

Excess free energy and Casimir forces in systems with long-range interactions of van der Waals type: General considerations and exact spherical-model results

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We consider systems confined to a d -dimensional slab of macroscopic lateral extension and finite thickness L that undergo a continuous bulk phase transition in the limit $L \rightarrow \infty$ and are describable by an $O(n)$ symmetrical Hamiltonian. Periodic boundary conditions are applied across the slab. We study the effects of long-range pair interactions whose potential decays as $b x^{-(d+\sigma)}$ as $x \rightarrow \infty$, with $2 < \sigma < 4$ and $2 < d + \sigma \leq 6$, on the Casimir effect at and near the bulk critical temperature $T_{c,\infty}$, for $2 < d < 4$. These interactions decay sufficiently fast to leave bulk critical exponents and other universal bulk quantities unchanged—i.e., they are irrelevant in the renormalization group (RG) sense. Yet they entail important modifications of the standard scaling behavior of the excess free energy and the Casimir force \mathcal{F}_C . We generalize the phenomenological scaling *Ansätze* for these quantities by incorporating these long-range interactions. For the scaled reduced Casimir force per unit cross-sectional area, we obtain the form $L^d \mathcal{F}_C / k_B T \approx \Xi_0(L/\xi_\infty) + g_\omega L^{-\omega} \Xi_\omega(L/\xi_\infty) + g_\sigma L^{-\omega_\sigma} \Xi_\sigma(L/\xi_\infty)$. Here Ξ_0 , Ξ_ω , and Ξ_σ are universal scaling functions; g_ω and g_σ are scaling fields associated with the leading corrections to scaling and those of the long-range interaction, respectively; ω and $\omega_\sigma = \sigma + \eta - 2$ are the associated correction-to-scaling exponents, where η denotes the standard bulk correlation exponent of the system without long-range interactions; ξ_∞ is the (second-moment) bulk correlation length (which itself involves corrections to scaling). The contribution $\propto g_\sigma$ decays for $T \neq T_{c,\infty}$ algebraically in L rather than exponentially, and hence becomes dominant in an appropriate regime of temperatures and L . We derive exact results for spherical and Gaussian models which confirm these findings. In the case $d + \sigma = 6$, which includes that of nonretarded van der Waals interactions in $d = 3$ dimensions, the power laws of the corrections to scaling proportional to b of the spherical model are found to get modified by logarithms. Using general RG ideas, we show that these logarithmic singularities originate from the degeneracy $\omega = \omega_\sigma = 4 - d$ that occurs for the spherical model when $d + \sigma = 6$, in conjunction with the b dependence of g_ω .

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I. INTRODUCTION

When macroscopic bodies are immersed into a medium, the forces acting between them in its absence are usually altered. Moreover, additional (effective) forces not present without the medium may be induced by fluctuations occurring in it. A well-known example of fluctuation-induced forces is the so-called *Casimir* force between metallic bodies, named after its discoverer Casimir [1], which is induced by vacuum fluctuations of the electromagnetic field and was recently verified through high-precision experiments [2,3].

Although the Casimir effect was well received at the time of its discovery, interest in it diminished soon afterward, and for a long time it did not attract much attention. Since approximately 1970 there has been a resurgence of interest in it, which has evolved into an enormous research activity during the past decades [4–13].

There are a number of good reasons for this development. To begin with, fluctuation-induced forces are ubiquitous in nature. Casimir's original work [1] was concerned with the force induced by vacuum fluctuations of the electromagnetic field. Subsequently it has been realized that analogous forces exist that are not mediated by massless particles such as photons, but are induced by low-energy excitations such as spin waves—or, more generally, Goldstone modes in systems with a spontaneously broken continuous symmetry—or ther-

mal fluctuations. Since Goldstone modes are massless, the associated fluctuations are scale invariant and induce a long-ranged Casimir force. The same applies to thermal fluctuations at critical points because of the divergence of the correlation length. The upshot is that Casimir forces have turned out to be of interest for many diverse fields of physics, such as quantum field theories [4–8], condensed matter physics, the physics of fluids and quantum fluids [9–11], wetting phenomena [14–16], microfluidics, and nanostructured materials [17].

Second, owing to the progress in experimental techniques made in recent years, detailed investigations of Casimir forces have become possible [2,3,18–23]. Third, a further important reason for the ongoing interest in Casimir forces is that they exhibit *universal* features: Microscopic details of both the fluctuating medium as well as the immersed macroscopic bodies do not normally matter, at least as long as long-range interactions are absent or may be safely ignored.

Last but not least, an equally important reason has been the theoretical progress in dealing with interacting field theories with boundaries that has been achieved since the 1980s [24–30]. This has led to detailed investigations of the Casimir effect for interacting field theories [13,28,31–35].

In this paper we will be concerned with the *thermodynamic Casimir effect*—i.e., the Casimir effect induced by *thermal fluctuations*. Our aim is to study the effects of long-

range interactions of van der Waals type on the Casimir force in systems undergoing a continuous bulk phase transition. To this end we shall consider long-range two-body interactions with a pair potential $v^{(\sigma)}(x)$ that behaves as

$$v^{(\sigma)}(x) \underset{x \rightarrow \infty}{\approx} \text{const} \times x^{-(d+\sigma)} \quad (1.1)$$

in the large-distance limit. The familiar dispersion forces in fluids belong to this category: Important examples are the nonretarded and retarded van der Waals interactions of a ($d=3$)-dimensional fluid, which correspond to the cases $\sigma=3$ and $\sigma=4$, respectively.

According to scaling considerations (to be recalled in Sec. II), the leading infrared singularities at the critical point of systems with short-range forces do not get modified by such long-range interactions because the associated pair potentials decay sufficiently fast at large distances. They are irrelevant in the renormalization group (RG) sense, giving corrections to the leading critical behavior. Long-range interactions of this kind have been termed “subleading long-range interactions” [36–39]. They are generically present in fluids [40–42] but occur also in other, for example, magnetic, systems.

For typical three-dimensional systems of the n -vector type with $n < \infty$, the associated correction-to-scaling exponent ω_σ is *larger* than the familiar exponent ω that governs the leading corrections to scaling (see, e.g., Ref. [43]). Hence such long-range interactions yield *next-to-leading* corrections to scaling.

Despite their irrelevance, they have important consequences, even for the near-critical behavior of bulk systems. Since they involve pair potentials that decrease as inverse powers of the distance x in the limit $x \rightarrow \infty$, the usual exponential large- x decay of correlations away from the critical point gets replaced by an algebraic one.

Their consequences for the medium-induced force between two macroscopic bodies immersed into the medium a distance L apart is of a similar kind and importance: They yield contributions that decay quite generally as an inverse power of L , irrespective of whether or not the temperature T is close to the bulk critical temperature $T_{c,\infty}$ of the medium. When $T \approx T_{c,\infty}$, they compete with the long-ranged Casimir force produced by critical or near-critical fluctuations. As previous work [36–39,44] suggests, and will be shown in detail below, they actually become the *dominant* part of the medium-induced force in a certain regime of temperatures and L .

We will consider the case of a slab geometry of cross-sectional area $A=L_\parallel^{d-1}$ and thickness L . Reliable results for this geometry are important for the interpretation of Monte Carlo simulations of appropriate models with subleading long-range interactions.

In view of our above remarks, a most obvious system class to consider would be fluids. To describe the long-distance physics of classical fluids near their liquid-gas critical point, a one-component order parameter is used. Instead of considering this case, we will focus our attention on systems that involve an n -component order parameter and can

be modeled by an $O(n)$ symmetrical Hamiltonian, and investigate them in the limit $n \rightarrow \infty$. For simplicity, we will restrict ourselves to the case of *periodic boundary conditions* along all—namely, both the perpendicular as well as the $d-1$ principal parallel—directions. Under these conditions, the large- n limit of the $O(n)$ model is equivalent to the spherical model [45–47]. We will present *exact* results for the Casimir force at and above the bulk critical temperature T_c , for both spherical and Gaussian models with subleading long-range interactions.

Our motivation for considering spherical models is twofold. First, studying the effects of such long-range interactions on the Casimir force for such models is an interesting problem in its own right. Second, the exact results obtained for these models provide nontrivial checks for the results of perturbative field-theoretic renormalization group approaches and are expected to give valuable guidance for acceptable approximations, an issue we plan to take up in a subsequent paper [48].

A special feature of the spherical model with $2 < d < 4$ is that the correction-to-scaling exponents ω_σ and ω become equal when $d+\sigma=6$, a condition satisfied, for example, for nonretarded van der Waals interactions in $d=3$ dimensions. As our exact results show, the corrections to scaling induced by the long-range interaction (1.1) then get modified by logarithms.

The remainder of this paper is organized as follows. In the next section, we provide the required background on Casimir forces. We begin by recalling the definition of the Casimir force. Then we discuss its scaling form when all interactions are short ranged, specify the form of the subleading long-range interactions to be considered, and recapitulate the scaling arguments which show that they do not modify the leading critical singularities. Next, we generalize the finite-size scaling *Ansatz* by incorporating them. In Sec. III we introduce the spherical model with subleading long-range interactions which we solve for $2 < d < 4$ to produce exact large- n results for the Casimir force. The finite-size behavior of the equation of state is analyzed in Sec. IV. Section V deals with the finite-size behavior of the free energy and the Casimir force. Section VI contains a brief summary and discussion. Finally, there are three Appendixes in which various technical details are explained.

II. BACKGROUND

A. Definition and scaling form of Casimir force

We consider a statistical mechanical system, a model magnet or fluid, whose shape is a d -dimensional slab of thickness L and hyperquadratic cross section with area $A=L_\parallel^{d-1}$. As previously mentioned, we choose periodic boundary conditions (BCs) along all d principal hypercubic axes, so that the system has the topology of a d -torus. Unless stated otherwise, the dimensionality d is presumed to satisfy $2 < d < 4$.

Let $F_{L,A}(T)$ be the total free energy of the system. Taking the thermodynamic limit $L_\parallel \rightarrow \infty$ at fixed $L < \infty$, we denote the reduced free energy per cross-sectional area A as $f_L(T)$

$\equiv \lim_{A \rightarrow \infty} F_{L,A}/Ak_B T$. For $L \rightarrow \infty$, $f_L(T)/L$ approaches $f_{\text{bk}}(T)$, the reduced bulk free energy density [49]. We therefore introduce the reduced excess free energy by

$$f_{\text{ex}}(T,L) = f_L(T) - Lf_{\text{bk}}(T). \quad (2.1)$$

The limit $L \rightarrow \infty$ of this quantity exists, but depends on the boundary conditions: for periodic boundary conditions and the film geometry with boundary planes \mathfrak{B}_1 and \mathfrak{B}_2 introduced above, we have [49]

$$f_{\text{ex}}(T,H,\infty) = \begin{cases} 0, & \text{periodic BCs,} \\ f_{s,1} + f_{s,2}, & \text{film geometry,} \end{cases} \quad (2.2)$$

where $f_{s,i}$, $i=1,2$, are the surface excess free energies of the respective semi-infinite systems bounded by \mathfrak{B}_i .

In either case, the thermodynamic Casimir force per unit area is defined in terms of f_{ex} as

$$\mathcal{F}_C(T,L) = -k_B T \frac{\partial f_{\text{ex}}(T,L)}{\partial L}. \quad (2.3)$$

According to this definition, this quantity is a generalized force conjugate to the thickness L of the slab, which approaches zero as $L \rightarrow \infty$. We are interested in its behavior for $L \gg a$, where a is a typical microscopic length scale (we henceforth set it to unity). Suppose for the moment that all interactions are short ranged. Then finite-size scaling theory should be applicable in this limit. According to it, the Casimir force takes the scaling form [11,50]

$$\mathcal{F}_C(T,L)/k_B T = L^{-d} \Xi_0(L/\xi_\infty), \quad (2.4)$$

where ξ_∞ is the bulk correlation length [51], while Ξ_0 is a universal scaling function. This holds up to eventual contributions from regular background terms and irrelevant scaling fields, which we disregard for the moment but will come back to later, in particular, in Sec. II B 2.

As the temperature T approaches its bulk critical value $T_{c,\infty}$, with L fixed at a finite value, the correlation length ξ_∞ diverges and $L/\xi_\infty \rightarrow 0$. The corresponding limiting value of the scaling function Ξ_0 (which exists) is conventionally written as

$$\Xi_0(0) = (d-1)\Delta_C, \quad (2.5)$$

which defines the so-called Casimir amplitude Δ_C [14]. This quantity is related to the critical Casimir force via

$$\mathcal{F}_C(T_{c,\infty},L)/k_B T_{c,\infty} = (d-1) \frac{\Delta_C}{L^d}. \quad (2.6)$$

Just like the scaling function Ξ_0 , it is a *universal* quantity; it is independent of microscopic details, but depends on the bulk universality class considered and on other gross features such as boundary conditions.

Let us be a bit more precise. Suppose that instead of choosing periodic boundary conditions we considered a lattice model with free boundary conditions along the perpendicular direction. Then the topmost and lowest layers of the system would be free surfaces, corresponding to macroscopic planar boundaries between which the Casimir force acts. Provided (a) no symmetry-breaking boundary terms are included in the Hamiltonian and (b) no long-range surface or-

der is possible for $T > T_{c,\infty}$, one expects the long-distance physics of the system near the bulk critical point to be described by an $O(n)$ ϕ^4 model with *Dirichlet* boundary conditions. This is because upon coarse graining, the lattice model with free boundary conditions maps onto such a continuum field theory, albeit one satisfying *Robin boundary conditions* inside of averages [29,30].

If conditions (a) and (b) are satisfied, one has reason to believe that the theory belongs to the basin of attraction of the fixed point describing the so-called ordinary surface transition. This fixed point is infrared stable and corresponds to a Dirichlet boundary condition on large scales. The analogs of the Casimir amplitude Δ_C and the scaling function Ξ for this case of Dirichlet boundary conditions on both surface planes differ from their counterparts for periodic boundary conditions. Details of the mesoscopic Robin boundary condition—or microscopic details of the boundaries—do not matter as long as the resulting continuum theory belongs to the basin of attraction of the mentioned fixed point.

More generally, we have for a film geometry bounded in one direction by a pair of parallel boundary planes \mathfrak{B}_1 and \mathfrak{B}_2 the following situation. Universal quantities such as the Casimir amplitude Δ_C or the scaling function Ξ depend (for given bulk universality class and short-range interactions) on gross properties of *both* boundary planes. Let SUC_i denote the universality class pertaining to the surface critical behavior of the semi-infinite system with boundary plane \mathfrak{B}_i (“surface universality class” SUC), where $i=1$ or 2 . To specify universal quantities like the Casimir amplitude, we can write $\Delta_C^{\text{SUC}_1, \text{SUC}_2}$, where possible choices of SUC_1 and SUC_2 are “ord,” “sp,” and “norm,” the SUCs of the ordinary, special, and normal (or extraordinary [52]) transitions, respectively. The above-mentioned case of Dirichlet boundary conditions on \mathfrak{B}_1 and \mathfrak{B}_2 corresponds to the choices $\text{SUC}_1 = \text{SUC}_2 = \text{ord}$.

Systems with $O(n)$ -symmetrical Hamiltonian and short-range interactions have been studied in such film geometries for various choices of SUC_1 and SUC_2 by means of the ϵ expansion about the upper critical dimension $d^*=4$ [9,31–35], Monte Carlo simulations [10,53,54], and other techniques [11]. A fairly up-to-date survey of pertinent results may be found in the latter reference. More recent results are contained in Ref. [54]. Aside from these cases and the one of periodic boundary conditions, also slabs with antiperiodic boundary conditions have been considered for systems with short-range interactions [31,32].

Going back to the case of periodic boundary conditions, we now turn to the question of how to include subleading long-range interactions.

B. Subleading long-range interactions

We consider long-range two-body interactions with a pair potential $v^{(\sigma)}(x)$ of the kind (1.1). Let us begin by recalling how the relevance or irrelevance of such interactions for bulk critical behavior can be assessed.

1. Relevance-irrelevance criterion

Let \mathcal{H}_{sr} be the standard ϕ^4 Hamiltonian representing the bulk universality class of the n -vector model with short-

range interactions for d below $d^*=4$, its upper critical dimension. At the bulk critical point, the n -component order parameter field ϕ transforms as $\phi \rightarrow \ell^{-\Delta[\phi]}\phi$ under changes $\mu \rightarrow \mu\ell$ of the momentum scale, where the scaling dimension $\Delta[\phi]$ is given by

$$\Delta[\phi] = (d - 2 + \eta)/2. \quad (2.7)$$

Adding to \mathcal{H}_{sr} a long-range interaction term with pair potential $v^{(\sigma)}(x)$, we consider the Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\text{sr}} + b \int \mathcal{O}^{(\sigma)}(x) d^d x, \quad (2.8)$$

where $\mathcal{O}^{(\sigma)}(x)$ denotes the nonlocal operator

$$\mathcal{O}^{(\sigma)}(x) = \int d^d y v^{(\sigma)}(y) \phi\left(x - \frac{y}{2}\right) \phi\left(x + \frac{y}{2}\right), \quad (2.9)$$

and b is the associated coupling constant.

We now ask under what conditions the short-range fixed point remains infrared stable with respect to this $\mathcal{O}^{(\sigma)}$ perturbation. Upon insertion of the limiting form (1.1) into it, we can use Eq. (2.7) to conclude that the scaling dimension of the associated scaling operator, at the short-range fixed point, is given by

$$\Delta[\mathcal{O}^{(\sigma)}] = d - 2 + \eta + \sigma. \quad (2.10)$$

The corresponding scaling field $g_\sigma \sim b$ varies as $\ell^{-\nu_\sigma}$ in the infrared limit $\ell \rightarrow 0$, with the RG eigenexponent

$$\nu_\sigma \equiv -\omega_\sigma = d - \Delta[\mathcal{O}^{(\sigma)}] = 2 - \eta - \sigma. \quad (2.11)$$

Depending on whether the correction-to-scaling exponent $\omega_\sigma > 0$ or $\omega_\sigma < 0$, the short-range fixed point is locally stable or unstable to such perturbations. Hence we arrive at the following *irrelevance-relevance criterion*: The long-range perturbation proportional to b is irrelevant at the short-range fixed point if

$$\sigma > 2 - \eta, \quad (2.12)$$

and relevant if $\sigma < 2 - \eta$. Note that here and elsewhere in this paper, η always means the correlation exponent of the short-range case.

The case when this criterion suggests these long-range interactions to be relevant has been studied in the literature in the context of bulk critical behavior. For $\sigma < 2$, the upper critical dimension above which Landau theory holds is lowered from $d^*=4$ to $d_{\text{r}}^*(\sigma) = 2\sigma$. In the regime $\sigma < d < d_{\text{r}}^*(\sigma)$, the values of the critical exponents depend on σ , where the analog of η is given exactly by $\eta_{\text{r}} = 2 - \sigma$ [55–60]. For given d , a crossover from the critical behavior characterized by these critical exponents to one representative of systems with short-range interactions is predicted to occur at $\sigma = 2 - \eta$ [56,61–64]. This crossover has recently been reexamined for $d=2$ by numerical means [65].

Since we assume in our subsequent analysis that $2 < \sigma < 4$, the irrelevance criterion (2.12) is satisfied. Associated with the long-range interaction (2.9) therefore is an irrelevant scaling field $g_\sigma \sim b$ whose RG eigenexponent is given in Eq. (2.11). We next generalize the finite-size scaling ansatz for the free energy by incorporating g_σ .

2. Finite-size scaling

Allowing a magnetic field H to be present, we consider the reduced free energy per unit cross-sectional area $A = L_\perp^{d-1}$ of the previously specified slab with periodic boundary conditions, in the thermodynamic limit $L_\perp \rightarrow \infty$. According to the phenomenological theory of finite-size scaling [50,66,67], this quantity can be decomposed into a regular background contribution $f_L^{\text{reg}}(T, H)$ and a singular part $f_L^{\text{sing}}(T, H)$:

$$f_L(T, H) = f_L^{\text{sing}}(T, H) + f_L^{\text{reg}}(T, H). \quad (2.13)$$

This decomposition entails analogous decompositions of the bulk and excess free-energy densities $f_{\text{bk}}(T, H)$ and $f_{\text{ex}}(T, H, L)$, respectively.

