} \sum_{j=1}^{\infty} \frac{K_{(d-2)/2}(j\sqrt{r})}{j^{(d-2)/2}}, \tag{A13}$$

for $d\to d+2$, where $K_\nu(x)$ is a modified Bessel function of the second kind, and their well-known asymptotic behavior

$$K_\nu(x) \underset{x\to 0}{=} 2^{\nu-1}\Gamma(\nu)x^{-\nu} + O(x^{2-\nu}) \tag{A14}$$

for $\nu > 0$ [see, e.g., Eq. (8.446) of Ref. 66].

The result

$$\lim_{r\to 0} \frac{8\pi Q_{d+2,2}(r)}{r} = 2\pi^{-d/2}\Gamma\left(\frac{d}{2}\right)\zeta(d) \tag{A15}$$

can be expressed in terms of either one of the one-loop Casimir amplitude $\Delta_{C,[1]}^{(\wp)}$ given in Eq. (4.7). Inserting it into Eqs. (A11) and (A12) finally gives

$$J^{(\mathrm{per})}(L;\mathring{\tau}) = -\frac{2\Delta_{C,[1]}^{(\mathrm{per})}}{nL^d} + \frac{2}{L}\frac{A_{d-1}}{d-1}\mathring{\tau}^{(d-1)/2} - \frac{2A_d}{d}\mathring{\tau}^{d/2}$$

$$- \frac{8\pi Q_{d+2,2}(\mathring{\tau}L^2)}{\mathring{\tau}L^{d+2}} \tag{A16}$$

and

$$J^{(\mathrm{sp,sp})}(L;\mathring{\tau}) = -\frac{2\Delta_{C,[1]}^{(\mathrm{sp,sp})}}{nL^d} + \frac{1}{L}\frac{A_{d-1}}{d-1}\mathring{\tau}^{(d-1)/2} - \frac{2A_d}{d}\mathring{\tau}^{d/2}$$

$$- \frac{\pi Q_{d+2,2}(4\mathring{\tau}L^2)}{2^{d-1}\mathring{\tau}L^{d+2}}, \tag{A17}$$

respectively.

APPENDIX B: EVALUATION OF $f_{\psi,[1]}^{(\wp)}(L;0)$

In this appendix, we present the calculation of the one-loop free-energy contributions $f_{\psi,[1]}^{(\wp)}(L;\mathring{\tau})$ defined in Eq. (4.4) for $\mathring{\tau}=0$.

Upon applying Poisson's summation formula (A3), we obtain

$$f_{\psi,[1]}^{(\mathrm{per})}(L;0) = f_{\psi,0}^{(\mathrm{per})} + nL\sum_{j=1}^{\infty} \int_{q=(p,k)}^{(d)} \cos(kjL)\ln q^2 \tag{B1}$$

and

$$f_{\psi,[1]}^{(\mathrm{sp,sp})}(L;0) = f_{\psi,0}^{(\mathrm{sp,sp})} + nL\sum_{j=1}^{\infty} \int_{q=(p,k)}^{(d)} \cos(2kjL)\ln q^2, \tag{B2}$$

where

$$f_{\psi,0}^{(\wp)} = Lf_{b,0} + f_{\psi,s,0}^{(\wp)} \tag{B3}$$

with

$$f_{b,0} = \frac{n}{2}\int_q^{(d)} \ln q^2 \tag{B4}$$

and

$$f_{\psi,s,0}^{(\mathrm{per})} = 2f_{\psi,s,0}^{(\mathrm{sp,sp})} = -\frac{n}{2}\int_p^{(d-1)} \ln p^2. \tag{B5}$$

The expressions (B1) and (B2) can be evaluated along lines similar to those followed in Sec. V of Ref. 8. This gives

$$nL\sum_{j=1}^{\infty} \int_{q=(p,k)}^{(d)} \cos(kjL)\ln q^2 = L^{-(d-1)}\Delta_{C,[1]}^{(\mathrm{per})} \tag{B6}$$

and

$$nL\sum_{j=1}^{\infty} \int_{q=(p,k)}^{(d)} \cos(2kjL)\ln q^2 = L^{-(d-1)}\Delta_{C,[1]}^{(\mathrm{sp,sp})}, \tag{B7}$$

where $\Delta_{C,[1]}^{(\wp)}$ are the one-loop Casimir amplitudes of Eq. (4.7).

APPENDIX C: SERIES REPRESENTATIONS OF THE FUNCTIONS $Q_{d,\sigma}(r)$

In this appendix, we wish to derive representations of the functions $Q_{d,\sigma}(r)$ as generalized power series and to establish their relation (3.26) with the functions $g_{a,b}(z)$ utilized by KD.

