

Scaling and nonscaling finite-size effects in the Gaussian and the mean spherical model with free boundary conditions

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We calculate finite-size effects of the Gaussian model in a $L \times \tilde{L}^{d-1}$ box geometry with free boundary conditions in one direction and periodic boundary conditions in $d-1$ directions for $2 < d < 4$. We also consider film geometry ($\tilde{L} \rightarrow \infty$). Finite-size scaling is found to be valid for $d < 3$ and $d > 3$ but logarithmic deviations from finite-size scaling are found for the free energy and energy density at the Gaussian upper borderline dimension $d^* = 3$. The logarithms are related to the vanishing critical exponent $1 - \alpha - \nu = (d-3)/2$ of the Gaussian surface energy density. The latter has a cusplike singularity in $d > 3$ dimensions. We show that these properties are the origin of nonscaling finite-size effects in the mean spherical model with free boundary conditions in $d \geq 3$ dimensions. At bulk T_c , in $d = 3$ dimensions we find an unexpected *nonlogarithmic* violation of finite-size scaling for the susceptibility $\chi \sim L^3$ of the mean spherical model in film geometry, whereas only a logarithmic deviation $\chi \sim L^2 \ln L$ exists for box geometry. The result for film geometry is explained by the existence of the lower borderline dimension $d_l = 3$, as implied by the Mermin-Wagner theorem, that coincides with the Gaussian upper borderline dimension $d^* = 3$. For $3 < d < 4$ we find a power-law violation of scaling $\chi \sim L^{d-1}$ at bulk T_c for box geometry and a nonscaling temperature dependence $\chi_{\text{surface}} \sim \xi^d$ of the surface susceptibility above T_c . For $2 < d < 3$ dimensions we show the validity of universal finite-size scaling for the susceptibility of the mean spherical model with free boundary conditions for both box and film geometry and calculate the corresponding universal scaling functions for $T \geq T_c$.

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I. INTRODUCTION AND SUMMARY

Finite-size effects near phase transitions and the concept of finite-size scaling near critical points have been the subject of many studies over the past decades [1–4]. Consider, for example, the susceptibility $\chi(t, L)$ of a ferromagnetic system at the reduced temperature $t = (T - T_c)/T_c \geq 0$ near the bulk critical temperature T_c in a cubic geometry with a linear size L below the upper critical dimension $d = 4$. The property of finite-size scaling means that, for sufficiently large L and small t , χ has the asymptotic form

$$\chi(t, L) = \chi(t, \infty) f_\chi(L/\xi), \quad (1)$$

where $\chi(t, \infty) = A_\chi t^{-\gamma}$ is the bulk susceptibility and $\xi = \xi_0 t^{-\nu}$ is the bulk correlation length. An appealing feature of finite-size scaling is universality which means that all nonuniversal parameters of the confined system can be absorbed entirely in the bulk amplitude A_χ and in the *bulk* correlation length ξ , thus finite-size scaling functions such as $f_\chi(x)$ are expected to be independent of nonuniversal details (such as the lattice structure, the lattice spacing and the magnitude of coupling constants). This implies that the amplitude B_χ of the small- x behavior $f(x) = B_\chi x^{\gamma/\nu}$ for $T \rightarrow T_c$ at fixed L is also universal. The specific shape and the amplitude B_χ of such scaling functions do, of course, depend on the geometry and the kind of boundary conditions. A central prediction of finite-size scaling is the size dependence at the bulk critical temperature T_c

$$\chi(0, L) = A_\chi \xi_0^{-\gamma/\nu} B_\chi L^{\gamma/\nu} \quad (2)$$

with the *bulk* critical exponent γ/ν and the *universal* amplitude B_χ . For purely periodic boundary conditions and short-range interactions, universal finite-size scaling in the sense of Eqs. (1) and (2) has been largely confirmed, except for the *nonuniversal* exponential behavior in the region $L \gg \xi$ which has recently been shown [5–8] to depend on the lattice structure for lattice models and on the cutoff procedure for continuum models.

Of particular interest are nonperiodic boundary conditions, which are relevant for real systems. For example, for the superfluid transition of ^4He , Dirichlet boundary conditions of field theories are believed to be fairly realistic [9]. For this system, however, accurate experiments have detected nonscaling finite-size effects on both static [9–12] and dynamic [13,14] properties that are as yet unexplained. Furthermore there exist unexplained finite-size effects in the XY model with nonperiodic boundary conditions as detected by Monte Carlo simulations [15].

On the theoretical side, the true conditions for the validity of universal finite-size scaling for systems with nonperiodic boundary conditions are not established. This includes the important case of free boundary conditions for lattice models that are believed to be asymptotically equivalent to Dirichlet boundary conditions of continuum models. It is known that universal finite-size scaling in the sense of Eq. (1) fails for the mean spherical model in film geometry with free boundary conditions in $d = 3$ and $d = 4$ dimensions [2,16–18], and similarly for the ideal Bose gas with Dirichlet boundary conditions for cubic and film geometries [2,19–21]. In these models the bulk correlation length could not be used as the only reference length and nonscaling finite-size effects were

incorporated in nonuniversal shifts of the temperature variable [16–21]. Logarithmic nonscaling finite-size effects that depend on the lattice spacing exist also in Gaussian interface models [22] as well as in other models [4].

On the other hand, universal amplitude ratios have been found for critical systems contained in parallel plates with nonperiodic boundary conditions [23]. Furthermore, field-theoretic renormalization-group calculations have apparently confirmed the validity of universal finite-size scaling within the φ^4 field theory with Dirichlet boundary conditions: Universal finite-size amplitude ratios [24] and universal finite-size contributions to the free energy density and to the critical Casimir force were calculated both in the Gaussian (one-loop) approximation [25–27] as well as in two-loop order [26]. Universal finite-size scaling functions have also been predicted for the specific heat and the superfluid density in the presence of Dirichlet boundary conditions [9,28]. Related field-theoretic predictions have also been presented for surface quantities [29,30]. In these papers [24–30], however, the method of dimensional regularization was employed which neglects lattice and cutoff effects. Recent work on finite-size effects [5–8,31–35] has demonstrated that general renormalization-group arguments are not sufficient to prove the validity of universal finite-size scaling and that cutoff and lattice effects are nonnegligible for confined systems with periodic boundary conditions. Clearly these investigations need to be extended to the case of nonperiodic boundary conditions.

The corresponding analytic calculations, at finite cutoff and at finite lattice spacing, become quite difficult within the φ^4 theory beyond the lowest order. Before embarking on such an ambitious project it is, of course, necessary to first examine the lowest-order case under the simplest nontrivial conditions, i.e., with free (or Dirichlet) boundary conditions in only one direction. Therefore, as a first step, we consider the exactly solvable Gaussian model with short-range interaction on a simple-cubic lattice with a lattice constant \tilde{a} for a finite rectangular $L \times \tilde{L}^{d-1}$ box geometry with free boundary conditions in one direction and periodic boundary conditions in $d-1$ directions. Even at the Gaussian level, the analytic calculations at finite lattice spacing in the range $2 < d < 4$ turn out to be nontrivial.