Before turning to the singular parts, let us briefly comment on the regular background terms. For simple lattice systems with short-range interactions it has been found that the regular background terms of the excess free energy in the case of periodic boundary conditions agree to high accuracy with those of the bulk free energy [50]. This is understandable: Periodic boundary conditions preclude surface and edge contributions to the total free energy and hence terms of this kind that are analytic in temperature and magnetic field. Yet, it must be remembered that free energies and their regular background contributions are not universal properties, but depend on microscopic details of the system considered. Suppose a given system with periodic boundary conditions that belongs to the bulk universality class of the d -dimensional, n -component ϕ^4 model. Then we can choose a simple lattice n -vector model with nearest-neighbor interactions to investigate its universal critical behavior. However, inclusion of any irrelevant interaction—in particular, long-range interactions—that were dropped when making the transition from the original system to the lattice model is expected to modify the regular background contributions of the (bulk and excess) free energy. In other words, the empirical fact that the regular background contributions of the bulk and excess free energies of simple lattice models with short-range interactions can be chosen to be equal when periodic boundary conditions are applied does not imply that the same is true for microscopically more realistic models with additional (irrelevant) interactions. In particular, this must be kept in mind when adding irrelevant long-range interactions.

The singular parts $f_{\text{bk}}^{\text{sing}}$, $f_{\text{ex}}^{\text{sing}}$, and $f_{\text{ex}}^{\text{sing}}$ should have a scaling form. Specifically, $f_{\text{ex}}^{\text{sing}}(T, H, L)$ should take the finite-size scaling form

$$f_{\text{ex}}^{\text{sing}}(T, h, L) = L^{-(d-1)} X(g_t L^{1/\nu}, g_h L^{\Delta/\nu}, g_\sigma L^{-\omega_\sigma}, g_\omega L^{-\omega}, \dots) \quad (2.14)$$

on sufficiently large length scales, where ω is the previously mentioned standard correction-to-scaling exponent of short-range systems. Further, g_t , g_h , g_ω , and g_σ denote scaling fields. The first two are the leading even and odd relevant bulk scaling fields (namely, the “thermal” and “magnetic” scaling fields). For simple magnetic systems they behave as

$$g_t \approx a_t t, \quad t = (T - T_{c,\infty})/T_{c,\infty}, \quad (2.15)$$

and

$$g_h \approx a_h h, \quad h = H/k_B T_{c,\infty}, \quad (2.16)$$

near the bulk critical point $(T, H) = (T_{c,\infty}, 0)$, where a_t and a_h are nonuniversal metric factors; for fluid systems, both become linear combinations of t and $\delta\mu$, the deviation of the chemical potential from the critical point, because of “mixing” (see, e.g., Refs. [68,69]). For simplicity, we will use magnetic language and work with the above expressions henceforth.

Likewise, the previously introduced scaling field associated with the long-range interaction (2.9) is expected to vary as

$$g_\sigma \approx a_\sigma b \quad (2.17)$$

for small b . The ellipsis in Eq. (2.14) stands for analogous expressions involving further scaling fields, all of which we assume to be irrelevant; this means, in particular, that all *relevant* scaling fields other than g_t and g_h are taken to vanish. Moreover, we assume that none of the suppressed irrelevant scaling fields is *dangerous irrelevant* (see, e.g., Appendix D of Ref. [70]), so that all of them may be safely set to zero.

Current estimates of the correction-to-scaling exponent $\omega(n, d)$ of the d -dimensional n -vector model give $\omega(1, 3) \approx 0.81$ and somewhat smaller values for $n=2$ and 3, such as $\omega(3, 3) \approx 0.80$ [71–73]. On the other hand, the well-known exact spherical-model (SM) value is

$$\omega_{\text{SM}}(2 < d < 4) = \omega(\infty, 2 < d < 4) = 4 - d. \quad (2.18)$$

Let us compare these numbers with the appropriate analogs for the correction-to-scaling exponent ω_σ one can derive from Eq. (2.11). The cases of nonretarded and retarded van der Waals interactions in d dimensions correspond to the choices $\sigma=d$ and $\sigma=d+1$, giving $\omega_d = d-2+\eta$ and $\omega_{d+1} = d-1+\eta$, respectively. Both exponents are positive in the regime of dimensions $2 < d < 4$ we are concerned with. For finite n , where $\eta > 0$, the latter remains larger than ω in this whole regime, whereas ω_d would become smaller than ω slightly below $d=3$. In the spherical limit $n \rightarrow \infty$, this sign change of $\omega_d - \omega$ occurs at $d=3$ where $\omega_d = \omega = 1$. In our analysis of the spherical model given below we shall first assume that $d+\sigma < 6$. Then the possibility that $\omega > \omega_\sigma$ is ruled out. The borderline case $d+\sigma=6$ of the spherical model is special because $\omega = \omega_\sigma = 4-d$. Owing to this degeneracy, it requires special attention and will be discussed separately.

For the time being we therefore take it for granted that the irrelevant scaling fields g_ω and g_σ yield leading and next-to-leading corrections to scaling in the critical regime, respectively. However, away from the bulk critical point, the long-range interaction is expected to modify the large- L behavior of f_{ex} and the Casimir force in a *qualitative* manner so that they decay as inverse powers of L rather than exponentially [44]. To see how this translates into properties of the scaling function X , let us denote the scaling variables appearing in Eq. (2.14) as

$$\check{t} = g_t L^{1/\nu},$$

$$\check{h} = g_h L^{\Delta/\nu},$$

$$\check{g}_\sigma = g_\sigma L^{-\omega_\sigma},$$

$$\check{g}_\omega = g_\omega L^{-\omega}, \quad (2.19)$$

and expand X as

$$X(\check{t}, \check{h}; \check{g}_\sigma, \check{g}_\omega) = X_0(\check{t}, \check{h}) + \check{g}_\sigma X_\sigma(\check{t}, \check{h}) + \check{g}_\omega X_\omega(\check{t}, \check{h}) + \dots, \quad (2.20)$$

where it is understood that all suppressed scaling fields have been set to zero.

The scaling functions X_0 and X_ω obviously are properties of the *short-range* universality class. A similar though somewhat more restricted statement applies to X_σ : Just like the other two, it may be viewed as the expectation value of a quantity, computed at the infrared-stable fixed point of the ϕ^4 model with short-range interactions in a periodic slab of thickness $L=1$. However, it differs from those inasmuch as, in its case, this quantity is the nonlocal operator $\mathcal{O}^{(\sigma)}(\mathbf{x})$ associated with the long-range interaction, whereas the other do not involve this interaction at all.

At the bulk critical point $g_t = g_h = 0$, all three of these scaling functions are expected to take finite, nonzero values. Specifically, the critical value of X_0 yields the Casimir amplitude:

$$\Delta_C \equiv X_0(0, 0). \quad (2.21)$$

We denote its analogs for X_ω and X_σ as

$$\Delta_{\omega,C} \equiv X_\omega(0, 0), \quad (2.22)$$

$$\Delta_{\sigma,C} \equiv X_\sigma(0, 0). \quad (2.23)$$

The former controls the leading corrections to the asymptotic behavior of the critical excess free energy, the latter its contribution linear in g_σ originating from the long-range interaction (2.9).

Next, we turn to a discussion of the behavior as $L \rightarrow \infty$ when $T > T_{c,\infty}$. In this limit, either the scaling variable \check{t} , or both \check{t} and \check{h} , tend to infinity. As explained above, both functions X_0 and X_ω must decrease as $\sim \exp[-L/\xi^{\text{sr}}(T, H)]$, where $\xi^{\text{sr}}(T, H)$ is the true correlation length of the system with short-range interactions. Let us set $g_h = 0$ for the sake of simplicity. As $\check{t} \rightarrow \infty$ we then should have

$$X_0(\check{t}, 0) \underset{\check{t} \rightarrow \infty}{\sim} \exp[-|\text{const}| \check{t}^\nu + O(\ln \check{t})], \quad (2.24)$$

and similar asymptotic behavior for X_ω . However, for the function $X_\sigma(\check{t}, 0)$ we anticipate the limiting form

$$X_\sigma(\check{t}, 0) \underset{\check{t} \rightarrow \infty}{\approx} c_\sigma \check{t}^{-\nu\zeta}. \quad (2.25)$$

The exponent ζ introduced here characterizes the asymptotic dependence on L/ξ via $X_\sigma \sim (L/\xi)^{-\zeta}$. Our results for both the spherical ($n=\infty$) and the Gaussian model (GM) derived in the following sections yield

$$\zeta_{\text{SM}} = \zeta(n=\infty) = \zeta_{\text{GM}} = 2, \quad (2.26)$$

in conformity with Ref. [44].

In the regime $L/\xi \gg 1$ where X_0 and X_ω are exponentially small, the implied contribution $\sim g_\sigma$ to the excess free energy should become dominant:

$$f_{\text{ex}}(Lg_t^\nu \gg 1) \approx g_\sigma c_\sigma L^{-(d+\sigma+\eta+\zeta-3)} g_t^{-\nu\zeta}. \quad (2.27)$$

and imply a corresponding large- L behavior

$$\mathcal{F}_C \sim g_\sigma L^{-(d+\sigma+\eta+\zeta-2)} g_t^{-\nu\zeta} \quad (2.28)$$

of the Casimir force.

In the cases of the spherical and Gaussian models, where $\eta=0$ and ζ is given by Eq. (2.26), the large- L dependence of f_{ex} reduces to $\sim L^{-(d+\sigma-1)}$. Our exact results for the spherical and Gaussian models given below confirm these findings. In fact, there are reasons to expect that the latter L dependence applies more generally even when $\eta>0$. As proven some time ago by Iagolnitzer and Souillard [74], using the Griffiths-Sherman-Kelly inequalities [75], the two-point net correlation function of a ferromagnetic system whose interactions decay as $v^{(\sigma)}(x)$ in Eq. (1.1) cannot decay faster than the potential. Although we are not aware of any rigorous proof that they cannot decay slower than the potential either [76,77], it seems most natural to us to assume that this cumulant decays as $x \rightarrow \infty$ according to the same power law as the interaction potential, barring eventual logarithmic corrections in special cases.

Now, the correlation function

$$G(\mathbf{x}) \equiv \langle S(\mathbf{x})S(\mathbf{0}) \rangle - \langle S(\mathbf{x}) \rangle \langle S(\mathbf{0}) \rangle \quad (2.29)$$

of a slab of size $\infty^{d-1} \times L$ under periodic boundary conditions can be expressed in terms of its bulk counterpart G_∞ via

$$G_L^{\text{PBC}}(\mathbf{x}) = \sum_{j=-\infty}^{\infty} G_\infty(\mathbf{x} - jL\hat{\mathbf{e}}_1), \quad (2.30)$$

where $\hat{\mathbf{e}}_1$ is a unit vector along the finite 1 direction. For fixed \mathbf{x} , the terms with $j \neq 0$ yield L -dependent deviations from the $j=0$ bulk term that decay $\sim L^{-d-\sigma}$ as $L \rightarrow \infty$, provided the large-distance behavior (1.1) of $v^{(\sigma)}$ carries over to G_∞ . This suggests that (away from criticality) the excess contribution to the free energy of a d -dimensional volume is down by a factor $L^{-\sigma}$, so that the excess density f_{ex} behaves as $L^{1-d-\sigma}$. To ensure consistency with Eq. (2.27), we must therefore have

$$\zeta = 2 - \eta. \quad (2.31)$$

Although our results for the spherical and Gaussian models described below are in conformity with this prediction, they do not provide a nontrivial check of it because η vanishes. Such a check should in principle be possible within the framework of the ϵ expansion. To this end, one would have to compute the scaling function X_σ using RG improved perturbation theory to sufficiently high orders, verify its limiting behavior (2.25), and confirm its consistency with Eq. (2.31).

III. SPHERICAL MODEL

A. Definition of the model

Let $\mathcal{L} \subset \mathbb{Z}^d$ be the set of sites \mathbf{x} of a simple hypercubic lattice of size $L_1 \times L_2 \times \cdots \times L_d$. Imposing periodic boundary

conditions along all d principal directions, we consider a spherical model with the Hamiltonian

$$\frac{\mathcal{H}}{k_B T} = -\frac{1}{2} \sum_{\mathbf{x}, \mathbf{x}' \in \mathcal{L}} \frac{J(\mathbf{x} - \mathbf{x}')}{k_B T} S(\mathbf{x})S(\mathbf{x}') - h \sum_{\mathbf{x} \in \mathcal{L}} S(\mathbf{x}) + s \sum_{\mathbf{x} \in \mathcal{L}} S^2(\mathbf{x}) \quad (3.1)$$

whose spin variables $S(\mathbf{x}) \in \mathbb{R}$ satisfy the mean spherical constraint

$$\left\langle \sum_{\mathbf{x} \in \mathcal{L}} S^2(\mathbf{x}) \right\rangle = |\mathcal{L}|. \quad (3.2)$$

Here $|\mathcal{L}|$, the cardinality of the set \mathcal{L} , is the total number of sites (or spins). Further, s is a real positive variable, called the spherical field, whose value is to be determined from Eq. (3.2). For systems such as the one considered here, whose spins are all equivalent by translational invariance, the constraint (3.2) fixes all averages $\langle S^2(\mathbf{x}) \rangle$, $\forall \mathbf{x} \in \mathcal{L}$, to be unity.

As before, $h=H/k_B T$ denotes a reduced magnetic field. The pair interaction $J(\mathbf{x})$ consists of nearest-neighbor bonds and a long-ranged contribution of the type $v^{(\sigma)}$ specified in Eq. (1.1), with $2 < \sigma < 4$; we use the choice

$$J(\mathbf{x}) = J_1 \delta_{\mathbf{x},1} + \frac{J_2}{(\rho_0^2 + x^2)^{(d+\sigma)/2}}, \quad (3.3)$$

with $J_1 \geq 0$ and $J_2 > 0$, where $\rho_0 > 0$ sets a crossover length scale beyond which $J(\mathbf{x})$ varies approximately as $J_2 x^{-d-\sigma}$.

B. Properties of the interaction potential

In Appendix A we show that the Fourier transform

$$\tilde{J}(\mathbf{q}) \equiv \sum_{\mathbf{x}} J(\mathbf{x}) e^{-i\mathbf{q} \cdot \mathbf{x}} \quad (3.4)$$

of this interaction can be written as

$$\tilde{J}(\mathbf{q}) = \tilde{J}(\mathbf{0}) - K k_B T \Omega(\mathbf{q}) \quad (3.5)$$

with

$$K \equiv -\frac{1}{k_B T} \left. \frac{\partial \tilde{J}(\mathbf{q})}{\partial q^2} \right|_{\mathbf{q}=\mathbf{0}}, \quad (3.6)$$

where $\Omega(\mathbf{q})$ behaves as

$$\Omega(\mathbf{q}) = q^2 - b q^\sigma + b_4 q^4 + b_{4,1} \sum_{\alpha=1}^d q_\alpha^4 + o(q^4) \quad (3.7)$$

for small q , and $K > 0$, $b > 0$, $b_4 > 0$, and $b_4 + b_{4,1} > 0$. The term proportional to $b_{4,1}$ is anisotropic in \mathbf{q} space. It is a consequence of the fact that the hypercubic lattice breaks the Euclidean symmetry down to the symmetry of a hypercube. For other, less symmetric lattices more than two fourth-order invariants and hence additional anisotropic q^4 terms would appear.

Owing to our choice (3.3) of interaction constants, we have $J(\mathbf{x}) > 0$ for all lattice displacements \mathbf{x} . A straightforward consequence is that the Hamiltonian (3.1) has a unique ground state whose energy for $h=0$ is given by $\tilde{J}(\mathbf{0})$. Further-

more, $\tilde{J}(\mathbf{0}) > \tilde{J}(\mathbf{q})$ for all nontrivial wave vectors \mathbf{q} in the first Brillouin zone BZ_1 . It follows that the resulting values of $b, \dots, b_{4,1}$ must be such that the equation $1 - bq^{\sigma-2} + q^2[b_4 + b_{4,1}\sum_{\alpha} (q_{\alpha}/q)^4] = 0$ has no real-valued solutions \mathbf{q} .

Since the nonanalytic contribution $\sim q^{\sigma}$ arises from the large-distance tail of $J(x)$, its coefficient $k_B T K b$ should not depend on the details of how $J(x)$ behaves at small distances and hence should be independent of ρ_0 . Our result

$$b \frac{k_B T K}{J_2} = \frac{\pi^{d/2} \Gamma(-\sigma/2)}{2^{\sigma} \Gamma[(d+\sigma)/2]}, \quad (3.8)$$

derived in Appendix A, confirms this expectation. On the other hand, the coefficients of the analytic terms of orders q^2 and q^4 of $\tilde{J}(\mathbf{q})$ depend, of course, on J_1 and ρ_0 .

Note that the Fourier transform of the second term on the right-hand side of Eq. (3.3) yields a contribution to the nearest-neighbor coupling $J(x)|_{x=1}$ that depends on κ . This dependence can be utilized to modify this contribution and hence the nearest neighbor coupling for a given value of J_2 by varying κ . If we choose, for simplicity, the value zero for the coupling constant J_1 in Eq. (3.3), then the parameter b becomes (cf. Appendix A)

$$b = -\frac{1}{\pi} \Gamma(-\sigma/2) \Gamma(2-\sigma/2) \sin(\pi\sigma/2) (\rho_0/2)^{\sigma-2}, \quad (3.9)$$

which reduces to

$$b = \frac{2}{3} \rho_0, \quad d = \sigma = 3 \quad (3.10)$$

for the case of nonretarded van der Waals interactions in three dimensions.

C. Solution of the model, free energy, and constraint equation

Defining

$$v_2 \equiv -\frac{\partial}{\partial q^2} \ln \tilde{J}(\mathbf{q})|_{q=0} = \frac{K k_B T}{\tilde{J}(\mathbf{0})}, \quad (3.11)$$

we introduce the parameter

$$r \equiv \frac{1}{v_2} \left[\frac{2s k_B T}{\tilde{J}(\mathbf{0})} - 1 \right] \quad (3.12)$$

and the mode sum

$$U_{d,\Omega}(r|\mathbf{L}) = \frac{1}{2|\mathcal{L}|} \sum_{\mathbf{q} \in \text{BZ}_1} \ln[r + \Omega(\mathbf{q})], \quad (3.13)$$

where $\mathbf{L} \equiv (L_1, \dots, L_d)$. As is shown in Appendix A, the coefficient v_2 for our choice (3.3) of interaction constants takes the value

$$v_2 = \frac{\rho_0^2}{2(\sigma-2)} \quad (3.14)$$

when $J_1=0$.