Let us define the integral

$$I_{d,\sigma}(k,y) = K_{d-1} \int_0^\infty dp \, p^{d-2} \frac{(k^2 + p^2)^{(\sigma-2)/2}}{y + k^2 + p^2}, \quad \text{(C1)}$$

where K_d denotes the usual factor

$$K_d \equiv \int_q^{(d)} \delta(|q| - 1) = \frac{2^{1-d} \pi^{-d/2}}{\Gamma(d/2)}. \quad \text{(C2)}$$

Then the right-hand side of Eq. (3.24) can be written as

$$Q_{d,\sigma}(r) = \frac{r}{2} \left\{ \left[I_{d,\sigma}(0,1) - I_{d+1,\sigma}(0,1) \sqrt{r} \right] r^{(d+\sigma-5)/2} + \sum_{k \neq 0} I_{d,\sigma}(k,r) \right\}, \quad \text{(C3)}$$

where here and below the summation $\Sigma_{k \neq 0}$ extends over all nonzero $k \in 2\pi\mathbb{Z}$.

When $k=0$, the evaluation of the integral $I_{d,\sigma}(k,r)$ is straightforward, giving

$$I_{d,\sigma}(0,r) = \frac{2^{1-d} \pi^{(3-d)/2} r^{(d+\sigma-5)/2}}{\Gamma[(d-1)/2] \cos[\pi(d+\sigma)/2]}. \quad \text{(C4)}$$

In the case of nonzero values of k, we Taylor expand in r about $r=0$ to obtain

$$I_{d,\sigma}(k,r) = \sum_{j=0}^\infty I_{d,\sigma}^{(0,j)}(k,0) \frac{r^j}{j!}, \quad \text{(C5)}$$

where the required partial derivatives $I_{d,\sigma}^{(0,j)}(k,r) = \partial^j I_{d,\sigma}(k,r)/\partial r^j$ at $r=0$ are given by

$$I_{d,\sigma}^{(0,j)}(k,0) = \frac{(-1)^j \Gamma(j+1) \Gamma[j + (5-d-\sigma)/2]}{(4\pi)^{(d-1)/2} |k|^{2j+5-d-\sigma} \Gamma(j+2-\sigma/2)}. \quad \text{(C6)}$$

We now substitute the Taylor series (C5) into Eq. (C3) and interchange the summations over j and k in the last term. Recalling the series expansion

$$\zeta(s) = \sum_{n=1}^\infty \frac{1}{n^s} \quad \text{(C7)}$$

of Riemann's zeta function, one can perform the k summations analytically to obtain

$$\sum_{k \neq 0} I_{d,\sigma}^{(0,j)}(k,0) = 2 I_{d,\sigma}^{(0,j)}(2\pi,0) \zeta(2j+5-d-\sigma). \quad \text{(C8)}$$

Using this result together with Eq. (C4), one arrives at the representation

$$Q_{d,\sigma}(r) = \frac{2^{-d} \pi^{(3-d)/2}}{\Gamma[(d-1)/2] \cos[\pi(d+\sigma)/2]} r^{(d+\sigma-3)/2}$$
$$+ \frac{2^{-d-1} \pi^{1-d/2}}{\Gamma(d/2) \sin[\pi(d+\sigma)/2]} r^{(d+\sigma-2)/2} - \pi^{(d-1)/2}$$
$$\times \sum_{j=1}^\infty \left[\frac{\Gamma[j + (3-d-\sigma)/2]}{\Gamma(j+1-\sigma/2)} \frac{\zeta(2j+3-d-\sigma)}{(2\pi)^{2j-\sigma+2}} (-r)^j \right]. \quad \text{(C9)}$$

For general values of d and σ, the first two terms on the right-hand side of Eq. (C9) have branch-cut singularities. Cauchy's ratio test shows that the remaining power series (third term) is absolutely convergent for complex y inside a circle of radius $(2\pi)^2$.

As is known from Ref. 21, functions $Q_{d,\sigma}$ with noninteger values of σ are encountered in the study of finite-size effects of systems with long-range interactions. From the series expansion (C9), the asymptotic behavior of the functions $Q_{d,\sigma}(r)$ as $r \to 0$ can be read off easily even for such general values of σ. This representation may, of course, also be employed to compute the functions $Q_{d,\sigma}(r)$ by numerical means for values of r inside the radius of convergence of the series.

To establish the relation (3.26) between $Q_{d,\sigma}$ and the functions $g_{a,0}(z)$ [cf. Eq. (3.25)] employed by KD, it is convenient to use the expansion (A13). Substituting the Bessel functions in it by their integral representation

$$K_\nu(z) = \frac{(z/2)^\nu \sqrt{\pi}}{\Gamma(\nu + \frac{1}{2})} \int_1^\infty dt \, (t^2 - 1)^{\nu-1/2} e^{-zt} \quad \text{(C10)}$$

and interchanging the integration with the summation over j immediately gives Eq. (3.26).

APPENDIX D: NUMERICAL RESULTS FOR AND PROPERTIES OF THE REQUIRED FUNCTIONS $Q_{d,\sigma}(r)$

In the present work, only functions $Q_{d,\sigma}(r)$ with the special value $\sigma=2$ are needed. The purpose of the present appendix is to present numerical results for these functions.

The expansion (A13) of these functions in terms of modified Bessel functions lends itself well to numerical evaluation. Figure 9 shows plots of the functions $Q_{4,2}(r)$ and $Q_{6,2}(r)$, which were numerically determined via this representation.