For the specific heat and the susceptibility of the Gaussian model we find full agreement with universal finite-size scaling. With regard to the singular part of the free energy we find that the finite-size scaling form is indeed valid for $d < 3$ and $d > 3$ but logarithmic deviations from finite-size scaling occur at $d=3$ where the critical exponent $1 - \alpha - \nu = (d-3)/2$ of the surface energy density vanishes. In order to describe the logarithmic $d=3$ behavior it is necessary to keep the lattice spacing finite. We find that the same logarithmic deviations from finite-size scaling exist in the continuum version of the Gaussian model with Dirichlet boundary conditions provided that a finite cutoff is used. This implies that the method of dimensional regularization at infinite cutoff is not capable of correctly describing the $d=3$ behavior of the singular part of the free energy density and of the energy density since it yields unphysical divergences of

these quantities in the form of a pole term $\sim (d-3)^{-1}$ [36]. As discussed in Sec. III H, the dimension $d=3$ can be considered as an upper borderline dimension d^* of the Gaussian model with free boundary conditions above which the lattice and cutoff effects become non-negligible for the surface energy density.

For $d > 3$ we find that the surface energy density $U_{surface}(t)$ of the Gaussian model with free boundary conditions has a cusplike singularity at bulk T_c as T_c is approached from above. For the lattice model at finite lattice spacing \tilde{a} the height of the cusp is

$$\lim_{t \rightarrow 0^+} U_{surface}(t) = U_{surface}(0) = T_c \xi_0^{-2} \tilde{a}^{3-d} \tilde{B}_d \quad (3)$$

with

$$\tilde{B}_d = \frac{1}{8} \int_0^\infty dy \{ [1 + e^{-4y} - 2e^{-2y} I_0(2y)] [e^{-2y} I_0(2y)]^{d-1} \} > 0, \quad (4)$$

where $I_0(z)$ is the Bessel function of order zero. The temperature dependent part of $U_{surface}(t)$ has a universal scaling form $\sim \xi^{3-d}$, but it vanishes at T_c and is subleading compared to the nonuniversal finite regular part, Eq. (3), at T_c . The latter part yields a leading nonscaling contribution $2U_{surface}(0)/L$ to the total energy density. These results remain valid also for the Gaussian model in the film geometry ($\tilde{L} \rightarrow \infty$) with free boundary conditions.

In a second step we analyze the exactly solvable mean spherical model with the same boundary conditions. Previously this model has been studied for the film geometry at integer dimensions $d=3,4,5, \dots$ [16,17]. Here we extend this analysis to *continuous* dimensions in the range $2 < d < 4$ and consider both the film and box geometries. This reveals $d=3$ as a borderline dimension between a universal scaling ($d < 3$) and a nonuniversal nonscaling ($d \geq 3$) regime. In this paper we calculate the nonscaling effects for $3 \leq d < 4$ as well as the analytic form of the universal finite-size scaling function $f_\chi(L/\xi)$, Eq. (1), of the susceptibility for $2 < d < 3$ including the amplitude $B(s)$ of the scaling result, Eq. (2) with $\gamma/\nu=2$,

$$\chi(0,L) = B(s)L^2, \quad d < 3 \quad (5)$$

at an arbitrary shape factor $s = L/\tilde{L} \geq 0$. The amplitude $B(s)$ is shown to diverge for $d \rightarrow 3$.

The mean spherical model can be considered as a Gaussian model with a constraint where the constraint can be expressed in terms of the Gaussian energy density. Our results for the latter quantity explain the origin of logarithmic nonscaling terms in thermodynamic quantities of the mean spherical model at $d=3$ and of power-law violations of finite-size scaling for $3 < d < 4$. While previous work suggested the existence of only *logarithmic* deviations from finite-size scaling in $d=3$ dimensions [2,16–21] we find, quite unexpectedly, a *nonlogarithmic* violation of the scaling

prediction, Eq. (5), for the size dependence of the susceptibility at bulk T_c in $d=3$ dimensions

$$\chi(0,L) = B_{film} \tilde{a}^{-1} L^3 \quad (6)$$

for film geometry, whereas for box geometry, at a fixed finite shape factor $s=L/\tilde{L}>0$, we find the expected logarithmic deviation from scaling

$$\chi(0,L) = B_{box}(s) L^2 \ln(L/\tilde{a}). \quad (7)$$

As will be shown in detail in Sec. IV C, the special result of Eq. (6) for the film geometry at $d=3$ is due to the simultaneous appearance of two logarithmic effects at $d=3$ where two borderline dimensions coincide: it is a combined effect of the logarithmic *surface* term of the Gaussian model at the (upper) borderline dimension $d^*=3$, where the exponent $1-\alpha-\nu$ vanishes, and of a logarithmic *finite-size* term arising from the mode continuum of the film system just at the (lower) borderline dimension $d_l=3$ at which the film critical temperature vanishes in accordance with the Mermin-Wagner theorem [37]. Most striking is the *discontinuous* change of the exponent 2 of the power law $\chi_{film} = B(0)L^2$ for $d<3$, Eq. (5), to 3 of the power law $\chi_{film} = B_{film} \tilde{a}^{-1} L^3$ for $d=3$, Eq. (6).

The result of Eq. (6) is not contained in the work of Barber and Fisher [16] who calculated χ for the film geometry in $d=3$ dimensions only for $T \geq \tilde{T}(L)$ where $\tilde{T}(L) > T_c$ is some temperature that they called ‘‘quasicritical.’’ Our $d=3$ result for $\chi(t,L)$ covers the entire critical region $T \geq T_c$ including the regime $T \geq \tilde{T}(L)$. In the latter regime, the explicit form of our result is at variance with the simpler form of Barber and Fisher.

For box geometry in $3 < d < 4$ dimensions we find a power-law violation of scaling at T_c

$$\chi(0,L) = B_{box}(s,d) \tilde{a}^{3-d} L^{d-1}, \quad (8)$$

where the amplitude $B_{box}(s,d)$ is proportional to the amplitude \tilde{B}_d , Eq. (4), of the cusp of the Gaussian surface energy density. A nonscaling form is also found for the temperature dependence of the surface susceptibility for $3 < d < 4$ above T_c ,

$$\chi_{surface} = \tilde{A}_{surface} \tilde{a}^{3-d} \xi^d \sim t^{-d/(d-2)} \quad (9)$$

with $\xi \sim t^{-\nu}$, $\nu = (d-2)^{-1}$, whereas the scaling form, Eq. (1), would imply $\chi_{surface} \sim O(\chi_b \xi) \sim t^{-3/(d-2)}$ for the mean spherical model. Again the amplitude $\tilde{A}_{surface}$ in Eq. (9) is proportional to \tilde{B}_d .

For the film geometry in $d > 3$ dimensions we find an anomalous enhancement of the film critical temperature $T_{c,d}(L)$ above the bulk critical temperature $T_{c,d}(\infty)$. A corresponding shift was first found for $d \geq 4$ by Barber and Fisher [16]. This enhancement is most naturally expressed in terms of the dimensionless parameter $2J\beta_{c,d}(L) = 2J[k_B T_{c,d}(L)]^{-1}$ where J is the nearest-neighbor coupling. The result is, for $d > 3$,

$$2J[\beta_{c,d}(\infty) - \beta_{c,d}(L)] \\ = 4\tilde{B}_d \tilde{a}/L - \tilde{C}_d (\tilde{a}/L)^{d-2} + O(\tilde{a}^{d/2} L^{-d/2}) \quad (10)$$

with the nonuniversal amplitude \tilde{B}_d , Eq. (4), and with a universal amplitude $\tilde{C}_d > 0$. Eq. (10) implies $T_{c,d}(L) > T_{c,d}(\infty)$ for large $L \gg \tilde{a}$. The leading term $\sim L^{-1}$ in Eq. (10) has a nonscaling L dependence whereas the subleading universal term has the scaling L dependence $\sim L^{1/\nu}$.