Expressed in terms of the above quantities, the total free energy $F_{\mathbf{L}}(K, h)$ of our model is given by [11]

$$\frac{F_{\mathbf{L}}(K, h)}{k_B T |\mathcal{L}|} = f^{(0)}(K) + \frac{1}{2} \sup_{r>0} \left\{ 2U_{d,\Omega}(r|\mathbf{L}) - Kr - \frac{h^2}{Kr} \right\} \quad (3.15)$$

with

$$f^{(0)}(K) = \frac{1}{2} \left(\ln \frac{K}{2\pi} - \frac{K}{v_2} \right). \quad (3.16)$$

To determine the required supremum, we differentiate Eq. (3.15) with respect to r . This yields as the condition from which $r \equiv r_{\mathbf{L}}(K, h)$ —or, equivalently, the spherical field s of Eq. (3.12)—is to be determined the constraint equation

$$K = \frac{h^2}{K r_{\mathbf{L}}^2} + W_{d,\Omega}(r_{\mathbf{L}}|\mathbf{L}) \quad (3.17)$$

with

$$W_{d,\Omega}(r_{\mathbf{L}}|\mathbf{L}) = \frac{1}{|\mathcal{L}|} \sum_{\mathbf{q} \in \text{BZ}_1} \frac{1}{r_{\mathbf{L}} + \Omega(\mathbf{q})}. \quad (3.18)$$

The latter quantity is obviously related to $U_{d,\Omega}$ via

$$U_{d,\Omega}(r_{\mathbf{L}}|\mathbf{L}) = U_{d,\Omega}(0|\mathbf{L}) + \frac{1}{2} \int_0^{r_{\mathbf{L}}} W_{d,\Omega}(x|\mathbf{L}) dx. \quad (3.19)$$

Let us recall that the constraint equation (3.17) can be recast in the form of an equation of state [11]. To see this, note that Eq. (3.15) yields for the magnetization density $m_{\mathbf{L}}$ the result

$$m_{\mathbf{L}}(K, h) = -\frac{\partial F_{\mathbf{L}}(K, h)/|\mathcal{L}|}{\partial h} = \frac{h}{K r_{\mathbf{L}}(K, h)}, \quad (3.20)$$

whenever the supremum is attained for the solution $r_{\mathbf{L}}$ of Eq. (3.17). Using this to eliminate $r_{\mathbf{L}}$ in favor of $m_{\mathbf{L}}$ and h gives us the equation of state

$$(1 - m_{\mathbf{L}}^2) K = W_{d,\Omega} \left(\frac{h}{m_{\mathbf{L}} K} | \mathbf{L} \right). \quad (3.21)$$

In view of this correspondence between the constraint equation (3.17) and the equation of state (3.21), we will take the liberty of referring to the former henceforth as the equation of state.

From Eq. (3.20) one can easily read off that $r_{\mathbf{L}}$ for $h=0$ has the familiar meaning of an inverse susceptibility. Let us define the susceptibility by

$$\chi_{\mathbf{L}}(K, h) \equiv \frac{\partial m_{\mathbf{L}}(K, h)}{\partial h}. \quad (3.22)$$

Taking the derivative of the above-mentioned equation with respect to h at $h=0$ then gives the desired relation

$$[r_{\mathbf{L}}(K, 0)]^{-1} = \chi_{\mathbf{L}}(K, 0) K. \quad (3.23)$$

We are interested in the limit where all linear dimensions $L_2, \dots, L_d \rightarrow \infty$ while L_1 remains fixed at the finite value $L_1 \equiv L$. Let us employ the following convenient convention: Whenever the bold symbol \mathbf{L} in quantities such as $W_{d,\Omega}(r|\mathbf{L})$ or $r_{\mathbf{L}}$ has been replaced by L , it is understood that the so-

specified thermodynamic limit has been taken. For instance, $U_{d,\Omega}(r|L)$ stands for

$$U_{d,\Omega}(r|L) \equiv \lim_{L_2, \dots, L_d \rightarrow \infty} U_{d,\Omega}(r|L), \quad (3.24)$$

and $U_{d,\Omega}(r_L|L)$ means this function, taken at the corresponding limiting value $r_L \equiv \lim_{L_2, \dots, L_d \rightarrow \infty} r_L$ of the supremum r_L , i.e., of the solution to Eq. (3.17).

IV. FINITE-SIZE BEHAVIOR OF THE EQUATION OF STATE (3.17)

A. Decomposition of mode sums into bulk and size-dependent contributions

In order to determine the finite-size behavior of the excess free energy and its consequences for the Casimir force, we must investigate the L dependence of the mode sums $U_{d,\Omega}(r_L|L)$ and $W_{d,\Omega}(r_L|L)$ for large L . Let us first focus our attention on the explicit L dependence of these quantities by considering them at an arbitrary L -independent value of r . Writing

$$U_{d,\Omega}(r|L) = U_{d,\Omega}(r|\infty) + \Delta U_{d,\Omega}(r|L) \quad (4.1)$$

and

$$W_{d,\Omega}(r|L) = W_{d,\Omega}(r|\infty) + \Delta W_{d,\Omega}(r|L), \quad (4.2)$$

we split off their L -independent bulk parts

$$U_{d,\Omega}(r|\infty) = \frac{1}{2} \int_{\mathbf{q} \in \text{BZ}_1}^{(d)} \ln[r + \Omega(\mathbf{q})] \quad (4.3)$$

and

$$W_{d,\Omega}(r|\infty) = \int_{\mathbf{q} \in \text{BZ}_1}^{(d)} \frac{1}{r + \Omega(\mathbf{q})}, \quad (4.4)$$

where

$$\int_{\mathbf{q} \in \text{BZ}_1}^{(d)} \equiv \prod_{\alpha=1}^d \int_{-\pi}^{\pi} \frac{dq_\alpha}{2\pi} \quad (4.5)$$

is a convenient shorthand, from their L -dependent remainders $\Delta U_{d,\Omega}(r|L)$ and $\Delta W_{d,\Omega}(r|L)$. Using Poisson's summation formula (A4) (see Appendix A), the latter can be written as

$$\Delta U_{d,\Omega}(r|L) = \sum_{k=1}^{\infty} \int_{\mathbf{q} \in \text{BZ}_1}^{(d)} \cos(q_1 k L) \ln[r + \Omega(\mathbf{q})] \quad (4.6)$$

and

$$\Delta W_{d,\Omega}(r|L) = \sum_{k=1}^{\infty} \int_{\mathbf{q} \in \text{BZ}_1}^{(d)} \frac{2 \cos(q_1 k L)}{r + \Omega(\mathbf{q})}, \quad (4.7)$$

respectively.

B. Bulk equation of state

Next, we consider the equation of state (3.17) in the bulk limit $L \rightarrow \infty$. At the bulk critical point $K = K_{c,L=\infty}$, $h = 0$, its

solution $r \equiv r_{L=\infty}$ must vanish. Hence the critical coupling $K_{c,\infty}$ is given by

$$K_{c,\infty}(b) = W_{d,\Omega}(0|\infty). \quad (4.8)$$

As indicated, this quantity depends on the interaction parameter b as well as on all other interaction parameters $b_4, b_{4,1}$, etc. appearing in $\Omega(\mathbf{q})$. Defining the scaling fields g_t and g_h as

$$g_t = K_{c,\infty} - K, \quad g_h = h/\sqrt{K}, \quad (4.9)$$

we find from Eq. (3.17) that the bulk quantity r_∞ is to be determined from

$$-g_t = (g_h/r_\infty)^2 + W_{d,\Omega}(r_\infty|\infty) - W_{d,\Omega}(0|\infty), \quad (4.10)$$

the ‘‘bulk equation of state.’’

1. The case $d + \sigma < 6$ with $2 < d < 4$ and $2 < \sigma < 4$

To study its solutions near the bulk critical point, we must know how $W_{d,\Omega}$ behaves for small r . Since the long-ranged interaction proportional to b does not modify the leading infrared behavior, it is justified to expand in b . A straightforward calculation (see Appendix A) shows that provided $2 < d < 4$, $2 < \sigma < 4$, and $d + \sigma < 6$,

$$W_{d,\Omega}(r|\infty) - W_{d,\Omega}(0|\infty) \underset{r \rightarrow 0}{\approx} -A_d r^{d/2-1} + (w_d + b w_{d,\sigma})r + O(r^2) - b B_{d,\sigma} r^{(d+\sigma)/2-2} [1 + o(r)] + O(b^2), \quad (4.11)$$

where

$$A_d = -\frac{\Gamma(1-d/2)}{(4\pi)^{d/2}} > 0 \quad (4.12)$$

and

$$B_{d,\sigma} = \frac{\pi(d+\sigma-2)}{2(4\pi)^{d/2} \Gamma(d/2) \sin[\pi(d+\sigma)/2]} > 0. \quad (4.13)$$

We insert the above result into the bulk equation of state (4.10), keeping only the explicitly shown contributions. The resulting equation for the scaled inverse susceptibility $r_\infty g_t^{-\gamma}$ is expected to take a scaling form. To the linear order of our analysis in b and the irrelevant scaling fields g_σ and g_ω , this is the case provided a term linear in b is included in g_ω . Such a contribution is anticipated on general grounds because in a ϕ^4 theory with coupling constant u , the RG flow of the running variable $\bar{u}(\ell)$ should be affected by terms linear in b ; technically, this may be attributed to the fact that single insertions of the long-ranged operator (2.9) require contributions linear in b of the ϕ^4 counterterm.

On the other hand, the scaling field g_σ should have no contribution of zeroth order in b because, given an initial Hamiltonian without long-range interactions ($b=0$), no long-range interaction can be generated under a RG transformation.

In conformity with these ideas, the choices

$$g_\omega(b) = w_d + b w_{d,\sigma}, \quad g_\sigma(b) = b \quad (4.14)$$

(up to nonlinear contributions and a redefinition of the scales of these fields) turn out to be appropriate. They entail that the resulting bulk equation of state scales, so that solutions r_∞ to it can be written as

$$r_\infty \approx g_t^\gamma \mathcal{R}^{(\infty)}(g_h g_t^{-\Delta}, g_\omega g_t^{\nu\omega}, g_\sigma g_t^{\nu\omega\sigma}), \quad (4.15)$$

where the critical exponents $\gamma = \nu(2 - \eta)$, ν , η , $\Delta = (\nu/2)(d + 2 - \eta)$, ω_σ , and ω take the spherical-model values

$$\gamma_{\text{SM}} = 2\nu_{\text{SM}} = \frac{2}{d-2},$$

$$\eta_{\text{SM}} = 0, \quad \Delta_{\text{SM}} = \frac{d+2}{2(d-2)},$$

$$\omega_{\sigma,\text{SM}} = \sigma - 2, \quad (4.16)$$

and (2.18), respectively. The function $\mathcal{R}^{(\infty)}$ is given by

$$\begin{aligned} \mathcal{R}^{(\infty)}(x_h, x_\omega, x_\sigma) &= \mathcal{R}_0^{(\infty)}(x_h) + x_\omega \mathcal{R}_\omega^{(\infty)}(x_h) + x_\sigma \mathcal{R}_\sigma^{(\infty)}(x_h) \\ &+ o(x_\omega, x_\sigma), \end{aligned} \quad (4.17)$$

where $\mathcal{R}_0^{(\infty)}(x_h)$ is the solution to the asymptotic scaled bulk equation of state

$$1 + x_h^2 [\mathcal{R}_0^{(\infty)}(x_h)]^{-2} = A_d [\mathcal{R}_0^{(\infty)}(x_h)]^{(d-2)/2}, \quad (4.18)$$

while the remaining two functions are given by

$$\mathcal{R}_\omega^{(\infty)}(x_h) = \frac{2[\mathcal{R}_0^{(\infty)}(x_h)]^4}{(d-2)A_d[\mathcal{R}_0^{(\infty)}(x_h)]^{d/2+1} + 4x_h^2} \quad (4.19)$$

and

$$\mathcal{R}_\sigma^{(\infty)}(x_h) = \frac{-2B_{d,\sigma}[\mathcal{R}_0^{(\infty)}(x_h)]^{(d+\sigma+2)/2}}{(d-2)A_d[\mathcal{R}_0^{(\infty)}(x_h)]^{d/2+1} + 4x_h^2}. \quad (4.20)$$

For zero magnetic field, the above findings simplify considerably, giving

$$\begin{aligned} r_\infty|_{h=0} &\approx \left(\frac{g_t}{A_d}\right)^\gamma \left[1 + \frac{2g_\omega(b)}{(d-2)A_d} \left(\frac{g_t}{A_d}\right)^{\nu\omega} \right. \\ &\quad \left. - \frac{2g_\sigma(b)B_{d,\sigma}}{(d-2)A_d} \left(\frac{g_t}{A_d}\right)^{\nu\omega\sigma} \right], \end{aligned} \quad (4.21)$$

where again the spherical-model values (4.16) and (2.18) must be substituted for the critical exponents γ , ν , ω_σ , and ω .

2. Logarithmic anomalies and the case $d+\sigma=6$ with $2 < d < 4$

The above results get modified by the appearance of logarithmic anomalies when $d=4$ or $d+\sigma=6$. Our ultimate interest is to understand the consequences this has for finite-size scaling and the Casimir force in the latter case. Since logarithmic anomalies occur already in the bulk theory, it will be helpful to clarify their origin first in this simpler context.

That the finite-size behavior gets modified by the presence of logarithmic anomalies when $d+\sigma=6$ was recognized al-

ready in a paper by Chamati and one of us [37]. However, no explanation of their cause within the general context of RG theory was given there. Here we wish to fill this gap. As we shall see, despite some similarities with the situation at the upper critical dimension $d=4$, the mechanisms by which they are produced in the cases $d=4$ and $d+\sigma=6$ with $2 < d < 4$ are different.

Let us begin by recalling the well understood case $d=4$ [78]. The coefficients A_d and w_d both become singular as $d \rightarrow 4$ (see, e.g., Ref. [79] and Appendix A). Although w_d is nonuniversal, its pole part at $d=4$ (a single pole) is universal and equal to that of A_d , so that the sum of these two terms in Eq. (4.11) produces a finite $r \ln r$ contribution in the limit $d \rightarrow 4$. As a consequence, the leading thermal singularity of r_∞ takes the form

$$r_\infty|_{h=0} \sim g_t / |\ln g_t|. \quad (4.22)$$

In the framework of RG theory the appearance of logarithmic anomalies means that the Hamiltonian \mathcal{H} transforms under a change of momentum scale $\mu \rightarrow \mu\ell$ into a transformed one $\mathcal{H}(\{\bar{g}_j(\ell)\}, \ell)$ whose ℓ dependence cannot fully be absorbed through scale-dependent scaling fields $\bar{g}_j(\ell)$ but has an additional explicit dependence on ℓ . We follow here the notational conventions of Wegner [78,80,81]: The $\bar{g}_j(\ell)$ are nonlinear scaling fields with initial values $\bar{g}_j(1)=g_j$ and eigenexponents y_j ; i.e.,

$$\bar{g}_j(\ell) = \ell^{-y_j} g_j. \quad (4.23)$$

We denote their linear counterparts as $\bar{\mu}_j(\ell)$, and let $\bar{\mu}_0$ with $y_0=d$ be the special field associated with the volume. If the linearized RG operator is diagonal in the variables μ_i , then these fields usually satisfy flow equations, which to quadratic order can be written as

$$-\ell \frac{d\bar{\mu}_i(\ell)}{d\ell} = y_i \bar{\mu}_i + \frac{1}{2} \sum_{j,k} a_{ijk} \bar{\mu}_j \bar{\mu}_k, \quad (4.24)$$

where $a_{ijk}=a_{ikj}$ and $a_{ij0}=0$ [80]. Provided the conditions

$$y_i \neq y_j + y_k \quad (4.25)$$

are satisfied, one arrives at an expansion of the form

$$\bar{\mu}_i = \bar{g}_i + \frac{1}{2} \sum_{j,k} b_{ijk} \bar{g}_j \bar{g}_k + \dots \quad (4.26)$$

with

$$b_{ijk} = \frac{a_{ijk}}{y_j + y_k - y_i}. \quad (4.27)$$

Similar conditions involving sums of more than two eigenexponents, e.g., $y_i \neq y_j + y_k + y_l$, must hold in order that the contributions of third and higher orders have a corresponding form with scale-independent expansion coefficients.

When conditions such as Eq. (4.25) are violated so that y_i equals a sum of other RG eigenvalues, the coefficients of the expansion of the linear fields $\bar{\mu}_i$ in the nonlinear ones \bar{g}_i become scale dependent, involving logarithms of ℓ or even powers of such logarithms. For example, when $y_i = y_j + y_k$ for

a single triple (i, j, k) with $a_{ijk} \neq 0$, then b_{ijk} gets replaced by [78,80]

$$b_{ijk}(\ell) = -a_{ijk} \ln \ell. \quad (4.28)$$

Upon making the usual choice $\ell_t = \ell(g_t)$ such that $|\bar{g}_t(\ell_t)| = 1$, logarithms of t result.

Let us first consider the case $d + \sigma < 6$ with $d, \sigma \in (2, 4)$, and ignore the contributions from all irrelevant fields. Then the inequalities (4.25) as well as the condition that the linearized RG operator be diagonal at the critical fixed point in the (relevant) fields are satisfied.

The logarithmic singularities one encounters at the upper critical dimension $d=4$ have two sources [78]: (i) The exponent $\mu_0 = d$ is equal to twice the thermal RG eigenexponent $y_t = 1/\nu$; (ii) a marginal operator (ϕ^4) must be taken into account, so that an infinite number of eigenexponent inequalities (4.25) and its analogs involving more than three RG eigenexponents are violated. The known consequences are that the leading thermal singularities have logarithmic anomalies which for general values of n consist of nontrivial powers of $\ln g_t$.

Next, we turn to the case $d + \sigma = 6$ with $d, \sigma \in (2, 4)$. A similarity with the case $d=4$ is that the coefficient $w_{d,\sigma}$ (which is again universal) has a single pole at $d + \sigma = 6$ that cancels with the pole of $B_{d,\sigma}$ such that a contribution proportional to $r \ln r$ is produced in the limit $\sigma \rightarrow 6 - d$ of Eq. (4.11). Thus the analog of this equation for $d + \sigma = 6$ becomes

$$W_{d,\Omega}(r|\infty) - W_{d,\Omega}(0|\infty) \underset{r \rightarrow 0}{\approx} -A_d r^{d/2-1} + (w_d + \tilde{w}_d b) r + bK_d r \ln r + O(b^2) \quad (4.29)$$

with

$$\tilde{w}_d = \frac{K_d}{2} + w_{d,6-d}^{\text{reg}}, \quad (4.30)$$

where K_d denotes the conventional factor

$$K_d \equiv \int_q \delta(|q| - 1) = \frac{2}{(4\pi)^{d/2} \Gamma(d/2)} > 0, \quad (4.31)$$

while $w_{d,6-d}^{\text{reg}}$ means the regular part

$$w_{d,6-d}^{\text{reg}} = \lim_{\sigma \rightarrow 6-d} \left(\frac{2K_d}{\sigma + d - 6} + w_{d,\sigma} \right) \quad (4.32)$$

of $w_{d,\sigma}$ at $\sigma = 6 - d$.

Upon substituting the above result into the bulk equation of state (4.10), we see that instead of Eqs. (4.15)–(4.20) we now have

$$r_\infty \approx g_t^\gamma (\mathcal{R}_0^{(\infty)}(x_h) + g_t^{\nu\omega} \mathcal{R}_\omega^{(\infty)}(x_h) \times \{w_d + b\tilde{w}_d + bK_d \ln[g_t^\gamma \mathcal{R}_0^{(\infty)}(x_h)]\}), \quad (4.33)$$

which simplifies to

$$r_\infty|_{h=0} \approx \left(\frac{g_t}{A_d} \right)^\gamma \left[1 + \frac{2}{(d-2)A_d} \left(\frac{g_t}{A_d} \right)^{\nu\omega} \times \left(w_d + b\tilde{w}_d + b \frac{2K_d}{d-2} \ln \frac{g_t}{A_d} \right) \right] \quad (4.34)$$

when $h=0$.