The function $R_{d,2}(r)$ has an expansion in modified Bessel functions analogous to Eq. (A13), which follows from it by differentiation with respect to d. Using it we have determined $R_{6,2}(r)$ by numerical evaluation. The result is depicted in Fig. 10.

The asymptotic small-r forms of these functions can be determined in a straightforward fashion from the representation (C9). One obtains

$$\frac{Q_{4,2}(r)}{r} \underset{r \to 0}{=} \frac{1}{24} - \frac{\sqrt{r}}{8\pi} - \frac{r \ln r}{32\pi^2} + \frac{1 - 2C_E + 2\ln(4\pi)}{32\pi^2} r$$
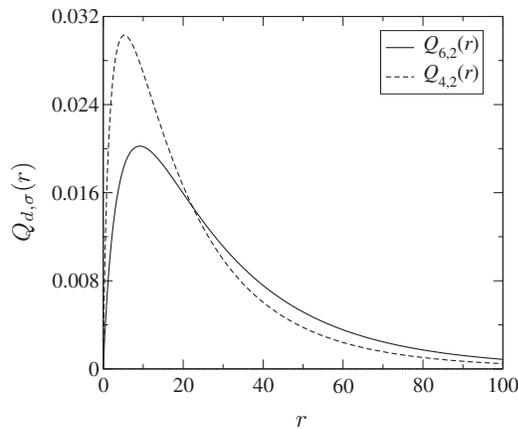$$+ \frac{\zeta(3)}{256\pi^4} r^2 - \frac{\zeta(5)}{2048\pi^6} r^3 + O(r^4), \quad \text{(D1)}$$

FIG. 9. Plots of the functions $Q_{4,2}(r)$ and $Q_{6,2}(r)$, obtained by numerical evaluation of the series expansion (A13).

$$\frac{Q_{6,2}(r)}{r} \underset{r\to 0}{=} \frac{\pi}{360} - \frac{r}{96\pi} + \frac{r^{3/2}}{48\pi^2} + \frac{r^2 \ln r}{256\pi^3}$$
$$- \frac{3/2 - 2C_E + 2\ln(4\pi)}{256\pi^3} r^2 + O(r^3), \quad \text{(D2)}$$

and

$$\frac{R_{6,2}(r)}{r} \underset{r\to 0}{=} \frac{C_E + \ln(4\pi) - 240\zeta'(-3) - 8/3}{720}\pi$$
$$- \frac{C_E - 2 + 24\zeta'(-1) + \ln(4\pi)}{192\pi} r$$
$$+ \frac{\ln(r/\pi) + C_E - 8/3}{96\pi^2} r^{3/2} + O(r^2 \ln^2 r). \quad \text{(D3)}$$

Their asymptotic forms for large values of r follow from [cf. Eq. (B33) of Ref. 21]
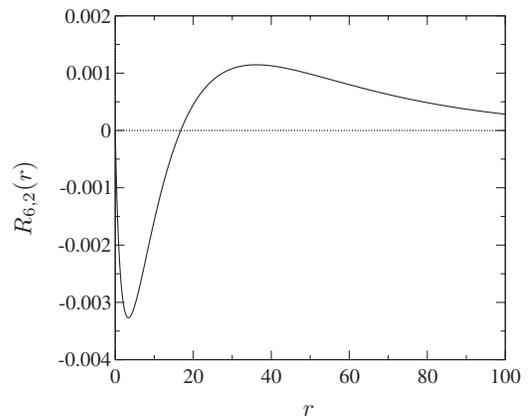

FIG. 10. Plot of the function $R_{6,2}(r)$ as numerically obtained from the series expansion that results from Eq. (A13) by differentiation with respect to d.

$$Q_{d,2}(r) \underset{r\to\infty}{=} \frac{r^{(d+1)/4}}{2(2\pi)^{(d-1)/2}} e^{-\sqrt{r}} [1 + O(r^{-1/2})], \quad \text{(D4)}$$

giving

$$\frac{Q_{4,2}(r)}{r} \underset{r\to\infty}{=} \frac{r^{1/4}}{2(2\pi)^{3/2}} e^{-\sqrt{r}} [1 + O(r^{-1/2})], \quad \text{(D5)}$$

$$\frac{Q_{6,2}(r)}{r} \underset{r\to\infty}{=} \frac{r^{3/4}}{2(2\pi)^{5/2}} e^{-\sqrt{r}} [1 + O(r^{-1/2})], \quad \text{(D6)}$$

and

$$\frac{R_{6,2}(r)}{r} \underset{r\to\infty}{=} \frac{r^{3/4}}{8(2\pi)^{5/2}} e^{-\sqrt{r}} \ln \frac{r}{4\pi^2} [1 + O(r^{-1/2})], \quad \text{(D7)}$$

respectively.

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[32] Our choice of additive counterterms differs from that of KD, who chose them L dependent, fixing them through normalization conditions for the L-dependent free energy. A second difference is that KD restricted themselves to the fixed-point values $c_j = 0$ and ∞, and, hence, did not take into account c-dependent additive surface counterterms.

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