In summary, we see that both the anomalous nonscaling enhancement of $T_{c,d}(L)$, Eq. (10), and the power-law violations, Eqs. (8) and (9), for $d > 3$ can be traced back to the same amplitude \tilde{B}_d , Eq. (4), of the nonscaling cusp of the Gaussian model. Thus the analysis of the Gaussian model provides a better understanding of the origin of the power-law nonscaling finite-size effects in the mean spherical model for $d > 3$, and, for box geometry, of the logarithmic deviations at the Gaussian upper borderline dimension $d^* = 3$. For film geometry, however, the Gaussian logarithmic effect at $d^* = 3$ is enhanced by a second logarithmic effect due to the lower borderline dimension $d_l = 3$ (where the film critical temperature vanishes), which then yields the power law Eq. (6).

We point out that all nonscaling effects are tied to the finite lattice constant $\tilde{a} > 0$, as seen explicitly in Eqs. (3) and (6)–(10). We expect that similar effects exist in the ideal Bose gas with Dirichlet boundary conditions [19–21]. These effects are not captured by the standard method of dimensional regularization. It remains to be seen whether the mechanism for nonscaling finite-size effects in the mean spherical model and the ideal Bose gas is an artifact restricted to these models or whether some of these features are of more general significance. This question is of particular interest below T_c where an explanation of the pronounced nonscaling finite-size effects in ^4He remains a challenge for future research.

In Sec. II we summarize the predictions implied by the finite-size scaling hypothesis. Section III contains the detailed results for the finite-size effects in the Gaussian lattice model with free boundary conditions and in the Gaussian continuum model with Dirichlet boundary conditions. In Sec. IV we analyze the consequences of our results for the mean spherical model with free boundary conditions. The derivation of our results is presented in appendixes.

II. FINITE-SIZE SCALING PREDICTIONS

In the subsequent sections we shall present exact results for the finite-size effects on the free energy density, energy density, specific heat and susceptibility of lattice models in a rectangular $L \times \tilde{L}^{d-1}$ box geometry with free boundary conditions in the direction of size L and periodic boundary conditions in the $d-1$ directions of size \tilde{L} . For the sake of clarity, we first summarize the predictions implied by the finite-size scaling hypothesis, which, for this geometry and these boundary conditions, have not yet been formulated explicitly in the literature. We denote the critical temperature of the d -dimensional bulk ($L \rightarrow \infty, \tilde{L} \rightarrow \infty$) system by $T_{c,d}$. In

the limit $\tilde{L} \rightarrow \infty$ at fixed L , the box becomes a film of thickness L , which may have its own critical temperature $T_{c,d}(L) \neq T_{c,d} \equiv T_{c,d}(\infty)$. In general one expects $T_{c,d}(L) < T_{c,d}$, but it turns out (see Sec. IV, see also Ref. [16]) that for the mean spherical model with $d > 3$ the film critical temperature $T_{c,d}(L)$ exceeds the bulk critical temperature $T_{c,d}$. For simplicity, in this section, we assume a d -dimensional box with a *finite* shape factor $L/\tilde{L} > 0$ and confine ourselves to $T \geq T_{c,d}$.

First we consider the free energy density $f(t, L, \tilde{L})$ (in units of $k_B T$) at the reduced temperature $t = (T - T_{c,d})/T_{c,d} \geq 0$ and at vanishing external field. It is expected that, for small t , f can be decomposed into a singular and a “nonsingular” part [38,39]

$$f(t, L, \tilde{L}) = f_s(t, L, \tilde{L}) + f_{ns}(t, L, \tilde{L}), \quad (11)$$

where $f_{ns}(t, L, \tilde{L})$ has a regular t dependence. In the bulk limit, the corresponding decomposition is

$$f_b(t) \equiv f(t, \infty, \infty) = f_{bs}(t) + f_0(t), \quad (12)$$

where the regular part $f_0(t) \equiv f_{ns}(t, \infty, \infty)$ can be identified unambiguously. For systems with short-range interactions, below the upper critical dimension $d=4$ and for large L, \tilde{L} and ξ , it is expected that the singular part $f_s(t, L, \tilde{L})$ has the finite-size scaling form [1,38]

$$f_s(t, L, \tilde{L}) = L^{-d} \mathcal{F}(L/\xi, L/\tilde{L}), \quad (13)$$

where $\xi(t) = \xi_0 t^{-\nu}$ is the (second-moment) correlation length of the d -dimensional bulk system. For a given shape factor $s = L/\tilde{L}$, the scaling function $\mathcal{F}(x, s)$ is expected to be universal. More specifically, the singular and nonsingular parts of the free energy density are expected to have the asymptotic (small t , large L , large \tilde{L}) form [1,4,38,39]

$$f_s(t, L, \tilde{L}) = Y \xi^{-d} + 2A_{surface}^+ \xi^{1-d} L^{-1} + L^{-d} \mathcal{G}(L/\xi, L/\tilde{L}) \quad (14)$$

and

$$f_{ns}(t, L, \tilde{L}) = f_0(t) + 2\Psi_1(t)/L \quad (15)$$

with a universal bulk amplitude Y and a universal surface amplitude $A_{surface}^+$, and with a universal finite-size part $\mathcal{G}(L/\xi, L/\tilde{L})$ of the scaling function

$$\mathcal{F}(L/\xi, L/\tilde{L}) = Y(L/\xi)^d + 2A_{surface}^+(L/\xi)^{d-1} + \mathcal{G}(L/\xi, L/\tilde{L}). \quad (16)$$

Equations (14)–(16) imply that there exists the surface free energy

$$f_{surface}(t) = \lim_{L \rightarrow \infty} \left\{ [f(t, L, \tilde{L}) - f_b(t)] \frac{L}{2} \right\} = A_{surface}^+ \xi^{1-d} + \Psi_1(t) \quad (17)$$

with a universal amplitude $A_{surface}^+$ of the singular part. The nonsingular surface contribution $\Psi_1(t)$ is a *regular* function of t . Nonasymptotic Wegner [40] corrections to scaling are neglected in Eqs. (13), (14), (16), and (17). The phenomenological finite-size scaling theory does not make specific predictions about the dependence on L and \tilde{L} of higher-order terms in Eq. (15).

Equations (11)–(17) are expected to hold also for continuum models with Dirichlet boundary conditions in one direction, with the same universal quantities as for free boundary conditions of lattice systems. As noted in the Introduction, however, there exist *nonuniversal* exponential terms in the regime $L \gg \xi, \tilde{L} \gg \xi$, where the lattice-dependent and cutoff-dependent exponential correlation length [7,8,41] becomes the appropriate reference length.