The origin of the logarithmic corrections proportional to b is due to the previously mentioned mixing of the b -independent linear part of the irrelevant scaling field g_ω (which we denote as μ_σ) with $\mu_\sigma \propto b$, which led us to conclude that the scaling fields g_ω and g_σ can be chosen as in Eq. (4.14) up to nonlinear contributions. Recalling that μ_σ is expected to contribute to the change of μ_ω under RG transformations, but μ_σ cannot be generated when $2 < \sigma < 4$ if the initial Hamiltonian does not involve any long-range interactions, one concludes that this translates into flow equations of the form

$$\begin{aligned} -\ell \frac{d}{d\ell} \bar{\mu}_\omega &= y_\omega \bar{\mu}_\omega + a_{\omega\sigma} \bar{\mu}_\sigma + \dots, \\ -\ell \frac{d}{d\ell} \bar{\mu}_\sigma &= y_\sigma \bar{\mu}_\sigma + \dots, \end{aligned} \quad (4.35)$$

with $a_{\omega\sigma} \neq 0$. As long as $d + \sigma < 6$, the eigenexponents y_σ and y_ω differ. In that case these flow equations yield

$$\bar{\mu}_\omega(\ell) = \bar{g}_\omega(\ell) + \frac{a_{\omega\sigma}}{y_\sigma - y_\omega} \bar{g}_\sigma(\ell) + \dots, \quad (4.36)$$

$$\bar{\mu}_\sigma(\ell) = \bar{g}_\sigma(\ell) + \dots, \quad (4.37)$$

which in turn implies that g_ω involves a linear combination of μ_ω and μ_σ in conformity with Eq. (4.14).

For $d + \sigma = 6$, the spherical model yields $y_\sigma = y_\omega = d - 4$ [cf. Eq. (2.11)]. Owing to this degeneracy, the expansion (4.36) gets replaced by

$$\bar{\mu}_\omega(\ell) = \bar{g}_\omega(\ell) - a_{\omega\sigma} \bar{g}_\sigma(\ell) \ln \ell, \quad (4.38)$$

which in turns leads to the logarithmic temperature anomaly in Eq. (4.34).

The general mechanism we have identified here as producing the logarithmic anomalies in the case $d + \sigma = 6$ is, of course, not new; a brief discussion of it may be found in Sec. V.E.1 of Ref. [80].

C. Finite-size scaling form of equation of state

We now proceed with our analysis of the finite-size behavior. To this end we must work out the large- L dependence of the functions $\Delta W_{d,\Omega}$ and $\Delta U_{d,\Omega}$. Expanding again to linear order in b gives

$$\Delta W_{d,\Omega}(r|L) = \Delta W_{d,\Omega}^{(0)}(r|L) + b \Delta W_{d,\Omega}^{(1)}(r|L) + O(b^2), \quad (4.39)$$

where the superscripts (0) and (1) on the right-hand side indicate, respectively, the function $\Delta W_{d,\Omega}(r|L)$ and its first derivative with respect to b , taken at $b=0$. From Eqs. (3.7) and (4.4) we obtain

$$\Delta W_{d,\Omega}^{(0)}(r|L) = \sum_{k=1}^{\infty} \int_{\mathbf{q} \in \text{BZ}_1}^{(d)} \frac{2 \cos(q_1 k L)}{r + \Omega(\mathbf{q})} \quad (4.40)$$

and

$$\Delta W_{d,\Omega}^{(1)}(r|L) = \sum_{k=1}^{\infty} \int_{\mathbf{q} \in \text{BZ}_1}^{(d)} \frac{2q^\sigma \cos(q_1 k L)}{[r + \Omega(\mathbf{q})]^2}. \quad (4.41)$$

The \mathbf{q} integrations (cosine transforms) appearing in these equations are well defined as long as $r > 0$ and $L > 0$. In order to obtain the asymptotic behavior of the functions (4.40) and (4.41) for $r \rightarrow 0$, we extend the \mathbf{q} integrations to the full \mathbf{q} space \mathbb{R}^d and make the replacement $\Omega(\mathbf{q}) \rightarrow q^2$ in their denominators. This amounts to the omission of contributions that are regular in r or less singular than those retained. The resulting expression for the right-hand side of Eq. (4.40) is easily evaluated by noting that it is nothing else than the difference between the free propagator G_L^{PBC} of Eq. (2.30) and its bulk counterpart G_∞ , given by

$$G_\infty(d|r;x) \equiv \int_{\mathbf{q}} \frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{r + q^2} = r^{(d-2)/2} \frac{K_{d/2-1}(x\sqrt{r})}{(2\pi)^{d/2} (x\sqrt{r})^{d/2-1}}, \quad (4.42)$$

with $x \equiv |\mathbf{x}|$.

One thus arrives at

$$\begin{aligned} \Delta W_{d,\Omega}^{(0)}(r|L) &\approx \frac{2}{L^{d-2}} \sum_{k=1}^{\infty} G_\infty(d|rL^2;k) \\ &= \frac{K_{d-1}}{L^{d-2}} \int_0^\infty \frac{p^{d-2}}{\sqrt{rL^2 + p^2}} \frac{dp}{e^{\sqrt{rL^2 + p^2}} - 1}, \end{aligned} \quad (4.43)$$

where the second line follows from the first one with the aid of the representation

$$G_\infty(d|r;x) = \int_{\mathbf{q}_\parallel} \frac{e^{-|x_\parallel|(r + q_\parallel^2)^{1/2}}}{2(r + q_\parallel^2)^{1/2}} e^{i\mathbf{x}_\perp \cdot \mathbf{q}_\perp} \quad (4.44)$$

upon interchanging the summation over k with the integration over the $(d-1)$ -dimensional wave vector \mathbf{q}_\parallel conjugate to $\mathbf{x}_\parallel = (x_2, \dots, x_d)$, the component of \mathbf{x} perpendicular to $\hat{\mathbf{e}}_1$.

In order to compute the analogous approximation for $\Delta W_{d,\Omega}^{(1)}(r|L)$, we proceed as follows. Applying the identity

$$\frac{q^\sigma}{(r + q^2)^2} = \partial_r \left(\frac{r q^{\sigma-2}}{r + q^2} \right) \quad (4.45)$$

to the integrand of Eq. (4.41), we see that the right-hand side of this equation is the derivative ∂_r of an expression that differs from the right-hand side of Eq. (4.40) merely through an extra power of $q^{\sigma-2}$ in the integrand. This tells us that the roles of the film propagator $G_L(d|r;x)$ and its bulk counterpart $G_\infty(d|r;x)$ in Eq. (4.43) now are taken over by the modified film propagator

$$G_L(d,\sigma|r;x) = \frac{1}{L} \sum_{\mathbf{q}_\perp \in (2\pi/L)\mathbb{Z}} \int_{\mathbf{q}_\parallel}^{(d-1)} \frac{q^{\sigma-2} e^{i\mathbf{q}\cdot\mathbf{x}}}{r + q^2} \quad (4.46)$$

and its $L=\infty$ analog, respectively, which obviously reduce to the former two when $\sigma=2$.

Let us define the function

$$\begin{aligned} Q_{d,\sigma}(y) &\equiv \frac{y}{2} [G_{L=1}(d,\sigma|y;\mathbf{0}) - G_\infty(d,\sigma|y;\mathbf{0})] \\ &= y \sum_{k=1}^{\infty} \int_{\mathbf{q}}^{(d)} \frac{q^{\sigma-2} \cos(q_1 k)}{y + q^2}. \end{aligned} \quad (4.47)$$

Here the second representation follows again by Poisson's summation formula (A4).

In terms of this function, the analog of Eq. (4.43) becomes

$$\Delta W_{d,\Omega}^{(1)}(r|L) \approx \frac{2}{L^{d+\sigma-4}} Q'_{d,\sigma}(rL^2), \quad (4.48)$$

where the prime indicates a derivative, i.e., $Q'_{d,\sigma}(y) \equiv \partial Q_{d,\sigma}(y)/\partial y$. Furthermore, our result (4.43) for $\Delta W_{d,\Omega}^{(0)}(r|L)$ can be written as

$$\Delta W_{d,\Omega}^{(0)}(r|L) \approx L^{-(d-2)} \frac{2}{rL^2} Q_{d,2}(rL^2). \quad (4.49)$$

Explicit results for the propagator $G_\infty(d,\sigma|r;x)$ and the functions $Q_{d,\sigma}(y)$ are derived in Appendix B. As is shown there, $G_\infty(d,\sigma|r;x)$ can be calculated for general values of $\sigma \in (2,4)$ and expressed in terms of generalized hypergeometric functions. From these results the asymptotic behavior of the functions $Q_{d,\sigma}(y)$ for large and small values of y can be inferred in a straightforward manner (see Appendix B 2). We managed to express $Q_{d,\sigma}(y)$ for general values of (d,σ) in terms of elementary and special functions up to a series of the form $\sum_{j=1}^{\infty} (\cdot)$, but have not been able to obtain closed-form analytic results for these series in general. However, for a variety of special choices (d,σ) , we succeeded in deriving explicit analytic expressions for the functions $Q_{d,\sigma}$. In particular, all functions $Q_{d,\sigma}$ required for the analysis of the case $d=\sigma=3$ of nonretarded van der Waals interactions in three dimensions are determined analytically in Appendix B.

From the above results the finite-size scaling form of the equation of state near the bulk critical point follows in a straightforward fashion. Let us choose the scaling variables \check{t} and \check{h} in Eq. (2.19) as

$$\check{t} = (K_{c,\infty} - K)L^{d-2}, \quad (4.50)$$

$$\check{h} = hK^{-1/2}L^{(d+2)/2}, \quad (4.51)$$

\check{g}_ω and \check{g}_σ in accordance with Eq. (4.14), and introduce the scaled inverse susceptibility

$$\check{r}_L \equiv r_L L^{\gamma/\nu} = r_L L^2, \quad (4.52)$$

where again the spherical-model values (4.16) were utilized for the exponents Δ/ν and γ/ν .

Upon subtracting from the equation of state (3.21) its bulk analog at the critical point and inserting Eqs. (4.2), (4.11), (4.48), and (4.49), we obtain for the case $2 < d < 4$, $2 < \sigma < 4$, and $d + \sigma < 6$

$$\check{t} \approx -(\check{h}/\check{r}_L)^2 + A_d \check{r}_L^{d/2-1} - 2\check{r}_L^{-1} Q_{d,2}(\check{r}_L) - \check{g}_\omega \check{r}_L + \check{g}_\sigma [B_{d,\sigma} \check{r}_L^{(d+\sigma-4)/2} - 2Q'_{d,\sigma}(\check{r}_L)]. \quad (4.53)$$

The result has the expected scaling form. We can solve for \check{r}_L (at least in principle) to determine it as a function \mathcal{R} of the other scaled variables. Hence we have shown, to linear order in g_ω , g_σ , and b , that the inverse susceptibility r_L can be written as

$$r_L = L^{-2} \mathcal{R}(\check{t}, \check{h}, \check{g}_\omega, \check{g}_\sigma) \quad (4.54)$$

in the appropriate finite-size scaling regime. By analogy with the expansion (4.17) made in the bulk case, we write

$$\mathcal{R}(\check{t}, \check{h}, \check{g}_\omega, \check{g}_\sigma) = \mathcal{R}_0(\check{t}, \check{h}) + \check{g}_\omega \mathcal{R}_\omega(\check{t}, \check{h}) + \check{g}_\sigma \mathcal{R}_\sigma(\check{t}, \check{h}) + o(\check{g}_\omega, \check{g}_\sigma). \quad (4.55)$$

Here $\mathcal{R}_0(\check{t}, \check{h})$ is the solution to Eq. (4.53) with \check{g}_ω and $\check{g}_\sigma = 0$ set to zero. The other two functions are found to be given by

$$\mathcal{R}_\omega(\check{t}, \check{h}) = \frac{2[\mathcal{R}_0(\check{t}, \check{h})]^4}{\mathcal{N}(\check{t}, \check{h})} \quad (4.56)$$

and

$$\mathcal{R}_\sigma(\check{t}, \check{h}) = \frac{4\mathcal{R}_0^3 Q'_{d,\sigma}(\mathcal{R}_0) - 2B_{d,\sigma} \mathcal{R}_0^{(d+\sigma+2)/2}}{\mathcal{N}(\check{t}, \check{h})} \quad (4.57)$$

with

$$\mathcal{N}(\check{t}, \check{h}) = (d-2)A_d \mathcal{R}_0^{d/2+1} + 4\check{h}^2 + 4\mathcal{R}_0 [Q_{d,2}(\mathcal{R}_0) - \mathcal{R}_0 Q'_{d,2}(\mathcal{R}_0)], \quad (4.58)$$

where \mathcal{R}_0 stands for $\mathcal{R}_0(\check{t}, \check{h})$.

In the large- L limit the foregoing results must reduce to our above ones for the bulk, Eqs. (4.15) and (4.17)–(4.21). This implies the limiting behavior

$$\mathcal{R}[\check{t}(L), \check{h}(L), \check{g}_\omega(L), \check{g}_\sigma(L)] \underset{L \rightarrow \infty}{\approx} \check{t}^{2\nu} \mathcal{R}^{(\infty)}(g_h g_t^{-\Delta}, g_\omega g_t^{\nu\omega}, g_\sigma g_t^{\nu\omega\sigma}) \quad (4.59)$$

and corresponding relations between the other \mathcal{R} functions and their bulk counterparts, namely,

$$\mathcal{R}_a[\check{t}(L), \check{h}(L)] \underset{L \rightarrow \infty}{\approx} \check{t}^{2\nu} \mathcal{R}_a^{(\infty)}(g_h g_t^{-\Delta}), \quad a = 0, \omega, \sigma. \quad (4.60)$$

For $d + \sigma = 6$ with $2 < d < 4$ and $2 < \sigma < 4$, logarithmic anomalies appear again in the equation of state and its solution. A simple way to obtain these is to take the limits $\sigma \rightarrow 6 - d$ of Eqs. (4.53)–(4.58). This yields

$$\check{t} \approx -(\check{h}/\check{r}_L)^2 + A_d \check{r}_L^{d/2-1} - 2\check{r}_L^{-1} Q_{d,2}(\check{r}_L) - (w_d + \tilde{w}_d b) L^{d-4} \check{r}_L - \check{g}_\sigma \left(2Q'_{d,6-d}(\check{r}_L) + K_d \check{r}_L \ln \frac{\check{r}_L}{L^2} \right) \quad (4.61)$$

and

$$r_L \approx L^{-2} \left(\mathcal{R}_0(\check{t}, \check{h}) + L^{-(4-d)} \mathcal{R}_\omega(\check{t}, \check{h}) \{w_d + \tilde{w}_d b + 2bQ'_{d,6-d}[\mathcal{R}_0(\check{t}, \check{h})][\mathcal{R}_0(\check{t}, \check{h})]^{-1} + bK_d \ln[L^{-2} \mathcal{R}_0(\check{t}, \check{h})]\} \right). \quad (4.62)$$

The logarithmic anomalies manifest themselves through the contributions that depend explicitly on $\ln L^2$ (rather than merely on scaled variables).

D. Relation between finite-size and bulk inverse susceptibility

The results of the previous section can be combined with those for the bulk equation of state to express the inverse scaled finite-size susceptibility \check{r}_L in terms of its bulk counterpart

$$\check{r}_\infty \equiv r_\infty L^{\gamma/\nu} = r_\infty L^2, \quad (4.63)$$

rather than the scaled temperature field \check{t} . The relationship between \check{r}_L and \check{r}_∞ will be needed in the next section to determine the excess free energy as a function of the inverse bulk susceptibility r_∞ . Since the second-moment correlation length ξ_∞ of the spherical model is given by $r_\infty^{-1/2}$ (up to a normalization factor), this gives us r_L and the excess free energy expressed in terms of ξ_∞ .

1. The case $d + \sigma < 6$ with $2 < d < 4$ and $2 < \sigma < 4$

We equate the finite-size equation of state (4.53) with its analog for \check{r}_∞ ,

$$\check{t} \approx -\check{h}^2 \check{r}_\infty^{-2} + A_d \check{r}_\infty^{(d-2)/2} - \check{g}_\omega \check{r}_\infty + \check{g}_\sigma B_{d,\sigma} \check{r}_\infty^{(d+\sigma-4)/2}, \quad (4.64)$$

and substitute for \check{r}_L the Ansatz

$$\check{r}_L \approx \mathbf{R}_0(\check{r}_\infty, \check{h}) + \check{g}_\sigma \mathbf{R}_\sigma(\check{r}_\infty, \check{h}) + \check{g}_\omega \mathbf{R}_\omega(\check{r}_\infty, \check{h}). \quad (4.65)$$

This yields for $\mathbf{R}_0 = \mathbf{R}_0(\check{r}_\infty, \check{h})$ the equation

$$2\mathbf{R}_0^{-1} Q_{d,2}(\mathbf{R}_0) = A_d (\mathbf{R}_0^{(d-2)/2} - \check{r}_\infty^{(d-2)/2}) - \check{h}^2 (\mathbf{R}_0^{-2} - \check{r}_\infty^{-2}) \quad (4.66)$$

and for the other functions the solutions

$$\mathbf{R}_\omega(\check{r}_\infty, \check{h}) = \frac{2\mathbf{R}_0}{\mathbf{N}} (\mathbf{R}_0 - \check{r}_\infty) \quad (4.67)$$

and

$$\mathbf{R}_\sigma(\check{r}_\infty, \check{h}) = \frac{2\mathbf{R}_0}{\mathbf{N}} [B_{d,\sigma} \check{r}_\infty^{(d+\sigma-4)/2} - \mathbf{R}_0^{(d+\sigma-4)/2}] + 2Q'_{d,\sigma}(\mathbf{R}_0), \quad (4.68)$$

where \mathbf{N} means the function

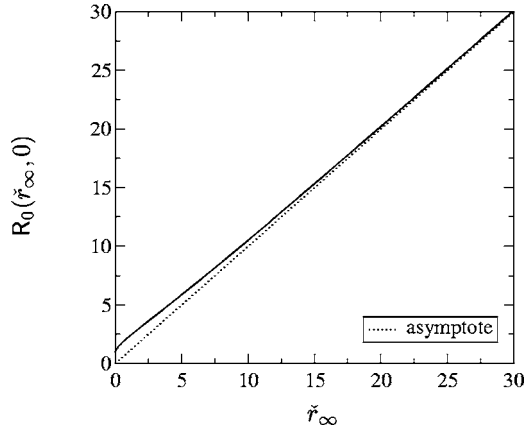


FIG. 1. Scaling function $R_0(\check{r}_\infty, 0)$ for $d=3$, as given by Eq. (4.72). The dotted line represents the asymptote $R_{0,as}(\check{r}_\infty, 0) = \check{r}_\infty$ that this function approaches for large values of \check{r}_∞ in an exponential manner.

$$N(\check{r}_\infty, \check{h}) = 4\check{h}^2 R_0^{-2} + (d-2)A_d R_0^{(d-2)/2} + 4R_0^{-1} Q_{d,2}(R_0) - 4Q'_{d,2}(R_0). \quad (4.69)$$

2. The case $d+\sigma=6$ with $2 < d < 4$

The analog of Eq. (4.64) is given by Eq. (4.61) with \check{r}_L replaced by \check{r}_∞ and the terms involving $Q_{d,2}$ and $Q'_{d,6-d}$ dropped. Owing to the presence of the logarithmic anomaly $\propto b$, the *Ansatz* (4.65) must be modified so as to allow for an explicit L dependence of R_σ :

$$\check{r}_L \approx R_0(\check{r}_\infty, \check{h}) + \check{g}_\sigma R_\sigma(\check{r}_\infty, \check{h}; L) + (w_d + \tilde{w}_d b) L^{d-4} R_\omega(\check{r}_\infty, \check{h}). \quad (4.70)$$

Instead of Eq. (4.68), we now have

$$R_\sigma(\check{r}_\infty, \check{h}; L) = \frac{2R_0}{N} \left[K_d \left(R_0 \ln(R_0/L^2) - \check{r}_\infty \ln \frac{\check{r}_\infty}{L^2} \right) + 2Q'_{d,6-d}(R_0) \right], \quad (4.71)$$

where the function N continues to be given by Eq. (4.69). Likewise, Eqs. (4.66) and (4.67) for R_0 and R_ω remain valid.

In the case of primary interest, $d=3$, these results can be augmented by determining the explicit solution to Eq. (4.66) for $h=0$. To this end, we substitute the result (B19) derived in Appendix B 1 for the function $Q_{3,2}$. Straightforward algebraic manipulations then lead to

$$R_0(\check{r}_\infty, 0) = 4 \operatorname{arcsch}^2[2 \exp(-\sqrt{\check{r}_\infty}/2)] = 4 \ln^2 \left[\frac{1}{2} \left(e^{\sqrt{\check{r}_\infty}/2} + \sqrt{4 + e^{\sqrt{\check{r}_\infty}/2}} \right) \right]. \quad (4.72)$$

This and the associated scaling function that follows from it via Eq. (4.67) are depicted in Figs. 1 and 2, respectively. Figure 3 shows the function $R_\sigma(\check{r}_\infty, 0; L)$ defined in Eq. (4.71).

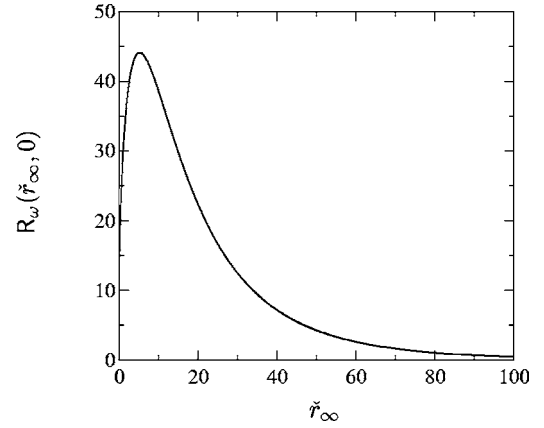


FIG. 2. Scaling function $R_\omega(\check{r}_\infty, 0)$ for $d=3$ that one obtains by inserting Eq. (4.72) into (4.67).

In conjunction with Eqs. (4.67), (4.68), and (4.70), the result (4.72) gives us the asymptotic behavior of r_L for $h=0$ in three dimensions including corrections to scaling, in an explicit analytic form.

V. FINITE-SIZE BEHAVIOR OF FREE ENERGY AND CASIMIR FORCE

We now turn to the computation of the finite-size free energy (3.15), beginning again with the case $d+\sigma < 6$.

A. The case $d+\sigma < 6$ with $2 < d < 4$ and $2 < \sigma < 4$

In order to use Eq. (3.19), we need the L -dependent part of $U_{d,\Omega}(0|L)$. The calculation is performed in Appendix C, giving

$$\Delta U_{d,\Omega}(0|L) \approx L^{-d} [\Delta_C^{\text{GM}}(d) + \check{g}_\sigma \Delta_{\sigma,C}^{\text{GM}}(d, \sigma) + O(b^2)]. \quad (5.1)$$

Here

$$\Delta_C^{\text{GM}}(d) = -\pi^{-d/2} \Gamma(d/2) \zeta(d) \quad (5.2)$$

and

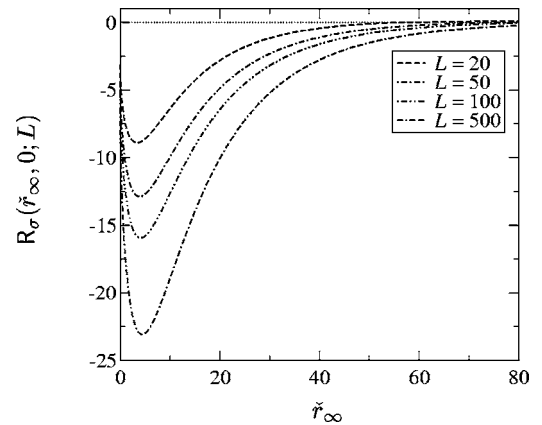


FIG. 3. Function $R_\sigma(\check{r}_\infty, 0; L)$ for $d=3$ and the indicated values of L , as obtained by insertion of Eq. (4.72) into (4.71).

$$\Delta_{\sigma,C}^{\text{GM}}(d,\sigma) = -\frac{2^{\sigma-2}\zeta(d+\sigma-2)\Gamma[(d+\sigma-2)/2]}{\pi^{d/2}\Gamma(1-\sigma/2)} \quad (5.3)$$

are the values of the Casimir amplitudes (2.21) and (2.22) for our Gaussian model, where $\zeta(d)$ is the Riemann zeta function.

Upon exploiting the relation (B5) between the derivatives of $Q_{d+2,2}(r)/r$ and $Q_{d,2}(r)/r$ derived in Appendix B, one can readily integrate Eq. (4.49) to obtain

$$\Delta U_{d,\Omega}^{(0)}(r|L) \approx -L^{-d} \left(\Delta_{\sigma,C}^{\text{GM}}(d) + \frac{4\pi}{rL^2} Q_{d+2,2}(rL^2) \right). \quad (5.4)$$

Likewise, $\Delta U_{d,\Omega}^{(1)}(r|L)$ follows by integration of Eq. (4.48). A simple integration by parts yields

$$\Delta U_{d,\Omega}^{(1)}(r|L) \approx L^{-(d+\sigma-2)} Q_{d,\sigma}(rL^2). \quad (5.5)$$

The above results can now be combined in a straightforward fashion to determine the scaled free-energy density $f_L L^{d-1}$. One gets

$$L^{d-1}(f_L - Lf^{(0)}) \approx Y(\check{r}, \check{r}, \check{h}, \check{g}_\omega, \check{g}_\sigma) \Big|_{\check{r}=\check{r}_L} \quad (5.6)$$

with

$$\begin{aligned} Y(\check{r}, \check{r}, \check{h}, \check{g}_\omega, \check{g}_\sigma) \equiv & \frac{1}{2} \check{r} \check{t} - \frac{\check{h}^2}{2\check{r}} - \frac{A_d}{d} \check{r}^{d/2} - \frac{4\pi}{\check{r}} Q_{d+2,2}(\check{r}) \\ & + \frac{\check{g}_\omega}{4} \check{r}^2 + \check{g}_\sigma \left(\Delta_{\sigma,C}^{\text{GM}}(d,\sigma) + Q_{d,\sigma}(\check{r}) \right. \\ & \left. - \frac{B_{d,\sigma}}{d+\sigma-2} \check{r}^{(d+\sigma-2)/2} \right), \end{aligned} \quad (5.7)$$

where $f^{(0)} \equiv f^{(0)}(K)$ denotes the smooth background term (3.16). As indicated, the function Y in the first equation must be taken at the solution \check{r}_L of the scaled equation of state $\partial Y(\check{r}, \check{r}, \check{h}, \check{g}_\omega, \check{g}_\sigma) / \partial \check{r} = 0$, Eq. (4.53).

The bulk free-energy density (per volume) f_{bk} follows from this in a straightforward manner. As is shown in Appendix B, the functions $Q_{d,2}(r)$ and $Q_{d,\sigma \neq 2}(r)$ behave for large values of r as

$$Q_{d,2}(r) = \frac{r^{(d+1)/4}}{r \rightarrow \infty} \frac{1}{2(2\pi)^{(d-1)/2}} e^{-\sqrt{r}} [1 + O(r^{-1/2})] \quad (5.8)$$

and

$$Q_{d,\sigma}(r) = -\Delta_{\sigma,C}^{\text{GM}}(d,\sigma) - \frac{D_\sigma(d)}{r} + O(r^{-2}), \quad (5.9)$$

respectively, where

$$D_\sigma(d) = \frac{2^\sigma \Gamma[(d+\sigma)/2]}{\pi^{d/2} \Gamma(-\sigma/2)} \zeta(d+\sigma), \quad (5.10)$$

according to Eq. (B33). Though not needed here, the value of this coefficient appears in our subsequent analysis; it is positive for $2 < \sigma < 4$ and vanishes at both $\sigma=2$ and 4 . Since the same applies to $\Delta_{\sigma,C}^{\text{GM}}(d+2,\sigma)$, the results (5.8) and (5.9) are in conformity with each other.

Hence neither the term $\propto Q_{d+2,2}$ in Eq. (5.6) nor the sum of $Q_{d,\sigma}$ and $\Delta_{\sigma,C}^{\text{GM}}(d,\sigma)$ contribute in the thermodynamic bulk limit. The remaining terms yield

$$\begin{aligned} f_{\text{bk}} - f^{(0)} \approx & \frac{r_\infty}{2} g_t - \frac{g_\omega^2}{2r_\infty} - \frac{A_d}{d} r_\infty^{d/2} + \frac{g_\omega}{4} r_\infty^2 \\ & - g_\sigma \frac{B_{d,\sigma}}{d+\sigma-2} r_\infty^{(d+\sigma-2)/2}. \end{aligned} \quad (5.11)$$

The difference of the right-hand sides of Eqs. (5.6) and (5.11) gives us the scaled excess free-energy density $L^{d-1} f_{\text{ex}}^{\text{sing}}$. In the result, the scaling function \mathcal{R} of Eq. (4.54) must be substituted for \check{r} , and for r_∞ , we have the scaling form (4.15) and the relationship (4.59) between the scaling functions \mathcal{R} and \mathcal{R}_∞ . Obviously, the resulting expression for $L^{d-1} f_{\text{ex}}^{\text{sing}}$ therefore complies with the scaling form (2.14).

To derive and describe what this means in terms of explicit results for scaling functions, it is advantageous to eliminate the temperature field g_t in favor of the inverse bulk susceptibility r_∞ (which in the spherical model is related to the bulk correlation length ξ_∞ via $r_\infty \propto \xi_\infty^{-2}$). The advantage originates from the explicit results we have been able to get for the dependence of \check{r}_L on \check{r}_∞ . Denoting the corresponding analogs of the scaling functions X, \dots, X_ω in Eqs. (2.14) and (2.20) by Y, \dots, Y_ω , we write

$$f_{\text{ex}}^{\text{sing}} \approx L^{-(d-1)} Y(r_\infty L^2, h L^{\Delta/\nu}, g_\omega L^{-\omega}, g_\sigma L^{-\omega\sigma}) \quad (5.12)$$

with

$$Y(\check{r}_\infty, \check{h}, \check{g}_\omega, \check{g}_\sigma) = Y_0(\check{r}_\infty, \check{h}) + \check{g}_\omega Y_\omega(\check{r}_\infty, \check{h}) + \check{g}_\sigma Y_\sigma(\check{r}_\infty, \check{h}) + \dots \quad (5.13)$$

The above results in conjunction with those of Secs. IV C and IV D yield the scaling functions

$$\begin{aligned} Y_0(\check{r}_\infty, \check{h}) = & -\frac{A_d}{2} \check{r}_\infty^{(d-2)/2} [\check{r}_\infty - \mathbf{R}_0(\check{r}_\infty, \check{h})] + \frac{A_d}{d} [\check{r}_\infty^{d/2} \\ & - \mathbf{R}_0^{d/2}(\check{r}_\infty, \check{h})] - \frac{4\pi Q_{d+2,2}[\mathbf{R}_0(\check{r}_\infty, \check{h})]}{\mathbf{R}_0(\check{r}_\infty, \check{h})} \\ & - \frac{\check{h}^2 [\check{r}_\infty - \mathbf{R}_0(\check{r}_\infty, \check{h})]^2}{2\check{r}_\infty^2 \mathbf{R}_0(\check{r}_\infty, \check{h})}, \end{aligned} \quad (5.14)$$

$$Y_\omega(\check{r}_\infty, \check{h}) = \frac{1}{4} [\check{r}_\infty - \mathbf{R}_0(\check{r}_\infty, \check{h})]^2, \quad (5.15)$$

and

$$\begin{aligned} Y_\sigma(\check{r}_\infty, \check{h}) = & \Delta_{\sigma,C}^{\text{GM}}(d,\sigma) + Q_{d,\sigma}[\mathbf{R}_0(\check{r}_\infty, \check{h})] \\ & + B_{d,\sigma} \left(\frac{\check{r}_\infty^{(d+\sigma-2)/2} - \mathbf{R}_0^{(d+\sigma-2)/2}(\check{r}_\infty, \check{h})}{d+\sigma-2} \right. \\ & \left. - \frac{\check{r}_\infty - \mathbf{R}_0(\check{r}_\infty, \check{h})}{2} \check{r}_\infty^{(d+\sigma-4)/2} \right). \end{aligned} \quad (5.16)$$

Note that \check{r}_∞ is the full inverse bulk susceptibility, which itself has corrections to scaling $\sim g_\omega$ and g_σ according to Eq.

(4.54). Expanding it in powers of g_ω and g_σ to express $f_{\text{ex}}^{\text{sing}}$ in terms of $\check{r}|_{g_\omega=g_\sigma=0}$ would produce contributions linear in g_ω and g_σ , in addition to those involving Y_ω and Y_σ .

1. Behavior at bulk criticality

At the bulk critical point (BCP) $T=T_{c,\infty}$, $h=0$, the above results reduce to

$$f_{\text{ex,BCP}}^{\text{sing}} \approx L^{-(d-1)} \left(\Delta_C^{\text{SM}}(d) + \Delta_{\omega,C}^{\text{SM}}(d) \frac{g_\omega(b)}{L^{4-d}} + \Delta_{\sigma,C}^{\text{SM}}(d, \sigma) \frac{g_\sigma(b)}{L^{\sigma-2}} + \dots \right), \quad (5.17)$$

where Δ_C^{SM} , $\Delta_{\omega,C}^{\text{SM}}$ and $\Delta_{\sigma,C}^{\text{SM}}$, the spherical-model values of the amplitudes (2.21)–(2.23), are given by [82,83]

$$\Delta_C^{\text{SM}}(d) \equiv Y_0(0,0) = -\frac{A_d}{d} \mathbf{R}_{0,\text{BCP}}^{d/2} - \frac{4\pi Q_{d+2,2}(\mathbf{R}_{0,\text{BCP}})}{\mathbf{R}_{0,\text{BCP}}}, \quad (5.18)$$

$$\Delta_{\omega,C}^{\text{SM}}(d) \equiv Y_\omega(0,0) = \mathbf{R}_{0,\text{BCP}}^2/4, \quad (5.19)$$

and

$$\Delta_{\sigma,C}^{\text{SM}}(d, \sigma) \equiv Y_\sigma(0,0) = \Delta_{\sigma,C}^{\text{GM}}(d, \sigma) + Q_{d,\sigma}(\mathbf{R}_{0,\text{BCP}}) - \frac{B_{d,\sigma}}{d + \sigma - 2} \mathbf{R}_{0,\text{BCP}}^{(d+\sigma-2)/2}. \quad (5.20)$$

Here $\mathbf{R}_{0,\text{BCP}} \equiv \mathbf{R}_0(0,0)$ is the d -dependent solution to Eq. (4.66) at the bulk critical point.

Thus at bulk criticality, the scaling fields g_ω and g_σ indeed give leading and next-to-leading corrections to the familiar first term involving the Casimir amplitude $\Delta_C^{\text{SM}}(d)$ of the spherical model with short-range interactions.

2. Behavior for $T > T_{c,\infty}$ and $h=0$

Next, we consider the case $T > T_{c,\infty}$ and $h=0$. As $L \rightarrow \infty$, the scaled inverse finite-size and bulk susceptibilities \check{r}_L and \check{r}_∞ both tend toward $+\infty$. Hence, to obtain the asymptotic large- L behavior, we must study the behavior of the functions \mathbf{R}_0 , \mathbf{R}_ω , and \mathbf{R}_σ in the limit $\check{r}_\infty \rightarrow \infty$. Clearly, $\mathbf{R}_0(\check{r}_\infty, \check{h}) \rightarrow \check{r}_\infty$ as $\check{r}_\infty \rightarrow \infty$. To determine the asymptotic large- \check{r}_∞ behavior of $\mathbf{R}_0(\check{r}_\infty, 0)$, we choose \check{r}_∞ so large that the function $Q_{d,2}(\mathbf{R}_0)$ in Eq. (4.66) can safely be replaced by the first term of its asymptotic expansion (5.8). Solving for $\mathbf{R}_0(\check{r}_\infty, 0)$ then yields

$$\mathbf{R}_0(\check{r}_\infty, 0) \approx \check{r}_\infty + \frac{2(2\pi)^{(1-d)/2}}{(d-2)A_d} \check{r}_\infty^{(5-d)/4} e^{-\check{r}_\infty^{1/2}} [1 + O(\check{r}_\infty^{-1/2})], \quad (5.21)$$

where \check{r}_∞ now also is to be taken at $h=0$.

Using this result together with Eqs. (5.8) and (5.9), one can derive the large- \check{r}_∞ behavior of the scaling functions Y_0 , Y_ω , and Y_σ in a straightforward fashion. One obtains

$$Y_0(\check{r}_\infty, 0) \approx -\frac{1 + O(\check{r}_\infty^{-1/2})}{(2\pi)^{(d-1)/2}} \check{r}_\infty^{(d-1)/4} e^{-\check{r}_\infty^{1/2}}, \quad (5.22)$$

$$Y_\omega(\check{r}_\infty, 0) \approx \frac{(2\pi)^{1-d}}{(d-2)^2 A_d^2} \check{r}_\infty^{(5-d)/2} e^{-2\check{r}_\infty^{1/2}} [1 + O(\check{r}_\infty^{-1/2})], \quad (5.23)$$

and

$$Y_\sigma(\check{r}_\infty, 0) \approx -D_\sigma(d) \check{r}_\infty^{-1} + O(\check{r}_\infty^{-2}), \quad (5.24)$$

where $D_\sigma(d)$ is the constant introduced in Eq. (5.10). Unlike $Y_0(\check{r}_\infty, 0)$ and $Y_\omega(\check{r}_\infty, 0)$, which decay exponentially, the scaling function $Y_\sigma(\check{r}_\infty, 0)$ decays in an algebraic manner.