Although the energy density (internal energy per unit volume) divided by k_B

$$U(t, L, \tilde{L}) = -T^2 \frac{\partial f(t, L, \tilde{L})}{\partial T} \quad (18)$$

is completely determined by the free energy density $f(t, L, \tilde{L})$, it turns out that a separate discussion of the energy density is warranted because of its important role played in the mean spherical model in Sec. IV. From Eqs. (11)–(15) one obtains the prediction

$$U(t, L, \tilde{L}) = U_s(t, L, \tilde{L}) + U_{ns}(t, L, \tilde{L}), \quad (19)$$

where the singular part

$$U_s(t, L, \tilde{L}) = T_c \xi_0^{-1/\nu} L^{-(1-\alpha)/\nu} \mathcal{U}(L/\xi, L/\tilde{L}) \quad (20)$$

has the universal scaling function

$$\begin{aligned} \mathcal{U}(x, s) &= -\nu x^{1-1/\nu} \partial \mathcal{F}(x, s) / \partial x \\ &= -d\nu Y x^{d-1/\nu} - 2(d-1)\nu A_{surface}^+ x^{d-1-1/\nu} \\ &\quad - \nu x^{1-1/\nu} \partial \mathcal{G}(x, s) / \partial x \end{aligned} \quad (21)$$

and where the leading nonsingular part

$$U_{ns}(t, L, \tilde{L}) = U_0(t) + 2U_1(t)/L \quad (23)$$

has a regular t dependence with $U_0(t) = -T^2 \partial f_0(t) / \partial T$ and

$$U_1(t) = -T^2 \partial \Psi_1(t) / \partial T. \quad (24)$$

For the surface energy density, Eq. (14) implies asymptotically

$$U_{surface}(t) = -T^2 \partial f_{surface}(t) / \partial T \quad (25)$$

$$= U_1(t) - T_c \xi_0^{-1/\nu} (d-1) \nu A_{surface}^+ \xi^{-(1-\alpha-\nu)/\nu}. \quad (26)$$

In Eqs. (20) and (26) we have used the hyperscaling relation

$$d\nu = 2 - \alpha. \quad (27)$$

These scaling predictions have been confirmed by several field-theoretic renormalization-group calculations of $f_s(t, L, \infty)$ [26] and of $U_{surface}$ [24,36,42,43] based on the φ^4 continuum Hamiltonian with Dirichlet boundary conditions for the field $\varphi(\mathbf{x})$. All calculations, however, were carried out within the dimensional regularization scheme that neglects cutoff effects. As pointed out by Dohm [9,36], an unresolved feature of the dimensionally regularized perturbative results for $U_{surface}$ [24,26,36,42,43] is a pole term $\sim (d-3)^{-1}$ that diverges in three dimensions.

We note that the critical exponent of $U_{surface}(t)$

$$1 - \alpha - \nu = (d-1)\nu - 1 \quad (28)$$

is positive for ordinary critical points of the $O(n)$ universal class with $d > 2$ which implies a *finite* critical value $U_{surface}(0) = U_1(0)$. By contrast, for the Gaussian model, $1 - \alpha - \nu = (d-3)/2$ is positive only for $d > 3$, thus $U_{surface}(t)$ diverges for $t \rightarrow 0$ in $d \leq 3$ dimensions (see Sec. III).

We shall also consider the specific heat (divided by k_B)

$$C(t, L, \tilde{L}) = \frac{\partial U(t, L, \tilde{L})}{\partial T} = C_s(t, L, \tilde{L}) + C_{ns}(t, L, \tilde{L}). \quad (29)$$

From Eqs. (19)–(23) we obtain the predictions

$$C_s(t, L, \tilde{L}) = \xi_0^{-2/\nu} L^{\alpha/\nu} C(L/\xi, L/\tilde{L}) \quad (30)$$

and

$$C_{ns}(t, L, \tilde{L}) = \partial U_0(t)/\partial t + 2L^{-1} \partial U_1(t)/\partial t \quad (31)$$

with the universal scaling function

$$\mathcal{C}(x, s) = \nu x^{1-1/\nu} \partial U(x, s)/\partial x. \quad (32)$$

The scaling structure implies that the surface specific heat $C_{surface}(t) = \partial U_{surface}(t)/\partial T$ has a divergent singular part,

$$C_{surface}(t) = \xi_0^{1-d} A_{C,surface}^+ t^{-\alpha_s} + \partial U_1(t)/\partial T \quad (33)$$

with the surface scaling exponent

$$\alpha_s = \alpha + \nu \quad (34)$$

and with a universal amplitude

$$A_{C,surface}^+ = -(1 - \alpha - \nu)(d-1) \nu A_{surface}^+. \quad (35)$$

Finally we recall the prediction for the asymptotic scaling form of the susceptibility

$$\chi(t, L, \tilde{L}) = \chi_b(t) f_\chi(L/\xi, L/\tilde{L}) \quad (36)$$

according to Eq. (1), where $\chi_b(t) = \chi(t, \infty) = A_\chi t^{-\gamma}$ is the bulk susceptibility. For $L \gg \xi, \tilde{L} \gg \xi$, the scaling function is expected to have the expansion

$$f_\chi(L/\xi, L/\tilde{L}) = 1 + c_\chi \xi/L + O(\xi^2/L^2, e^{-\tilde{L}/\xi}) \quad (37)$$

with the universal coefficient c_χ . For $t > 0$, this implies

$$\chi_{surface}(t) = \lim_{L \rightarrow \infty} \left\{ [\chi(t, L, \tilde{L}) - \chi_b(t)] \frac{L}{2} \right\} = A_{\chi,surface}^+ t^{-\gamma_s} \quad (38)$$

with the surface scaling exponent

$$\gamma_s = \gamma + \nu \quad (39)$$

and with the surface amplitude

$$A_{\chi,surface}^+ = \frac{1}{2} A_\chi \xi_0 c_\chi. \quad (40)$$

For $T \rightarrow T_{c,d}$, the small L/ξ behavior of the scaling function is expected to be

$$f_\chi(L/\xi, L/\tilde{L}) \sim B_\chi(L/\tilde{L})(L/\xi)^{\gamma/\nu} \quad (41)$$

with a finite universal amplitude $B_\chi(L/\tilde{L}) > 0$, which implies

$$\chi(0, L, \tilde{L}) = A_\chi \xi_0^{-\gamma/\nu} B_\chi(L/\tilde{L}) L^{\gamma/\nu}. \quad (42)$$

In the following, we examine the range of validity of these predictions for the exactly solvable Gaussian and mean spherical models in $2 < d < 4$ dimensions.

III. GAUSSIAN LATTICE MODEL WITH FREE BOUNDARY CONDITIONS

A. Lattice Hamiltonian

We consider N continuous scalar variables $\varphi_j, -\infty \leq \varphi_j \leq \infty$, on the lattice points \mathbf{x}_j of a simple-cubic lattice with a lattice spacing \tilde{a} in a finite rectangular $L \times \tilde{L}^{d-1}$ box of volume $V = L\tilde{L}^{d-1} = N\tilde{a}^d$. We assume a Gaussian statistical weight $\sim \exp(-H)$ with the lattice Hamiltonian

$$H = \tilde{a}^d \left[\sum_j \frac{r_0}{2} \varphi_j^2 + \sum_{\langle ij \rangle} \frac{J}{2\tilde{a}^2} (\varphi_i - \varphi_j)^2 \right] \quad (43)$$

with a nearest-neighbor coupling $J > 0$. The factor $(k_B T)^{-1}$ is absorbed in H . The dimensionless partition function is

$$Z = \left[\prod_j \int_{-\infty}^{\infty} \frac{d\varphi_j}{\tilde{a}^{1-d/2}} \right] \exp(-H). \quad (44)$$

In the bulk limit $\tilde{L} \rightarrow \infty, L \rightarrow \infty$, this model has a critical point at $r_0 = 0$ for arbitrary $d > 0$. We assume that the temperature T enters only through

$$r_0 = a_0 \frac{T - T_c}{T_c}, \quad a_0 > 0. \quad (45)$$

A serious shortcoming of this model is the fact that it has no low temperature phase, i.e., no bulk limit exists for $r_0 < 0$. Nevertheless, there exist nontrivial finite-size effects for $r_0 \geq 0$, as we shall see.