Thus the contribution due to this latter slowly decaying term governs the large- L behavior of the excess free energy $f_{\text{ex}}^{\text{sing}}$ for $T > T_{c,\infty}$ whenever the coupling constant b of the long-range potential does not vanish. One has

$$f_{\text{ex}}^{\text{sing}} \approx -g_\sigma(b) \frac{D_\sigma(d)}{r_\infty} L^{-(d+\sigma-1)} \approx -g_\sigma(b) L^{-(d+\sigma-1)} D_\sigma(d) \left(\frac{g_t}{A_d} \right)^{-\gamma}, \quad (5.25)$$

where we substituted Eq. (4.21) for r_∞ to obtain the second line. This strongly contrasts with the asymptotic form that applies in the absence of long-range interactions:

$$f_{\text{ex}}^{\text{sing}}|_{b=0} \approx - (2\pi L)^{-(d-1)/2} \left(\frac{g_t}{A_d} \right)^{[(d-1)/4]\gamma} e^{-(g/A_d)^\nu L}. \quad (5.26)$$

B. The case $d+\sigma=6$ with $2 < d < 4$

Proceeding along similar lines as in the foregoing subsection, one can derive the analogs of Eqs. (5.6) and (5.11)–(5.13). They read

$$L^{d-1}(f_L - Lf^{(0)}) \approx \frac{1}{2} \check{r}_L \check{t} - \frac{\check{h}^2}{2\check{r}_L} - \frac{A_d}{d} \check{r}_L^{d/2} - \frac{4\pi}{\check{r}_L} Q_{d+2,2}(\check{r}_L) + \frac{1}{4} (w_d + \tilde{w}_d b) L^{d-4} \check{r}_L^2 + \check{g}_\sigma \left(\Delta_{6-d,C}^{\text{GM}}(d) + Q_{d,6-d}(\check{r}_L) + \frac{K_d}{4} \check{r}_L^2 \ln \frac{\check{r}_L}{L^2} \right), \quad (5.27)$$

$$f_{\text{bk}} - f^{(0)} \approx \frac{r_\infty}{2} g_t - \frac{g_h^2}{2r_\infty} - \frac{A_d}{d} r_\infty^{d/2} + \frac{w_d + b\tilde{w}_d}{4} r_\infty^2 + g_\sigma \frac{K_d}{4} r_\infty^2 \ln r_\infty, \quad (5.28)$$

and

$$L^{d-1} f_{\text{ex}}^{\text{sing}} \approx Y_0(\check{r}_\infty, \check{h}) + (w_d + \tilde{w}_d b) L^{d-4} Y_\omega(\check{r}_\infty, \check{h}) + \check{g}_\sigma Y_\sigma(\check{r}_\infty, \check{h}; L) + \dots, \quad (5.29)$$

where

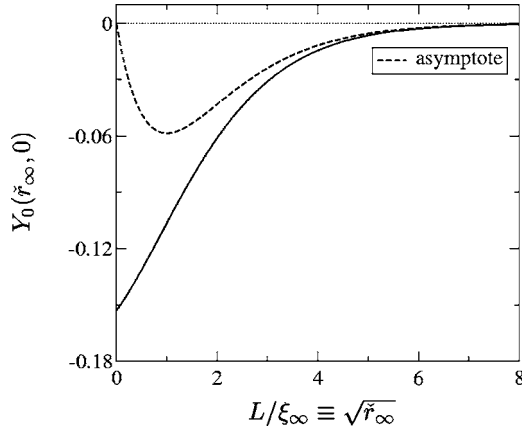


FIG. 4. Scaling function $Y_0(\check{r}_\infty, 0)$ for $d=3$ (full line). The dashed line represents the asymptote (5.22). The value $Y_0(0, 0) = \Delta_C^{\text{SM}}(d=3)$ which $Y_0(\check{r}_\infty, 0)$ approaches as $\check{r}_\infty \rightarrow 0$ is known exactly: According to Ref. [82], it is given by $\Delta_C^{\text{SM}}(3) = -2\zeta(3)/(5\pi) = -0.15305\dots$

$$Y_\sigma(\check{r}_\infty, \check{h}; L) = \Delta_{\sigma, C}^{\text{GM}}(d, 6-d) + Q_{d, 6-d}[\mathbf{R}_0(\check{r}_\infty, \check{h})] + \frac{K_d}{4} \left([\check{r}_\infty - 2\mathbf{R}_0(\check{r}_\infty, \check{h})] \check{r}_y \ln \frac{\check{r}_\infty}{L^2} + \mathbf{R}_0^2(\check{r}_\infty, \check{h}) \ln \frac{\mathbf{R}_0(\check{r}_\infty, \check{h})}{L^2} \right). \quad (5.30)$$

while the functions Y_0 and Y_ω remain given by Eqs. (5.14) and (5.15), respectively. Owing to the presence of logarithmic anomalies, the analogs of the scaling functions Y and Y_σ in Eq. (5.13) have an additional explicit dependence on L . It should also be remembered that logarithmic anomalies reside also in the temperature dependence of the b -dependent corrections to scaling of \check{r}_∞ .

The scaling functions $Y_0(\check{r}_\infty, 0)$ and $Y_\omega(\check{r}_\infty, 0)$ for the three-dimensional case are plotted in Figs. 4 and 5, respectively. In Fig. 6, the function $Y_\sigma(\check{r}_\infty, h=0; L)$ is displayed for the case $d=\sigma=3$ and some values of L .

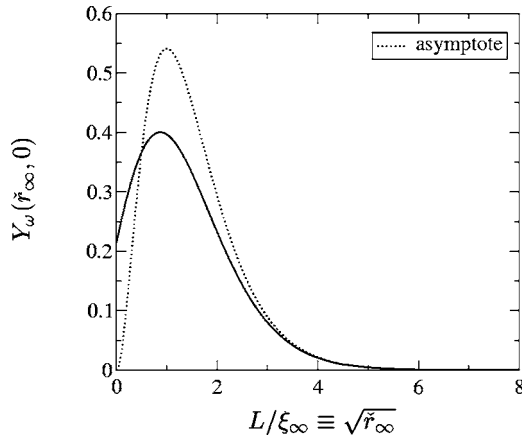


FIG. 5. Scaling function $Y_\omega(\check{r}_\infty, 0)$ for $d=3$ (full line). The dashed line represents the asymptote (5.23).

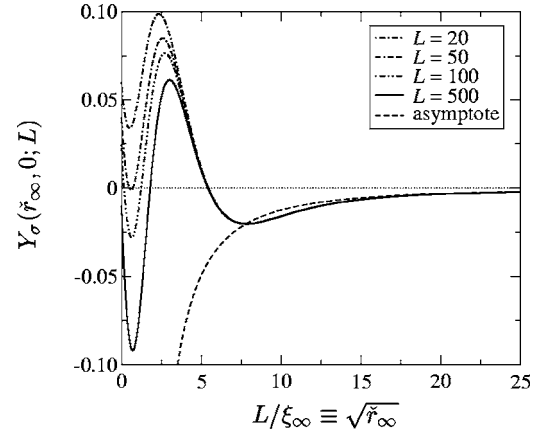


FIG. 6. Function $Y_\sigma(\check{r}_\infty, 0; L)$ for $d=\sigma=3$ and the indicated values of L (dashed-dotted and full lines). The dashed line represents the corresponding asymptote (5.24) with $d=\sigma=3$.

1. Behavior at bulk criticality

Let us again see how these results simplify at the bulk critical point. From Eqs. (5.29) and (5.30) one easily deduces the asymptotic behavior

$$f_{\text{ex,BCP}}^{\text{sing}} \approx L^{-(d-1)} \left[\Delta_C^{\text{SM}}(d) + \frac{g_\sigma(b)}{L^{4-d}} \left(\frac{K_d}{4} \mathbf{R}_{0,\text{BCP}}^2 \ln \frac{\mathbf{R}_{0,\text{BCP}}}{L^2} + \Delta_{\sigma, C}^{\text{GM}}(d, 6-d) + Q_{d, 6-d}(\mathbf{R}_{0,\text{BCP}}) \right) + \Delta_{\omega, C}^{\text{SM}}(d) \frac{w_d + \tilde{w}_d b}{L^{4-d}} + \dots \right]. \quad (5.31)$$

The leading correction to scaling now results from the b -dependent contribution involving the logarithmic anomaly.

2. Behavior for $T > T_{c, \infty}$ and $h=0$

Turning to the case of $T > T_{c, \infty}$ and $h=0$, let us again consider the asymptotic behavior of $f_{\text{ex}}^{\text{sing}}$ for $L \rightarrow \infty$ at fixed $T > T_{c, \infty}$. Upon inserting the large- \check{r}_∞ form (5.21) of \mathbf{R}_0 into the result (5.30) for Y_σ , one sees that the contribution in large parentheses decays exponentially and hence is asymptotically negligible compared to the algebraically decaying contribution from the sum of the two terms in the first line of this equation. This means that the limiting form (5.24) carries over to the present case, except that we must set $\sigma=6-d$. Since the expressions (5.14) and (5.15) for the scaling functions Y_0 and Y_ω —and hence their limiting forms (5.22) and (5.23)—continue to hold, the results (5.25) and (5.26) for the leading asymptotic behavior of $f_{\text{ex}}^{\text{sing}}$ when $b \neq 0$ or $b=0$, respectively, also remain valid.

3. The case $d=\sigma=3$

In Fig. 7 the scaled excess free-energy densities (5.29) of the three-dimensional case with nonretarded van der Waals-type interactions ($\sigma=3$) and without are compared for the chosen value $L=50$ of the slab thickness L . For simplicity, we have set the nonuniversal constants w_d and \tilde{w}_d to unity.

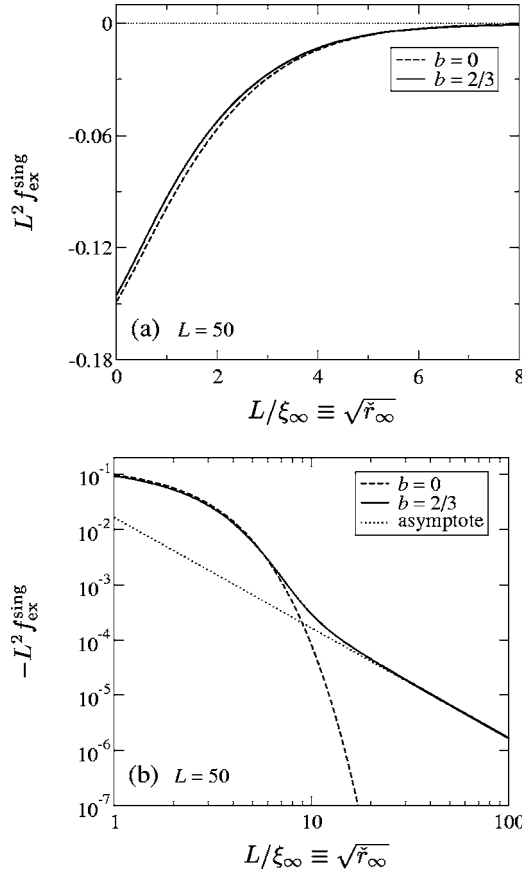


FIG. 7. Scaled excess free-energy density (5.29) of the three-dimensional spherical model in an $L \times \infty^2$ slab with periodic boundary conditions for $L=50$, plotted versus the finite-size scaling variable $L/\xi_{\infty} \equiv \sqrt{\check{r}_{\infty}}$ (a). The solid line corresponds to the case $\sigma=3$ of nonretarded van der Waals-type interactions with $g_{\sigma}(b) \equiv b=2/3$; the dashed line shows results for the short-range case $b=0$ for comparison. In (b) the graphs displayed in (a) are plotted in a double-logarithmic manner. In this representation the asymptote (5.24) (dotted line) becomes a straight line with the slope -2 . The nonuniversal constants w_d and \tilde{w}_d both have been set to unity.

As can clearly be seen from the double-logarithmic plot (b), the asymptotic behavior for large L/ξ_{∞} when $b \neq 0$ is characterized by the asymptote (5.24) and differs strongly from its counterpart for the short-range case $b=0$.

In order to illustrate the effect of the explicit dependence of the scaled excess free-energy density (5.29) for nonvanishing interaction constant b on L , we display in Fig. 8 linear and double-logarithmic plots of $L^2 f_{\text{ex}}^{\text{sing}}$ for a variety of values of L , including $L=\infty$. For the sake of simplicity, we have set the nonuniversal constants w_d and \tilde{w}_d to unity.

C. The Casimir force

Using the results of the foregoing subsection for the excess free energy, the large-scale behavior of the Casimir force (2.3) can be derived in a straightforward fashion. Depending on whether $d+\sigma < 6$ or $d+\sigma = 6$, we have

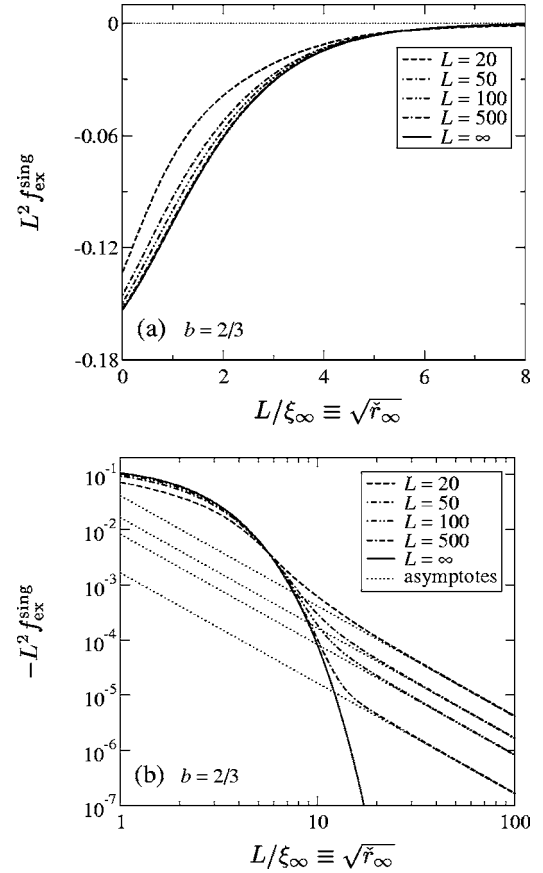


FIG. 8. Scaled excess free-energy densities (5.29) of the three-dimensional spherical model in an $L \times \infty^2$ slab with periodic boundary conditions and nonretarded van der Waals-type interactions ($\sigma=3$). The results for various choices of L including $L=\infty$ are shown as linear (a) and double-logarithmic plots (b). The asymptotes (dotted lines) correspond to the power-law behavior (5.24). The nonuniversal constants w_d and \tilde{w}_d both have been set to unity.

$$\begin{aligned} \frac{\mathcal{F}_C^{\text{sing}}}{k_B T} \approx L^{-d} [& \Xi_0(\check{r}_{\infty}, \check{h}) + g_{\omega}(b) L^{-\omega} \Xi_{\omega}(\check{r}_{\infty}, \check{h}) \\ & + g_{\sigma}(b) L^{-\omega_{\sigma}} \Xi_{\sigma}(\check{r}_{\infty}, \check{h}) + \dots] \end{aligned} \quad (5.32)$$

or

$$\begin{aligned} \frac{\mathcal{F}_C^{\text{sing}}}{k_B T} \approx L^{-d} [& \Xi_0(\check{r}_{\infty}, \check{h}) + (w_d + \tilde{w}_d b) L^{-\omega} \Xi_{\omega}(\check{r}_{\infty}, \check{h}) \\ & + g_{\sigma}(b) L^{-\omega} \Xi_{\sigma}(\check{r}_{\infty}, \check{h}; L) + \dots], \end{aligned} \quad (5.33)$$

where ω and ω_{σ} take their spherical-model values (2.18) and (4.16), respectively. The scaling form (5.32) should hold more generally for the n -vector model with $2 < d < 4$ even when $d+\sigma=6$, as long as ω and ω_{σ} are not degenerate. This applies, in particular, to the case $d=\sigma=3$ of nonretarded van der Waals interactions, albeit with the appropriate (different) values of ω and ω_{σ} , and different scaling functions.

By taking the derivatives of Eqs. (5.12) and (5.29) and with respect to L , one can express the above functions $\Xi_0, \dots, \Xi_{\sigma}$ in terms of the functions Y_0, \dots, Y_{σ} . One finds

$$\Xi_0(\check{r}_\infty, \check{h}) = \left(d - 1 - 2\check{r}_\infty \partial_{\check{r}_\infty} - \frac{\Delta}{\nu} \check{h} \partial_{\check{h}} \right) Y_0(\check{r}_\infty, \check{h}), \quad (5.34)$$

$$\Xi_\omega(\check{r}_\infty, \check{h}) = \left(d + \omega - 1 - 2\check{r}_\infty \partial_{\check{r}_\infty} - \frac{\Delta}{\nu} \check{h} \partial_{\check{h}} \right) Y_\omega(\check{r}_\infty, \check{h}), \quad (5.35)$$

$$\Xi_\sigma(\check{r}_\infty, \check{h}) = \left(d + \omega_\sigma - 1 - 2\check{r}_\infty \partial_{\check{r}_\infty} - \frac{\Delta}{\nu} \check{h} \partial_{\check{h}} \right) Y_\sigma(\check{r}_\infty, \check{h}), \quad (5.36)$$

and

$$\begin{aligned} \Xi_\sigma(\check{r}_\infty, \check{h}; L) \\ = \left(d + \omega_\sigma - 1 - 2\check{r}_\infty \partial_{\check{r}_\infty} - \frac{\Delta}{\nu} \check{h} \partial_{\check{h}} - L \partial_L \right) Y_\sigma(\check{r}_\infty, \check{h}; L), \end{aligned} \quad (5.37)$$

where again the spherical-model values (2.18) and (4.16) must be substituted for ω , ω_σ , and Δ/ν [84].

Noting that the limit of R_0 as \check{r}_∞ and \check{h} approach the bulk critical point exists,

$$R_0(\check{r}_\infty, \check{h}) \underset{\check{r}_\infty, \check{h} \rightarrow 0}{=} R_{0,\text{BCP}} + o(\check{r}_\infty, \check{h}), \quad (5.38)$$

one sees that the same applies to the scaling functions $Y_i(\check{r}_\infty, \check{h})$:

$$Y_i(\check{r}_\infty, \check{h}) \underset{\check{r}_\infty, \check{h} \rightarrow 0}{=} Y_i(0,0) + o(\check{r}_\infty, \check{h}), \quad i = 0, \omega, \sigma. \quad (5.39)$$

Hence the terms in Eqs. (5.34)–(5.37) involving the derivatives with respect to \check{r}_∞ and \check{h} yield vanishing contributions as the bulk critical point is approached. Using this in conjunction with Eqs. (5.18)–(5.20) and (5.31), one finds that the values of these functions at the bulk critical point become

$$\Xi_0(0,0) = (d-1)\Delta_C^{\text{SM}}(d), \quad (5.40)$$

$$\Xi_\omega(0,0) = (d+\omega-1)\Delta_{\omega,C}^{\text{SM}}(d), \quad (5.41)$$

$$\Xi_\sigma(0,0) = (d+\omega_\sigma-1)\Delta_{\sigma,C}^{\text{SM}}(d,\sigma), \quad (5.42)$$

and

$$\begin{aligned} \Xi_\sigma(0,0;L) = & 3[\Delta_{\sigma,C}^{\text{GM}}(d,6-d) + Q_{d,6-d}(R_{0,\text{BCP}})] \\ & + \frac{K_d}{4} R_{0,\text{BCP}}^2 \left(2 + 3 \ln \frac{R_{0,\text{BCP}}}{L^2} \right). \end{aligned} \quad (5.43)$$

To obtain the critical Casimir forces in the cases $d+\sigma < 6$ and $d+\sigma=6$, we must simply substitute the scaling functions Ξ_i in Eqs. (5.32) and (5.33), respectively, by their above values at the bulk critical point.

The asymptotic forms of the Casimir force as $L \rightarrow \infty$ at fixed temperature $T > T_{c,\infty}$ and zero magnetic field can be inferred in a straightforward fashion from the corresponding results (5.25) and (5.26) for the excess free-energy density.

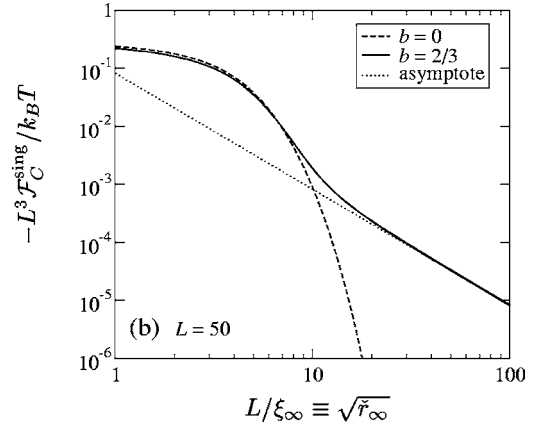
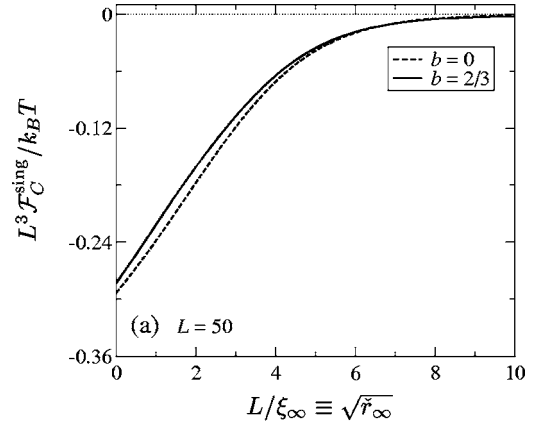


FIG. 9. Scaled Casimir force (5.33) of the three-dimensional spherical model in an $L \times \infty^2$ slab with periodic boundary conditions for $L=50$, plotted versus the finite-size scaling variable $L/\xi_\infty \equiv \sqrt{\check{r}_\infty}$ (a). The solid line corresponds to the case $\sigma=3$ of non-retarded van der Waals-type interactions with $g_\sigma(b) \equiv b=2/3$; the dashed line represents results for the short-range case $b=0$ for comparison. In (b) the graphs displayed in (a) are plotted in a double-logarithmic manner. In this representation the asymptote (5.44) $\sim \check{r}_\infty^{-1}$ (dotted line) becomes a straight line with the slope -2 . The nonuniversal constants w_d and \tilde{w}_d both have been set to unity.