We assume free boundary conditions in the d th (vertical) direction and periodic boundary conditions in the $d-1$ (horizontal) directions. The $d-1$ horizontal coordinates and the vertical coordinate of the lattice points $\mathbf{x}_j = (\mathbf{y}_j, z_j)$ are denoted by \mathbf{y}_j and z_j , respectively. The ‘‘bottom’’ and ‘‘top’’ surfaces perpendicular to the vertical direction have the coordinates $z_j = \tilde{a}$ and $z_j = L$, respectively, thus we have L/\tilde{a} layers of fluctuating variables. The variables in the bottom and top surfaces have only one neighboring layer. This is equivalent to assuming Dirichlet boundary conditions ($\varphi_j = 0$) in the (fictitious) layers $z_j = 0$ below the bottom surface and $z_j = L + \tilde{a}$ above the top surface. The variables φ_j can be represented as

$$\varphi_j = \tilde{L}^{-(d-1)}(L + \tilde{a})^{-1} \sum_{\mathbf{k}, p} \hat{\varphi}_{\mathbf{k}, p} \exp(i\mathbf{k} \cdot \mathbf{y}_j) \sqrt{2} \sin(pz_j) \quad (46)$$

with the Fourier amplitudes

$$\hat{\varphi}_{\mathbf{k}, p} = \tilde{a}^d \sum_j \varphi_j \exp(-i\mathbf{k} \cdot \mathbf{y}_j) \sqrt{2} \sin(pz_j). \quad (47)$$

The sum $\sum_{\mathbf{k}, p}$ runs over $(d-1)$ -dimensional \mathbf{k} vectors with components $k_i = 2\pi m_i / \tilde{L}$, $i = 1, \dots, d-1$ with integers $m_i = 0, \pm 1, \pm 2, \dots$, in the range $-\pi/\tilde{a} \leq k_i < \pi/\tilde{a}$ and over wave numbers $p = \pi n / (L + \tilde{a})$, $n = 1, 2, \dots, L/\tilde{a}$ in the range $0 < p < \pi/\tilde{a}$. Equation (47) follows from $\sum_z 2 \sin(pz_j) \sin(p'z_j) = (L + \tilde{a}) \tilde{a}^{-1} \delta_{p, p'}$. We see that, for L/\tilde{a} layers with free boundary conditions, the natural unit wave number in p space is $\pi/(L + \tilde{a})$ rather than π/L . For each given p , there are $(\tilde{L}/\tilde{a})^{d-1}$ variables $\hat{\varphi}_{\mathbf{k}, p}$. Equation (46) implies $\varphi_j = 0$ at $z_j = 0$ and $\varphi_j = 0$ at $z_j = L + \tilde{a}$ for arbitrary \mathbf{y}_j , thus we have a total number of $N = (L/\tilde{a})(\tilde{L}/\tilde{a})^{d-1}$ variables $\hat{\varphi}_{\mathbf{k}, p}$. Substituting Eq. (46) into Eq. (43) yields the diagonalized Hamiltonian

$$H = \frac{1}{2} \tilde{L}^{-(d-1)} (L + \tilde{a})^{-1} \sum_{\mathbf{k}, p} (r_0 + J_{\mathbf{k}, d-1} + J_p) \hat{\varphi}_{\mathbf{k}, p} \hat{\varphi}_{-\mathbf{k}, p} \quad (48)$$

with

$$J_{\mathbf{k}, d-1} = \frac{4J}{\tilde{a}^2} \sum_{i=1}^{d-1} [1 - \cos(k_i \tilde{a})], \quad (49)$$

$$J_p = \frac{4J}{\tilde{a}^2} [1 - \cos(p\tilde{a})]. \quad (50)$$

The Jacobian of the linear transformation $\varphi_j \rightarrow \hat{\varphi}_{\mathbf{k}, p}$ of Eq. (46) is

$$\left| \frac{\partial \varphi_j}{\partial \hat{\varphi}_{\mathbf{k}, p}} \right| = [\tilde{a}^d \tilde{L}^{d-1} (L + \tilde{a})]^{-N/2}. \quad (51)$$

Using Eqs. (44), (46), (48), and (51), we obtain the free energy density divided by $k_B T$

$$f(t, L, \tilde{L}) = -V^{-1} \ln Z = -\frac{1}{2} \tilde{a}^{-d} [\ln \pi + (\tilde{L}/\tilde{a})^{1-d} \ln 2] + \frac{1}{2} \tilde{L}^{-(d-1)} L^{-1} \sum_{\mathbf{k}, p} \ln[(r_0 + J_{\mathbf{k}, d-1} + J_p) \tilde{a}^2]. \quad (52)$$

In all calculations of this section, we shall keep the lattice spacing \tilde{a} finite.

In the following, we shall also consider film geometry (bulk limit in the $d-1$ horizontal directions). In Eq. (52), this corresponds to the replacement $\tilde{L}^{-(d-1)} \sum_{\mathbf{k}, p} \rightarrow \sum_p \int_{\mathbf{k}}$ where $\int_{\mathbf{k}} \equiv (2\pi)^{1-d} \int d^{d-1} k$ with $|k_i| \leq \pi/\tilde{a}$, $i = 1, 2, \dots, d-1$; hence

$$f(t, L, \infty) = -\frac{1}{2} \tilde{a}^{-d} \ln \pi + \frac{1}{2} L^{-1} \times \sum_p \int_{\mathbf{k}} \ln[(r_0 + J_{\mathbf{k}, d-1} + J_p) \tilde{a}^2]. \quad (53)$$

A simplifying (but unrealistic) feature of the Gaussian model is that the critical point of the film system of finite thickness L is also determined by $r_0 = 0$, i.e., it remains unshifted compared to the bulk critical point for all d . This differs from the case of the spherical model to be discussed in Sec. IV.

B. Bulk properties

First we briefly summarize some of the known bulk properties. The square of the second-moment bulk correlation length ξ above T_c is defined by

$$\xi^2 = \lim_{L \rightarrow \infty} \lim_{\tilde{L} \rightarrow \infty} \frac{1}{2d} \frac{\sum_{i,j} (\mathbf{x}_i - \mathbf{x}_j)^2 \langle \varphi_i \varphi_j \rangle}{\sum_{i,j} \langle \varphi_i \varphi_j \rangle}. \quad (54)$$

It is given by $\xi^2 = J_0 r_0^{-1}$ or

$$\xi = \xi_0 t^{-\nu}, \quad \nu = 1/2 \quad (55)$$

with

$$\xi_0 = (J_0/a_0)^{1/2}, \quad J_0 = 2J. \quad (56)$$

From Eq. (52) we have the bulk free energy density for $r_0 = a_0 t \geq 0$

$$f_b = -\frac{1}{2} \tilde{a}^{-d} \ln \pi + \frac{1}{2} \int_{\mathbf{q}} \ln[(r_0 + J_{\mathbf{q}, d}) \tilde{a}^2], \quad (57)$$

where $\int_{\mathbf{q}} = (2\pi)^{-d} \int d^d q$ with $|q_i| \leq \pi/\tilde{a}, i=1, \dots, d$. Equations (52)–(57) are defined for all integer dimensions $d = 1, 2, \dots$. They can be extended to continuous d , as usual, by means of analytic continuation via Euler's Gamma function Γ . From Eq. (57) one obtains the singular part of f_b for $0 < d < 2$ and $2 < d < 4$