Depending on whether a long-range interaction proportional to b is present or absent, one has

$$\left. \frac{\mathcal{F}_C^{\text{sing}}}{k_B T} \right|_{b \neq 0, L \rightarrow \infty} \approx -g_\sigma(b)(d+\sigma-1) \frac{D_\sigma(d)}{L^{d+\sigma}} \left(\frac{g_t}{A_d} \right)^{-\gamma} \quad (5.44)$$

or the exponential decay

$$\left. \frac{\mathcal{F}_C^{\text{sing}}}{k_B T} \right|_{b=0, L \rightarrow \infty} \approx - \frac{(g_t/A_d)^{(d+1)\gamma/4}}{(2\pi L)^{(d-1)/2}} e^{-L(g_t/A_d)^\nu}. \quad (5.45)$$

Here again the spherical-model values (4.16) must be substituted for γ and ν .

Figure 9 shows a comparison of the Casimir forces (5.33) of an $\infty^2 \times L$ slab of thickness $L=50$ with and without van der Waals-type interactions ($\sigma=3$), where we have again set the nonuniversal constants w_d and \tilde{w}_d to unity. The double-logarithmic plot (b) again nicely demonstrates the approach

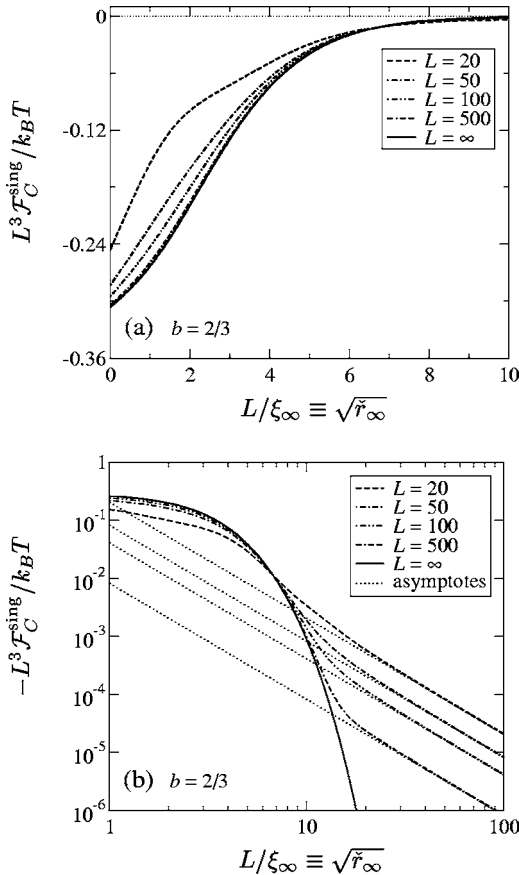


FIG. 10. Scaled Casimir force (5.33) of the three-dimensional spherical model in a $L \times \infty^2$ slab with periodic boundary conditions and nonretarded van-der-Waals-type interactions ($\sigma=3$). The results for various choices of L including $L=\infty$ are shown as linear (a) and double-logarithmic plots (b). The asymptotes (dotted lines) correspond to the power-law behavior $\sim \tilde{r}_\infty^{-1}$ of Eqs. (5.24) and (5.44). The nonuniversal constants w_d and \tilde{w}_d both have been set to unity.

to the asymptote $\sim \tilde{r}_\infty^{-1}$ and the qualitatively different behavior in the short-range case.

In Fig. 10 we illustrate how the scaled Casimir force for the case with van-der-Waals-type interactions ($\sigma=3$) varies under changes of the slab thickness L .

VI. SUMMARY AND CONCLUSIONS

In this paper we have studied the effects of long-range interactions whose pair potential decays at large distances as $x^{-d-\sigma}$ with $2 < \sigma < 4$. Prominent examples of such interactions are nonretarded and retarded van der Waals forces. The latter are ubiquitous in nature; in particular, they are present in fluids.

Application of the phenomenological theory of finite-size scaling revealed that such long-range interactions are of the kind termed “subleading long-range interactions” [36] and hence should yield corrections to scaling in the critical regime near the bulk critical point.

For systems belonging to the universality class of the n -component ϕ^4 model in d dimensions, the associated

correction-to-scaling exponent ω_σ , given in Eq. (2.11), has a larger value than its counterpart ω associated with the conventional leading corrections-to-scaling of $d \geq 3$ dimensional systems with short-range interactions. Hence the corrections-to-scaling governed by ω_σ are next to leading.

However, irrespective of whether ω is smaller or larger than ω_σ , the subleading long-range interactions yield a contribution to the Casimir force that decays in a power-law fashion as a function of the film thickness L , both at and away from the bulk critical temperature $T_{c,b}$. Since the fluctuation-induced Casimir force one has even in the absence of these long-range interactions, for $T > T_{c,b}$ decays exponentially on the scale of the correlation length, the contribution due to the long-range interactions becomes dominant for sufficiently large L .

To corroborate these findings we solved a mean spherical model with such long-range interactions—and hence the limit $n \rightarrow \infty$ of the corresponding n -vector model—exactly. For general values of $\sigma, d \in (2, 4)$, we confirmed the anticipated finite-size scaling behavior, and determined the scaling functions to first order in the irrelevant scaling fields g_ω and g_σ .

A crucial, though not unexpected, discovery was that the scaling field associated with the conventional leading corrections to scaling, g_ω , depends on the strength b of the long-range interactions. This dependence plays a role in the mechanism producing the logarithmic anomalies by which the finite-size scaling behavior of our model turned out to be modified when $d + \sigma = 6$. In these special cases—which include, in particular, the physically important one of nonretarded van der Waals interactions in three dimensions— anomalies of this kind showed up in b -dependent (leading) corrections to scaling. We were able to clarify their origin (see Sec. IV B 2): They are caused by the degeneracy $\omega = \omega_\sigma$ of the two correction-to-scaling exponents in conjunction with the b dependence of g_ω .

Thus, three-dimensional systems belonging to the universality classes of the scalar ϕ^4 model and its $O(n)$ counterparts with $n < \infty$ should not exhibit such logarithmic anomalies because their correction-to-scaling exponents ω and ω_σ are not degenerate.

It would be worthwhile to extend the present work in a number of different directions. We have focused our attention here on the case of temperatures $T \geq T_{c,\infty}$. An obvious next step is a detailed investigation of the model for temperatures below the bulk critical temperature $T_{c,\infty}$. For the spherical model with periodic boundary conditions considered here, such an extension, which we defer to a future publication, is relatively straightforward.

The scaling forms derived in this paper on the basis of phenomenological scaling ideas involved nontrivial critical indices, such as η and $\gamma/\nu = 2 - \eta$, and the correction-to-scaling exponent ω . Although the exact results for the spherical model we were able to present are in conformity with the predicted more general finite-size scaling forms, they permit us neither to corroborate the appearance of a nontrivial value of η nor to verify the n dependence of ω for the n -vector model. A desirable complementary check of the phenomenological predictions that is capable of identifying nontrivial values of η as well as the n dependence of it and other

exponents can be made by performing a two-loop RG analysis for small $\epsilon=4-d$. We have performed such an analysis; its results will be published elsewhere [48].

Valuable alternative checks of our phenomenological predictions should be possible by means of Monte Carlo simulations. Although it is quite a challenge to perform accurate Monte Carlo simulations of near-critical systems with long-range interactions, suitable algorithms were developed and demonstrated to be quite efficient recently [85–87]. We therefore believe that accurate tests of our predictions via such simulations are feasible.

An obviously important direction for further research is the extension of our work to other than periodic boundary conditions, namely, those of a kind giving a better representation of typical experimental situations. Important examples are slabs with Dirichlet boundary conditions on both boundary planes, or more generally, Robin boundary conditions. Although some aspects of our above findings should carry over to such boundary conditions—e.g., the form of the scaled variables encountered here and the power-law decrease of the Casimir away from the bulk critical temperature—it is clear that any quantitative comparison between theoretical predictions and results of a given experiment requires that appropriate boundary conditions have been chosen in the calculations. We leave such extensions to future work.

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APPENDIX A: FOURIER TRANSFORM OF THE INTERACTION POTENTIAL

In this appendix we wish to derive the small-momentum behavior of the Fourier transform (3.4) of the pair interaction $J(\mathbf{x})$ introduced in Eq. (3.3). To this end we introduce a lattice constant a_α for each of the principal directions of the simple hypercubic lattice in d dimensions we are concerned with. We assume that the lattice has an odd number $2N_\alpha+1$ (with $N_\alpha \in \mathbb{N}$) of layers perpendicular to the x_α axis, so that its linear extension along the x_α direction is $L_\alpha=(2N_\alpha+1)a_\alpha$.

With these conventions the lattice Fourier transform (3.4) of the pair interaction (3.3) becomes

$$\tilde{J}(\mathbf{q}) = \sum_{j_1=-N_1}^{N_1} \cdots \sum_{j_d=-N_d}^{N_d} J(\mathbf{x}^{(j)}) \prod_{\alpha=1}^d e^{-i\hat{q}_\alpha j_\alpha}, \quad (\text{A1})$$

where $\mathbf{x}^{(j)}=(j_\alpha a_\alpha)$ and we have introduced the dimensionless momentum components $\hat{q}_\alpha=q_\alpha a_\alpha$. The momentum \mathbf{q} takes values in the first Brillouin zone, i.e., $q_\alpha=2\pi\nu_\alpha/L_\alpha$ with $\nu_\alpha=-N_\alpha, -N_\alpha+1, \dots, N_\alpha$.

The contribution proportional to J_1 of Eq. (3.3) gives the usual result for nearest-neighbor interactions on a hypercubic lattice:

$$\tilde{J}_1(\mathbf{q}) = 2J_1 \sum_{\alpha=0}^d \cos(\hat{q}_\alpha) \quad (\text{A2})$$

$$= 2J_1 \left(d - \frac{1}{2}\hat{q}^2 + \frac{1}{24} \sum_{\alpha=1}^d [\hat{q}_\alpha^4 + O(\hat{q}_\alpha^6)] \right). \quad (\text{A3})$$

To compute the Fourier transform of the remaining part of the interaction (3.3), which we denote as $J_2(x)$, it is useful to recall Poisson's summation formula [[88], p. 31]

$$\sum_{j=-\infty}^{\infty} \delta(t-ja) = \frac{1}{a} \sum_{m=-\infty}^{\infty} e^{i2\pi mt/a}. \quad (\text{A4})$$

Applying the generalized functions on both sides to a test function $f(t)$ whose support is restricted to $[-L/2, L/2]$ gives

$$\sum_{j=-N}^N f(ja) = \sum_{m=-\infty}^{\infty} \int_{-L/2}^{L/2} \frac{dt}{a} e^{i2\pi mt/a} f(t). \quad (\text{A5})$$

Since we are interested in a system of macroscopic lateral extent, we take the limits $N_\alpha \rightarrow \infty$ for all $\alpha > 1$, keeping the associated lattice constants $a_\alpha > 0$ fixed. We thus obtain

$$\tilde{J}_2(\mathbf{q}) = \sum_{\mathbf{m} \in \mathbb{Z}^d} \int_{\mathfrak{V}_L} \frac{d^d x}{v_a} J_2(x) \prod_{\alpha=1}^d e^{-i(q_\alpha - 2\pi m_\alpha/a_\alpha)x_\alpha}, \quad (\text{A6})$$

where $v_a = \prod_{\alpha=1}^d a_\alpha$ is the volume of the unit cell, and the integration is over a slab $\mathfrak{V}_L = [-L/2, L/2] \times \mathbb{R}^{d-1}$ of thickness $L \equiv L_1$.

The terms with $\mathbf{m} \neq \mathbf{0}$ reflect the lattice structure of the model and give contributions anisotropic in \mathbf{q} space (as well as isotropic ones). Owing to the restricted integration regime, the $\mathbf{m}=\mathbf{0}$ term also yields \mathbf{q} -dependent contributions (which, however, are small for large L). These anisotropies add to those originating from the short-range contribution (A2) and produce, in particular, a nonzero value of the coefficient $b_{4,1}$ of the anisotropic q_α^4 terms in Eq. (3.7).

We have emphasized the importance of long-range van der Waals-type interactions for fluids before. Let us therefore consider the case of simple isotropic fluids. For such systems it is appropriate to take the continuum limit $a_\alpha \rightarrow 0$. Then the contributions of the $\mathbf{m} \neq \mathbf{0}$ terms vanish by the Riemann-Lebesgue lemma. We have

$$v_a \tilde{J}_2(\mathbf{q}) \xrightarrow{\{a_\alpha \rightarrow 0\}} \tilde{J}_{2,L}^{\text{cont}}(\mathbf{q}) \equiv \int_{\mathfrak{V}_L} d^d x J_2(x) e^{-i\mathbf{q} \cdot \mathbf{x}}. \quad (\text{A7})$$

In order that $\tilde{J}_2(\mathbf{q})$ have a nontrivial continuum limit, the coupling constant J_2 must be scaled such that J_2/v_a approaches a finite value $J_2^{\text{cont}} > 0$.

The Fourier transform has an explicit L dependence due to the restriction of the x_1 integration to a finite interval. However, the deviation from its bulk analog is small, unless L is very small: The integration over the parallel coordinates x_{\parallel} yields a function of x_1 that varies $\sim x_1^{-\sigma-1}$ for large x_1 . The

error resulting from $\int_L^\infty dx_1$ therefore decreases as $L^{-\sigma}$, i.e., decays $\sim N_1^{-\sigma}$ when $a_1 > 0$. Let us ignore this L dependence and determine the behavior of its bulk counterpart $\tilde{J}_{2,\infty}^{\text{cont}}(\mathbf{q})$ for small q .

The calculation of the latter is straightforward. The required angular integral is

$$\int d\Omega_d e^{i\mathbf{q}\cdot\mathbf{x}} = (2\pi)^{d/2} (qx)^{1-d/2} J_{(d-2)/2}(qx). \quad (\text{A8})$$

Performing the remaining radial integration gives

$$\tilde{J}_{2,\infty}^{\text{cont}}(\mathbf{q}) = J_2^{\text{cont}} 2\pi^{d/2} \left(\frac{q}{2\rho_0}\right)^{\sigma/2} \frac{K_{\sigma/2}(\rho_0 q)}{\Gamma[(d+\sigma)/2]}, \quad (\text{A9})$$

where $K_{\sigma/2}$ is a modified Bessel function. From its known asymptotic behavior for small values of q one easily derives the limiting form

$$\frac{\rho_0^\sigma \tilde{J}_{2,\infty}^{\text{cont}}(\mathbf{q})}{J_2^{\text{cont}}} = A_0 + A_2(\rho_0 q)^2 + A_4(\rho_0 q)^4 - A_\sigma(\rho_0 q)^\sigma + O(q^{\sigma+2}, q^6), \quad (\text{A10})$$

in which

$$A_0 = -2(\sigma-2)A_2 = -8(4-\sigma)(\sigma-2)A_4 = \frac{\pi^{d/2}\Gamma(\sigma/2)}{\Gamma[(d+\sigma)/2]}, \quad (\text{A11})$$

while A_σ is given by the right-hand side of Eq. (3.8).

The ratios $-A_2/A_0$ and A_σ/A_2 yield the values (3.11) and (3.9) of the coefficients v_2 and b , respectively, for the case of vanishing nearest-neighbor interaction constant J_1 .

APPENDIX B: CALCULATION OF THE FUNCTIONS $Q_{d,\sigma}(y)$

According to Eq. (4.47) the function $Q_{d,\sigma}(y)$ can be represented as

$$Q_{d,\sigma}(y) = \frac{y}{2} \left(\sum_{q_1 \in 2\pi\mathbb{Z}} \int_{q_{\parallel}}^{(d-1)} - \int_q^{(d)} \right) \frac{q^{\sigma-2}}{y+q^2} \quad (\text{B1})$$

$$= y^{(d+\sigma-2)/2} \sum_{k=1}^{\infty} G_\infty(d,\sigma|1;k\sqrt{y}). \quad (\text{B2})$$

To obtain the second form (B1), we have utilized the property

$$G_\infty(d,\sigma|r;x) = r^{(d+\sigma-4)/2} G_\infty(d,\sigma|1;x\sqrt{r}) \quad (\text{B3})$$

of the bulk propagator.

The case $\sigma=2$ is special in that the summation and integration over q_1 in Eq. (B1) can easily be performed to reduce $Q_{d,2}$ to a single integral, namely,

$$Q_{d,2}(y) = \frac{yK_{d-1}}{2} \int_0^\infty dp \frac{p^{d-2}}{(e^{\sqrt{y+p^2}} - 1)\sqrt{y+p^2}}. \quad (\text{B4})$$

Integrals of this kind were also encountered in Krech and Dietrich's work [31,32] on the Casimir effect in systems with short-range interactions.

From Eq. (B4) it is not difficult to derive a useful relation between $Q_{d+2,2}$ and $Q_{d,2}$:

$$\frac{\partial Q_{d+2,2}(y)}{\partial y} \frac{1}{y} = -\frac{Q_{d,2}(y)}{4\pi y}. \quad (\text{B5})$$

To do this, one simply must interchange the differentiation of $Q_{d+2,2}(y)/y$ with respect to y with the integration over p , replace the y derivative of the integrand's y -dependent part by a derivative with respect to p^2 , and then integrate by parts.

Returning to the case of general σ , we note that the representation (B2) has the advantage of linking the asymptotic behavior of $Q_{d,\sigma}(y)$ for large values of y to that of $G_\infty(d,\sigma|1;x)$. In addition, there are some special values of (d,σ) for which it allows one to derive closed-form analytical expressions for $Q_{d,\sigma}$ in a straightforward fashion. We therefore begin by computing the bulk propagator.