$$f_{bs} = Y \xi^{-d} \quad (58)$$

with the universal bulk amplitude

$$Y = -\frac{R_\xi^{+d}}{\alpha(1-\alpha)(2-\alpha)} = -\frac{A_d}{d(4-d)}, \quad (59)$$

$$A_d = \frac{\Gamma(3-d/2)}{2^{d-2} \pi^{d/2} (d-2)}. \quad (60)$$

For $0 < d < 2$ and $2 < d < 4$, the regular part of f_b reads,

$$f_0 = \tilde{a}^{-d} [\tilde{c}_1 + r_0 \tilde{a}^2 \tilde{c}_2 + r_0^2 \tilde{a}^4 \tilde{c}_3 + O(r_0^3 \tilde{a}^6)] \quad (61)$$

with d -dependent constants \tilde{c}_i . The constants \tilde{c}_1 , \tilde{c}_2 , and \tilde{c}_3 diverge for $d \rightarrow 0$, $d \rightarrow 2$, and $d \rightarrow 4$, respectively, where f_b attains a logarithmic dependence on $r_0 \tilde{a}^2$. The bulk susceptibility is simply, $\chi_b = r_0^{-1} = J_0^{-1} \xi^2$, which implies $A_\chi = a_0^{-1}$. The critical exponents are

$$\eta = 0, \quad \gamma = 2\nu = 1 \quad \text{for all } d > 0 \quad (62)$$

and

$$\alpha = (4-d)/2 \quad \text{for } 0 < d \leq 4 \quad (63)$$

above T_c , in agreement with the hyperscaling relation Eq. (27) for $d \leq 4$. Equations (59) and (63) imply $(R_\xi^+)^d = A_d(d-2)/8$ for $d < 4$. The prefactor in Eq. (2) is simply $A_\chi \xi_0^{-\gamma/\nu} = J_0^{-1}$.

The second-moment bulk correlation length ξ must be distinguished from the ‘‘exponential’’ bulk correlation length ξ_e in the direction of the unit vector $\mathbf{e} = (\mathbf{x}_i - \mathbf{x}_j)/|\mathbf{x}_i - \mathbf{x}_j|$, which is defined via the large-distance behavior of the anisotropic bulk correlation function $G(\mathbf{x}_i - \mathbf{x}_j) = \langle \varphi_i \varphi_j \rangle$ [41]. For the special case where $\mathbf{x} = (x, 0, 0, \dots)$ is directed along one of the cubic axes, the correlation function decays exponentially as [7]

$$G(\mathbf{x}) = \frac{\tilde{a}^{2-d}}{4J} \left(\frac{\tilde{a}}{2\pi|x|} \right)^{(d-1)/2} \left[\sinh \left(\frac{\tilde{a}}{\xi_1} \right) \right]^{(d-3)/2} \times e^{-|x|/\xi_1} [1 + O(|x|^{-1})] \quad (64)$$

with the exponential correlation length

$$\xi_1 = \left[\frac{2}{a} \operatorname{arcsinh} \left(\frac{\tilde{a}}{2\xi} \right) \right]^{-1}. \quad (65)$$

We shall see that it is ξ_1 rather than ξ that determines the exponential part of the finite-size effects above T_c not only for periodic boundary conditions [7] but also for free boundary conditions.

C. Free energy density

In Appendix A we derive from Eq. (52) the size dependent free energy density for box geometry for large L/\tilde{a} at fixed $L/\xi \geq 0$ and at fixed L/\tilde{L} for $d > 1$

$$f(t, L, \tilde{L}) = f_b + 2f_{\text{surface}}(t) L^{-1} + \mathcal{G}(L/\xi, L/\tilde{L}) L^{-d} - \frac{1}{2} \tilde{a}^{-1} \tilde{L}^{1-d} \ln 2 + O(\tilde{a} L^{-d-1}, \tilde{a}^4 L^{-4}), \quad (66)$$

where

$$f_{\text{surface}}(t) = \frac{\tilde{a}^{1-d}}{8} \int_0^\infty dy \{ y^{-1} [1 + e^{-4y} - 2e^{-2y} I_0(2y)] \times [e^{-2y} I_0(2y)]^{d-1} \exp(-y r_0 \tilde{a}^2 J_0^{-1}) \} \quad (67)$$

with the Bessel function of order zero,

$$I_0(z) = \frac{1}{\pi} \int_0^\pi d\theta \exp(z \cos \theta). \quad (68)$$

Equation (66) contains the universal finite-size part

$$\mathcal{G}(x, s) = \frac{1}{2} \int_0^\infty dy y^{-1} \left\{ \left(\frac{\pi}{y} \right)^{d/2} - \frac{1}{2} [sK(s^2 y)]^{d-1} \left[K \left(\frac{y}{4} \right) - 1 \right] - \frac{1}{2} \left(\frac{\pi}{y} \right)^{(d-1)/2} \right\} e^{-yx^2/4\pi^2} \quad (69)$$

with

$$K(z) = \sum_{m=-\infty}^{\infty} \exp(-m^2 z). \quad (70)$$

We note that f_{surface} depends on the lattice constant \tilde{a} , unlike the finite-size part $\mathcal{G}(x, s)$. Using $K(z) \sim (\pi/z)^{1/2}$ for $z \rightarrow 0$, we obtain for film geometry ($\tilde{L} \rightarrow \infty$)

$$\mathcal{G}(x, 0) = \frac{1}{2} \int_0^\infty dy y^{-1} \left[\left(\frac{\pi}{y} \right)^{1/2} - \frac{1}{2} K \left(\frac{y}{4} \right) \right] \times \left(\frac{\pi}{y} \right)^{(d-1)/2} e^{-yx^2/4\pi^2}. \quad (71)$$

The surface part remains, of course, identical with Eq. (67). Equations (66)–(71) are applicable to $T = T_c$ and to $T > T_c$ at fixed L/ξ . The correct exponential large- L/ξ behavior of $\mathcal{G}(L/\xi, L/\tilde{L})$ at fixed $T > T_c$ is not yet included in Eqs. (69) and (71) as it involves the ‘‘exponential’’ correlation length ξ_1 , Eq. (65). For large $L \gg \xi$ at fixed $T > T_c$, Eq. (69) must be replaced by

$$\begin{aligned} \mathcal{G}(L/\xi_1, L/\tilde{L}) &= -2^{-d} [L/(\pi\xi_1)]^{(d-1)/2} e^{-2L/\xi_1} \\ &\times [1 + O(\xi_1^2/L^2)] - (d-1) \\ &\times (L/\tilde{L})^{(d+1)/2} [L/(2\pi\xi_1)]^{(d-1)/2} e^{-\tilde{L}/\xi_1} \\ &\times [1 + O(\xi_1^{1/2}\tilde{L}^{-1/2})]. \end{aligned} \quad (72)$$

Correspondingly, Eq. (16) must be modified for large $L \gg \xi$. The nonuniversal last term $\sim \tilde{L}^{1-d}$ in Eq. (66) contributes to the regular part $f_{ns}(t, L, \tilde{L})$ of f , thus Eq. (15) should be complemented accordingly. In order to clarify to what extent the \tilde{a} dependent term $f_{surface}(t)$ contains universal contributions, we need to distinguish the cases $1 < d < 3$, $d = 3$, and $3 < d < 5$. For this purpose it will be useful to express the regular part linear in r_0 in terms of generalized Watson functions defined by [16]

$$W_d(z) = \frac{1}{(2\pi)^d} \int_0^{2\pi} \dots \int_0^{2\pi} \frac{d\theta_1 \dots d\theta_d}{z + 2 \sum_{j=1}^d (1 - \cos \theta_j)} \quad (73)$$

$$= \int_0^\infty dy e^{-zy} [e^{-2y} I_0(2y)]^d. \quad (74)$$

1. $1 < d < 3$

For $0 \leq r_0 \tilde{a}^2 \ll 1$ and $1 < d < 3$ we obtain from Eq. (67)

$$\begin{aligned} f_{surface}(t) &= f_{surface}(0) + A_{surface}^+ \xi^{1-d} - \tilde{b}_d r_0 \tilde{a}^{3-d} J_0^{-1} \\ &+ O(\tilde{a}/\xi^d) \end{aligned} \quad (75)$$

with the universal amplitude

$$A_{surface}^+ = -\frac{\Gamma((3-d)/2)}{2^{d+1} \pi^{(d-1)/2} (d-1)} < 0 \quad (76)$$

and with the nonuniversal constant

$$\begin{aligned} \tilde{b}_d &= \frac{1}{8} \int_0^\infty dy \{ [1 + e^{-4y} - 2e^{-2y} I_0(2y)] [e^{-2y} I_0(2y)]^{d-1} \\ &- (4\pi y)^{(1-d)/2} \}. \end{aligned} \quad (77)$$

This constant can be partially expressed in terms of generalized Watson function as

$$\begin{aligned} \tilde{b}_d &= \frac{1}{8} [W_{d-1}(4) - 2W_d(0)] + \frac{1}{8} \int_0^A dy [e^{-2y} I_0(2y)]^{d-1} \\ &+ \frac{1}{8} \int_A^\infty \{ [e^{-2y} I_0(2y)]^{d-1} - (4\pi y)^{(1-d)/2} \} \\ &+ 2^{-d-1} \pi^{(1-d)/2} (d-3)^{-1} A^{(3-d)/2} \end{aligned} \quad (78)$$

(see Appendix A). We note that \tilde{b}_d does not depend on the arbitrary finite constant $A > 0$.

The second term in Eq. (75) has the expected singular scaling form $\sim \xi^{1-d}$. The first term $f_{surface}(0)$ and the third term $\sim \tilde{b}_d$ contribute to the regular part $2\Psi_1(t)L^{-1}$ of $f_{ns}(t, L, \tilde{L})$. Thus the surface contribution is in accord with the predicted universal scaling structure of Eqs. (13), (15), (17), and (18). We expect that \tilde{b}_d depends on the lattice structure (see also Sec. III G). We note that both $A_{surface}^+$ and the coefficient \tilde{b}_d diverge for $d \rightarrow 3$ such that

$$\lim_{d \rightarrow 3^-} [\tilde{b}_d - A_{surface}^+] = \tilde{b} \quad (79)$$

has a finite limit \tilde{b} (see Appendix A). The explicit expression for the constant \tilde{b} is given in Eqs. (81) and (82) below.

2. $d = 3$

For $0 \leq r_0 \tilde{a}^2 \ll 1$ we obtain from Eq. (67) at $d = 3$

$$\begin{aligned} f_{surface}(t) &= f_{surface}(0) - (16\pi)^{-1} \xi^{-2} \ln(\xi/\tilde{a}) - \tilde{b} r_0 J_0^{-1} \\ &+ O(\tilde{a}/\xi^3). \end{aligned} \quad (80)$$

The analytic expression for the nonuniversal constant \tilde{b} is

$$\begin{aligned} \tilde{b} &= \frac{1}{8} \int_0^A dy [1 + e^{-4y} - 2e^{-2y} I_0(2y)] e^{-4y} [I_0(2y)]^2 \\ &+ \frac{1}{8} \int_A^\infty dy \{ [1 + e^{-4y} - 2e^{-2y} I_0(2y)] e^{-4y} [I_0(2y)]^2 \\ &- (4\pi y)^{-1} \} + (32\pi)^{-1} (1 - C_E - \ln A), \end{aligned} \quad (81)$$

where $C_E = 0.577$ is Euler's constant. This constant can be partially expressed in terms of generalized Watson functions as

$$\begin{aligned} \tilde{b} &= \frac{1}{8} [W_2(4) - 2W_3(0)] + \frac{1}{8} \int_0^A dy [e^{-2y} I_0(2y)]^2 \\ &+ \frac{1}{8} \int_A^\infty \{ [e^{-2y} I_0(2y)]^2 - (4\pi y)^{-1} \} + (32\pi)^{-1} \\ &\times (1 - C_E - \ln A). \end{aligned} \quad (82)$$

Note that \tilde{b} does not depend on the arbitrary finite constant $A > 0$. We expect that \tilde{b} depends on the lattice structure (see also Sec. III G).

While the first and third terms of Eq. (80) contribute to the nonuniversal regular part $2\Psi_1(t)L^{-1}$ of $f_{ns}(t, L, \tilde{L})$, the second (logarithmic) term is clearly a singular contribution to the free energy density. This implies that, for $d = 3$, Eqs. (13) and (16) must be replaced by

$$f_s(t, L, \tilde{L}, \tilde{a}) = L^{-3} \tilde{\mathcal{F}}(L/\xi, L/\tilde{L}, \tilde{a}/\xi), \quad (83)$$

where

$$\tilde{\mathcal{F}}(L/\xi, L/\tilde{L}, \tilde{a}/\xi) = \mathcal{F}(L/\xi, L/\tilde{L}) - (8\pi)^{-1} (L/\xi)^2 \ln(\xi/\tilde{a}) \quad (84)$$

contains a logarithmic nonscaling term that depends on the nonuniversal lattice constant \tilde{a} . We conjecture, however, that the coefficient $-(8\pi)^{-1}$ is universal, i.e., independent of the lattice structure (see also Sec. III G). The scaling part reads

$$\mathcal{F}(L/\xi, L/\tilde{L}) = (12\pi)^{-1}(L/\xi)^3 + \mathcal{G}(L/\xi, L/\tilde{L}), \quad (85)$$

where $\mathcal{G}(L/\xi, L/\tilde{L})$ is given by Eq. (69) for box geometry and by Eq. (71) for film geometry. Correspondingly, the universal scaling prediction of Eq. (14) must be replaced by

$$f_s(t, L, \tilde{L}, \tilde{a}) = Y\xi^{-3} - [(8\pi)^{-1}\xi^{-2}\ln(\xi/\tilde{a})]L^{-1} + L^{-3}\mathcal{G}(L/\xi, L/\tilde{L}) + O(L^{-4}), \quad (86)$$

with the universal bulk amplitude $Y = -(12\pi)^{-1}$ but *without a universal surface amplitude*. In Sec. III D we shall see that this logarithmic behavior is related to the vanishing of the surface critical exponent of the Gaussian energy density at $d=3$.