1. Calculation of the propagator $G_\infty(d,\sigma|r;x)$

We start from Eq. (4.46) and perform the angular integrations using our previous result (A8). This gives

$$G_\infty(d,\sigma|1;x) = \frac{x^{1-d/2}}{(2\pi)^{d/2}} \int_0^\infty dq \frac{q^{\sigma-2+d/2}}{1+q^2} J_{(d-2)/2}(qx). \quad (\text{B6})$$

The required integral can be evaluated with the aid of Eq. (6.565.8) of Ref. [89] or MATHEMATICA [90]. One obtains

$$G_\infty(d,\sigma|1;x) = \frac{\pi \csc[\pi(d+\sigma)/2]}{(4\pi)^{d/2}} \left[-{}_0F_1^{\text{reg}}\left(\frac{d}{2}; \frac{x^2}{4}\right) + \left(\frac{x}{2}\right)^{4-d-\sigma} {}_1F_2^{\text{reg}}\left(1; 2 - \frac{\sigma}{2}, 3 - \frac{d+\sigma}{2}; \frac{x^2}{4}\right) \right], \quad (\text{B7})$$

where ${}_0F_1^{\text{reg}}$ and ${}_1F_2^{\text{reg}}$ are regularized generalized hypergeometric function which can be expressed as

$${}_0F_1^{\text{reg}}(;d/2;x^2/4) = (x/2)^{1-d/2} I_{(d-2)/2}(x) \quad (\text{B8})$$

and

$${}_1F_2^{\text{reg}}(\alpha;\beta,\gamma;z) = \frac{{}_1F_2(\alpha;\beta,\gamma;z)}{\Gamma(\beta)\Gamma(\gamma)} \quad (\text{B9})$$

in terms of the modified Bessel function of the first kind I_ν and the generalized hypergeometric function ${}_1F_2(\alpha;\beta,\gamma;z)$, respectively. Their Taylor expansions read

$${}_0F_1^{\text{reg}}(;d/2;z) = \sum_{j=0}^{\infty} \frac{z^j}{j!\Gamma(j+d/2)} \quad (\text{B10})$$

and

$${}_1F_2^{\text{reg}}[1;2-\sigma/2,3-(d+\sigma)/2;z] = \sum_{j=0}^{\infty} \frac{z^j}{\Gamma(j+2-\sigma/2)\Gamma[j+3-(d+\sigma)/2]}. \quad (\text{B11})$$

For $\sigma=2$, we recover the familiar result for the free propagator of systems with short-range interactions:

$$G_\infty(d,2|1;x) = (2\pi)^{-d/2} x^{-(d-2)/2} K_{(d-2)/2}(x). \quad (\text{B12})$$

The latter is known to decay exponentially; the familiar asymptotic expansion of the Bessel functions K_ν implies that

$$\begin{aligned} G_\infty(d,2|1;x) &= \frac{x^{-(d-1)/2} e^{-x}}{2(2\pi)^{(d-1)/2}} \left(\sum_{j=0}^{m-1} \frac{\Gamma[(d-1+2j)/2]}{j! \Gamma[(d-1-2j)/2]} (2x)^{-j} + O(x^{-m}) \right). \end{aligned} \quad (\text{B13})$$

When $2 < \sigma < 4$, the Fourier transform of the propagator $G_\infty(d, \sigma | 1; x)$ is not regular in q at $q=0$. This entails that the propagator decays only as an inverse power of x . An easy way to obtain its asymptotic expansion for this case is to start from Eq. (B6), do a rescaling $q \rightarrow Q=qx$, expand the factor $(1+Qx^{-2})^{-1}$ of the resulting integrand in powers of x^{-2} , and integrate the series termwise. This leads to the asymptotic expansion

$$\begin{aligned} G_\infty(d, \sigma | 1; x) &= \frac{2^{\sigma-2}}{\pi^{d/2} x^{d+\sigma-2}} \sum_{j=0}^{m-1} \frac{\Gamma[j + (d + \sigma - 2)/2] (-4)^j}{\Gamma(1 - j - \sigma/2)} \frac{1}{x^{2j}} + O(x^{-2m}). \end{aligned} \quad (\text{B14})$$

Let us see how the above results can be employed to compute the required $Q_{d,\sigma}$. To treat the three-dimensional case, we need $Q_{d,2}(y)$ for $d=3$ and 5 , as well as $Q_{3,3}$, and their derivatives. Since $Q'_{3,2}(y)$ involves $Q_{1,2}(y)$, we also determine the latter. For these choices of d , the result (B12) reduces to

$$G_\infty(1,2|1;x) = \frac{1}{2} e^{-x}, \quad (\text{B15})$$

$$G_\infty(3,2|1;x) = \frac{1}{4\pi x} e^{-x}, \quad (\text{B16})$$

and

$$G_\infty(5,2|1;x) = \frac{1+x}{8\pi^2 x^3} e^{-x}, \quad (\text{B17})$$

respectively. Upon substituting these expressions into Eq. (B2), the series can be summed, giving

$$Q_{1,2}(y) = \frac{1}{2} \frac{\sqrt{y}}{\exp(\sqrt{y}) - 1}, \quad (\text{B18})$$

$$Q_{3,2}(y) = -\frac{y}{4\pi} \ln(1 - e^{-\sqrt{y}}), \quad (\text{B19})$$

and

$$Q_{5,2}(y) = \frac{y}{8\pi^2} [\text{Li}_3(e^{-\sqrt{y}}) + \sqrt{y} \text{Li}_2(e^{-\sqrt{y}})], \quad (\text{B20})$$

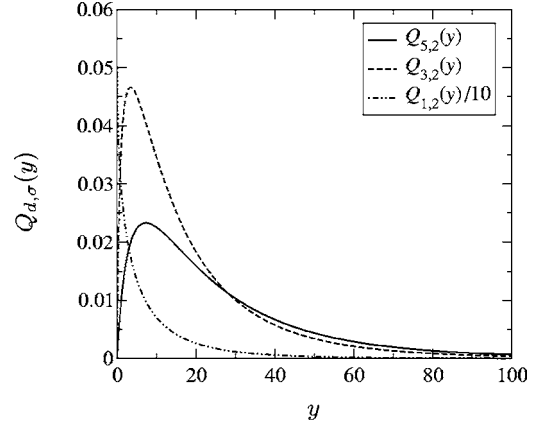


FIG. 11. The functions $Q_{5,2}(y)$ (full line), $Q_{3,2}(y)$ (dashed), and $Q_{1,2}(y)/10$ (dash-dotted), respectively.

where Li_p is the polylogarithmic function

$$\text{Li}_p(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^p}. \quad (\text{B21})$$

As can easily be checked, these results (B18)–(B20) are in conformity with Eq. (B5). Plots of the functions are displayed in Fig. 11.

For other choices of σ and d —including $\sigma=d=3$ —the series (B2) cannot in general be summed analytically. This suggests that one has to resort to numerical means. To this end a different representation of $Q_{d,\sigma}$ which we are now going to derive from Eq. (B1), proved to be more effective. Remarkably, this representation enabled us to derive even a closed-form analytical expression for $Q_{3,3}(y)$.

Note, first, that the subtracted q integral in Eq. (B1) is the bulk propagator at $x=0$. Both the limit $x \rightarrow 0$ of Eq. (B7) as well as the explicit calculation of the integral $\int_q^{(d)}$ yield

$$G_\infty(d, \sigma | y; 0) = -y^{(d+\sigma-4)/2} \frac{\pi}{2} K_d \csc[\pi(d + \sigma)/2]. \quad (\text{B22})$$

When $d + \sigma \geq 4$, this result involves analytic continuation in d since the integral is ultraviolet (uv) divergent in this case. The same L -independent uv divergences must occur in the first term of Eq. (B1), so that they cancel in the difference. We find it most convenient to handle uv divergences of this kind, which occur at intermediate steps, by means of dimensional regularization. Readers preferring to work with a large-momentum cutoff Λ are encouraged to utilize a smooth variant of it, since a sharp cutoff is known to give unphysical results in treatments of finite-size effects based on the small-momentum form of the inverse free propagator, i.e., of $\Omega(q)$ [36].

Next, consider a term of the series Σ_{q_1} in Eq. (B1). It is given by the integral

$$I_{d,\sigma}(q_1, y) = K_{d-1} \int_0^\infty dq_{\parallel} q_{\parallel}^{d-2} \frac{(q_1^2 + q_{\parallel}^2)^{(\sigma-2)/2}}{y + q_1^2 + q_{\parallel}^2}. \quad (\text{B23})$$

Its calculation for $q_1=0$ is straightforward, giving

$$I_{d,\sigma}(0, y) = K_{d-1} y^{(d+\sigma-5)/2} \frac{\pi}{2 \cos[\pi(d+\sigma)/2]}. \quad (\text{B24})$$

It can also be computed in closed form for $q_1 \neq 0$; the result involves a hypergeometric function ${}_2F_1$ and algebraic functions of y and q_1 . Rather than working with this expression directly, it is more convenient to split off appropriate terms containing the uv singularities they contribute to the series \sum_{q_1} in Eq. (B1). Whether and what kind of subtractions are necessary depends on the values of d and σ for which $Q_{d,\sigma}$ is needed. The $Q_{d,\sigma}(y)$ with the largest values of $d+\sigma$ encountered in our analysis of the three-dimensional case with $\sigma=3$ are $Q_{5,2}$ and $Q_{3,3}$. Thus the largest value of $d+\sigma$ for which $Q_{d,\sigma}$ is required is 7. Using power counting we see that the strongest possible uv singularity of the bulk integral $\int_q^{(d)}$ in Eq. (B1) is $\sim \Lambda^{d+\sigma-4}$. Hence it is sufficient to subtract from the integral (B23) its Taylor expansion to first order in y . This ensures that the difference, summed over q_1 , produces a uv finite result. All poles must originate from the subtracted terms and cancel with those of the bulk contribution in Eq. (B1).

Accordingly, we decompose $I_{d,\sigma}(q_1, y)$ as

$$I_{d,\sigma}(q_1, y) = \sum_{k=0}^1 I_{d,\sigma}^{(0,k)}(q_1, 0) \frac{y^k}{k!} + Z_{d,\sigma}(q_1, y), \quad (\text{B25})$$

where $I_{d,\sigma}^{(0,k)}$ denotes the k th derivative of the function $I_{d,\sigma}$ with respect to its second argument. Computing the integrals of the Taylor coefficients and the remainder $Z_{d,\sigma}$ yields

$$I_{d,\sigma}^{(0,k)}(q_1, 0) = \frac{(-1)^k}{2} k! K_{d-1} |q_1|^{d+\sigma-5-2k} \times B\left(\frac{d-1}{2}, \frac{5+2k-d-\sigma}{2}\right) \quad (\text{B26})$$

and

$$Z_{d,\sigma}(q_1, y) = \frac{K_{d-1} \pi}{2 \cos[\pi(d+\sigma)/2]} \left[\frac{y^{(\sigma-2)/2}}{(y+q_1^2)^{(3-d)/2}} - \frac{y^2 |q_1|^{d+\sigma-7} \Gamma[(d-1)/2]}{y+q_1^2 \Gamma(3-\sigma/2)} \times {}_2F_1^{\text{reg}}\left(1, \frac{d-1}{2}; \frac{d+\sigma-5}{2}; \frac{q_1^2}{y+q_1^2}\right) \right], \quad (\text{B27})$$

where $B(a, b)$ and ${}_2F_1^{\text{reg}}$ are the Euler beta function and the regularized hypergeometric function

$${}_2F_1^{\text{reg}}(a, b; c; z) = {}_2F_1(a, b; c; z) \Gamma(c), \quad (\text{B28})$$

respectively.

We now substitute the above results into the representation (B1) of $Q_{d,\sigma}$, utilizing the fact that series $\sum_{q_1 \neq 0}$ of pure powers of q_1 give ζ functions:

$$\sum_{\substack{q_1 \in 2\pi\mathbb{Z} \\ \neq 0}} |q_1|^{-s} = 2 \frac{\zeta(s)}{(2\pi)^s}. \quad (\text{B29})$$

The result is

$$Q_{d,\sigma}(y) = y \left(\frac{1}{2} y^{(d+\sigma-5)/2} I_{d,\sigma}(0, 1) + \sum_{j=1}^{\infty} Z_{d,\sigma}(2\pi j, y) + \frac{\zeta(5-d-\sigma)}{(2\pi)^{5-d-\sigma}} I_{d,\sigma}(1, 0) + y \frac{\zeta(7-d-\sigma)}{(2\pi)^{7-d-\sigma}} I_{d,\sigma}^{(0,1)}(1, 0) + \frac{K_d \pi}{4} y^{(d+\sigma-4)/2} \csc[\pi(d+\sigma)/2] \right). \quad (\text{B30})$$

Evaluating this expression for $(d, \sigma) = (3, 2)$ and $(5, 2)$ with the aid of MATHEMATICA [90], we have checked that the previous results (B18)–(B20) for $Q_{1,2}(y)$, $Q_{3,2}$, and $Q_{5,2}(y)$ are recovered. It can also be utilized to determine $Q_{3,3}(y)$ analytically. To this end one rewrites the series coefficient $Z_{3,3}$ as

$$Z_{3,3}(2\pi j, y) = \frac{y}{4\pi^2 j} - \frac{\sqrt{y}}{2\pi} \arccos\left(\frac{2\pi j}{\sqrt{y+4\pi^2 j^2}}\right) = \sqrt{y} \int_0^y dt \frac{\sqrt{t}}{8\pi^2 j(t+4\pi^2 j^2)} \quad (\text{B31})$$

and interchanges the integration over t with the summation over j . In this manner the series $\sum_j Z_{3,3}$ can be computed, and one obtains

$$Q_{3,3}(y) = \frac{y}{12} + \frac{y^2}{4\pi^2} \left[1 - \ln\left(\frac{\sqrt{y}}{2\pi}\right) \right] + \frac{y^{3/2}}{2\pi} \left\{ \frac{\pi}{4} + \text{Im} \left[\ln \Gamma\left(i \frac{\sqrt{y}}{2\pi}\right) \right] \right\}. \quad (\text{B32})$$

A plot of this function is shown in Fig. 12.

2. Asymptotic behavior of $Q_{d,\sigma}(y)$ for small and large values of y

The asymptotic behavior of the function $Q_{d,2}(y)$ for large values of y readily follows from the representation (B2) in conjunction with the asymptotic expansion (B13) of the bulk propagator (B12). The result one finds for general values of d ,

$$Q_{d,2}(y) = \frac{y^{(d+1)/4}}{y \rightarrow \infty 2(2\pi)^{(d-1)/2}} e^{-\sqrt{y}} [1 + O(y^{-1/2})], \quad (\text{B33})$$

can be verified to be in accordance with the large- y behavior of the explicit expressions (B18)–(B20) of these functions for $d=1, 3$, and 5.

To determine the large- y behavior of $Q_{d,\sigma}(y)$ with $2 < \sigma < 4$, we insert the asymptotic expansion (B14) into Eq. (B2). The summations over k can be performed for the expansion

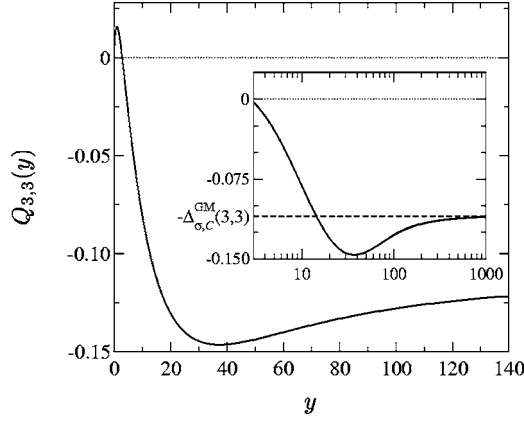


FIG. 12. The function $Q_{3,3}(y)$. The inset is a logarithmic-linear plot of this function, which illustrates the approach to the limiting value $-\Delta_{\sigma,C}^{GM}(3,3) = -\pi^2/90$ implied by Eqs. (5.9) and (5.3).

coefficients, giving ζ functions. In this way one arrives at the asymptotic expansion

$$Q_{d,\sigma}(y) \underset{y \rightarrow \infty}{=} \frac{2^{\sigma-2} m^{-1}}{\pi^{d/2}} \sum_{j=0} \left(\frac{\Gamma[j + (d + \sigma - 2)/2]}{\Gamma(1 - j - \sigma/2)} \right) \times \zeta(d + \sigma + 2j - 2) \frac{(-4)^j}{y^j} + O(y^{-m}). \quad (\text{B34})$$

Again, one can employ our explicit result (B32) for $Q_{3,3}$ to verify this asymptotic series. Note that the series (B34) truncates when σ is even, e.g., when $\sigma=2$. This ensures the consistency with the exponential decay (B33) one has for $\sigma=2$.

The asymptotic behavior of $Q_{d,2}(y)$ for small y can be conveniently obtained from Eq. (B30) for $1 < d < 7$. One finds that

$$Q_{d,2}(y) \underset{y \rightarrow 0}{=} \frac{\sqrt{\pi} \Gamma[(3-d)/2]}{(4\pi)^{d/2}} \left(y^{(d-1)/2} - \frac{B(1-d/2, 1/2)}{2\pi} y^{d/2} + \frac{2\zeta(3-d)}{(2\pi)^{3-d}} y + \frac{(d-3)\zeta(5-d)}{(2\pi)^{5-d}} y^2 + O(y^3) \right), \quad (\text{B35})$$

provided $d \neq 1, 3, 5$. The behavior in the latter cases follows by expansion about these values of d . The poles that the Γ function yields for individual terms at such odd integer values of d cancel, and logarithms of y emerge when $d=3$ or 5 . The expansions one gets in this manner,

$$Q_{1,2}(y) \underset{y \rightarrow 0}{=} \frac{1}{2} - \frac{\sqrt{y}}{4} + \frac{y}{24} - \frac{y^2}{1440} + O(y^3), \quad (\text{B36})$$

$$Q_{3,2}(y) \underset{y \rightarrow 0}{=} -\frac{y}{8\pi} \ln y + \frac{y^{3/2}}{8\pi} - \frac{y^2}{96\pi} + O(y^3), \quad (\text{B37})$$

and

$$Q_{5,2}(y) \underset{y \rightarrow 0}{=} \frac{\zeta(3)y}{8\pi^2} - \frac{1 - \ln y}{32\pi^2} y^2 - \frac{y^{5/2}}{48\pi^2} + O(y^3), \quad (\text{B38})$$

agree with those of the analytic expressions (B18)–(B20).

The small- y behavior of $Q_{d,\sigma}$ with $2 < \sigma < 4$ can be determined from Eq. (B30) in a similar fashion. One obtains

$$Q_{d,\sigma}(y) \underset{y \rightarrow 0}{=} \frac{K_{d-1}}{4} B\left(\frac{d+\sigma+1}{2}, \frac{1-d-\sigma}{2}\right) \left\{ y^{(d+\sigma-3)/2} + B\left(\frac{d-1}{2}, \frac{1}{2}\right) \frac{\cot[\pi(d+\sigma)/2]}{2\pi} y^{(d+\sigma-2)/2} + B\left(\frac{d-1}{2}, \frac{5-d-\sigma}{2}\right) \frac{4 \cos[(\pi(d+\sigma)/2]}{(2\pi)^{6-d-\sigma}} \times \left[\zeta(5-d-\sigma)y + \frac{(d+\sigma-5)\zeta(7-d-\sigma)y^2}{(4-\sigma)(2\pi)^2} \right] + O(y^3) \right\}. \quad (\text{B39})$$

To deal with the case of $Q_{3,3}$, one can set $\sigma=3$ and expand about $d=3$. This gives

$$Q_{3,3}(y) \underset{y \rightarrow 0}{=} \frac{y}{12} - \frac{y^{3/2}}{8} + \frac{y^2}{8\pi^2} \left(2 - 2C_E - \ln \frac{y}{4\pi^2} \right) + O(y^3), \quad (\text{B40})$$

where $C_E = 0.777\,215\,6\dots$ is the Euler-Mascheroni constant. The result is consistent with what one obtains from the analytic expression (B32) for $Q_{3,3}$.

APPENDIX C: CALCULATION OF $\Delta U_{d,\omega}(\mathbf{0}|L)$

We start from Eqs. (3.13) and (4.1), take the thermodynamic limit $L_{\parallel} \rightarrow \infty$, and utilize the continuum approximation. Upon transforming the discrete sum over the momentum component q_1 by means of Poisson's summation formula (A4) we arrive at:

$$\Delta U_{d,\Omega}(\mathbf{0}|L) = \sum_{j=1}^{\infty} \int_{\mathbf{q}}^{(d)} \cos(jq_1 L) \ln \Omega_{\mathbf{q}}. \quad (\text{C1})$$

We substitute for $\Omega_{\mathbf{q}}$ its small-momentum form (3.7), expand the logarithm as

$$\ln \Omega_{\mathbf{q}} = \ln[q^2 + O(q^4)] - bq^{\sigma-2} + O(b^2), \quad (\text{C2})$$

drop all suppressed terms, and extend the \mathbf{q} integration to \mathbb{R}^d .

The contribution from $\ln q^2$ is known from the short-range case [28,31,32], easily calculated, and given by the b -independent term on the right-hand side of Eq. (5.1). The $O(b)$ contribution involves a difference of critical bulk and finite-size propagators at $\mathbf{x}=\mathbf{0}$ for which one obtains, using Eqs. (B7), (B10), and (B11),

$$\frac{1}{2}(G_L - G_\infty)(d, \sigma + 2|0; \mathbf{0}) = \sum_{j=1}^{\infty} G_\infty(d, \sigma + 2|0; jL) = L^{2-d-\sigma} \frac{2^{\sigma-2} \Gamma[(d + \sigma - 2)/2] \zeta(d + \sigma - 2)}{\pi^{d/2} \Gamma(1 - \sigma/2)}. \quad (\text{C3})$$

Adding both contributions yields the result displayed in Eq. (5.1).

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