3. $3 < d < 5$

For $0 \leq \tilde{a}/\xi \ll 1$ we obtain, from Eq. (67), for $3 < d < 5$

$$f_{surface}(t) = f_{surface}(0) - \tilde{B}_d r_0 \tilde{a}^{3-d} J_0^{-1} + A_{surface}^+ \xi^{1-d} + O(\tilde{a}/\xi^d) \quad (87)$$

with the universal amplitude

$$A_{surface}^+ = \frac{\Gamma((5-d)/2)}{2^d \pi^{(d-1)/2} (d-1)(d-3)} > 0 \quad (88)$$

and with the nonuniversal constant

$$\tilde{B}_d = \frac{1}{8} \int_0^\infty dy \{ [1 + e^{-4y} - 2e^{-2y}I_0(2y)] [e^{-2y}I_0(2y)]^{d-1} \} > 0. \quad (89)$$

This constant can be expressed in terms of generalized Watson functions as

$$\tilde{B}_d = \frac{1}{8} [W_{d-1}(0) + W_{d-1}(4) - 2W_d(0)]. \quad (90)$$

We note that $W_{d-1}(0)$ exhibits a pole $\sim (d-3)^{-1}$ near $d=3$, where it can be represented as

$$W_{d-1}(0) = 2^{2-d} \pi^{(1-d)/2} (d-3)^{-1} A^{(3-d)/2} + \int_0^A dy [e^{-2y}I_0(2y)]^{d-1} + \int_A^\infty dy \{ [e^{-2y}I_0(2y)]^{d-1} - (4\pi y)^{(1-d)/2} \}. \quad (91)$$

The right-hand side of Eq. (91) is independent of the arbitrary constant $A > 0$. The first two terms in Eq. (87) contrib-

ute to the regular part $2\Psi_1(t)L^{-1}$ of $f_{ns}(t, L)$, whereas the third term has the expected singular scaling form $\sim \xi^{1-d}$. Thus the surface contribution is in accord with the predicted universal scaling structure of Eqs. (13), (14), (16), and (17).

We expect that \tilde{B}_d depends on the lattice structure (see also Sub. III G). We note that Eqs. (88) and (89) are the analytic continuations of Eqs. (76) and (77), respectively, from $d < 3$ to $d > 3$ and that both $A_{surface}^+$ and the coefficient \tilde{B}_d diverge for $d \rightarrow 3$ such that

$$\lim_{d \rightarrow 3^+} [\tilde{B}_d - A_{surface}^+] = \tilde{b} \quad (92)$$

has a finite limit \tilde{b} , Eq. (81) (see Appendix A).

D. Energy density

Equations (18) and (52) yield the Gaussian energy density (divided by k_B)

$$U(t, L, \tilde{L}) \equiv -\frac{T^2 a_0}{2T_c} E(r_0, L, \tilde{L}, \tilde{a}) \quad (93)$$

with

$$E(r_0, L, \tilde{L}, \tilde{a}) = \tilde{L}^{1-d} L^{-1} \sum_{\mathbf{k}, p} (r_0 + J_{\mathbf{k}, d-1} + J_p)^{-1}. \quad (94)$$

In the following, we must distinguish the cases $T = T_c$ and $T > T_c$. Using Eqs. (18) and (66)–(70) we obtain for $T > T_c$ and for large L/\tilde{a} and large ξ/\tilde{a} at fixed $L/\xi > 0$ and fixed \tilde{L}/L in $2 < d < 4$ dimensions

$$U(t, L, \tilde{L}) = U_b(t) + 2U_{surface}(t)L^{-1} + T_c \xi_0^{-2} \mathcal{E}(L/\xi, L/\tilde{L}) L^{2-d} + O(\tilde{a}L^{1-d}), \quad (95)$$

where $U_b(t) = -T^2 \partial f_b / \partial T$ is the bulk part of $U(t, L, \tilde{L})$. Near T_c the surface energy density is given by

$$U_{surface}(t) \equiv \frac{T_c \tilde{a}^{3-d}}{8\xi_0^2} E_{surface}(r_0 \tilde{a}^2 J_0^{-1}) \quad (96)$$

with

$$E_{surface}(z) = \int_0^\infty dy \{ [1 + e^{-4y} - 2e^{-2y}I_0(2y)] \times [e^{-2y}I_0(2y)]^{d-1} e^{-yz} \}, \quad (97)$$

where $z \equiv r_0 \tilde{a}^2 J_0^{-1}$. Equation (97) can be expressed completely in terms of generalized Watson functions as

$$E_{surface}(z) = W_{d-1}(z) + W_{d-1}(z+4) - 2W_d(z). \quad (98)$$

The universal function $\mathcal{E}(x, s) = -\frac{1}{2}x^{-1} \partial \mathcal{G}(x, s) / \partial x$ of the finite-size part reads

$$\mathcal{E}(x,s) = \frac{1}{8\pi^2} \int_0^\infty dy \left\{ \left(\frac{\pi}{y} \right)^{d/2} - \frac{1}{2} [sK(s^2y)]^{d-1} \left[K\left(\frac{y}{4}\right) - 1 \right] - \frac{1}{2} \left(\frac{\pi}{y} \right)^{(d-1)/2} \right\} e^{-yx^2/4\pi^2} \quad (99)$$

for box geometry and

$$\mathcal{E}(x,0) = \frac{1}{8\pi^2} \int_0^\infty dy \left[\left(\frac{\pi}{y} \right)^{1/2} - \frac{1}{2} K\left(\frac{y}{4}\right) \right] \left(\frac{\pi}{y} \right)^{(d-1)/2} e^{-yx^2/4\pi^2} \quad (100)$$

for film geometry. We note that $E_{surface}$ depends on the lattice constant \tilde{a} , unlike the finite-size part $\mathcal{E}(x,s)$. Equations (95)–(100) are not applicable to $T=T_c$ for $d \leq 3$, where the functions $U_{surface}(0)$ and $\mathcal{E}(0,0)$ diverge. For $3 < d < 4$, Eqs. (95)–(100) are applicable to both $T=T_c$ and $T > T_c$ at fixed $L/\xi \geq 0$. The correct exponential large- L behavior in terms of ξ_1 at fixed $T > T_c$ is not yet included in Eq. (100). It can be derived from $\mathcal{G}(L/\xi_1, L/\tilde{L})$, Eq. (72).

In order to see to what extent $E_{surface}$ contains universal contributions, we need to distinguish the cases $2 < d < 3$, $d = 3$, and $3 < d < 4$.

1. $2 < d < 3$

For $0 < r_0 \tilde{a}^2 \ll 1$ and $2 < d < 3$ we obtain, from Eqs. (25) and (75),

$$U_{surface}(t) = \frac{1}{2} T_c \xi_0^{-2} [-(d-1) A_{surface}^+ \xi^{3-d} + 2 \tilde{a}^{3-d} \tilde{b}_d] + O(\tilde{a}/\xi^{d-2}), \quad (101)$$

where \tilde{b}_d and $A_{surface}^+ < 0$ are given by Eqs. (77) and (76). Equation (101) implies a divergent surface energy density $\sim t^{1-\alpha-\nu}$ with a universal surface amplitude $(1-d)\nu A_{surface}^+ > 0$ and with the critical exponent

$$1 - \alpha - \nu = (d-3)/2 < 0, \quad (102)$$

in accordance with the singular finite-size scaling part of Eq. (26). Thus, for $2 < d < 3$, $U_s(t, L, \tilde{L})$ satisfies the scaling prediction of Eqs. (19) and (20) with the critical exponent $(1-\alpha)/\nu = d-2$ and with the universal scaling function for $x > 0$

$$\mathcal{U}(x,s) = -d\nu Y x^{d-2} - 2(d-1)\nu A_{surface}^+ x^{d-3} + 2\nu \mathcal{E}(x,s), \quad (103)$$

where the universal bulk amplitude Y is given by Eq. (58). The function $\mathcal{E}(x,s)$ diverges as $\sim x^{d-3}$ for $x \rightarrow 0$. This divergence is canceled by the surface term, which implies the finite limit

$$\mathcal{U}(0,s) = \lim_{x \rightarrow 0} \mathcal{U}(x,s) = \mathcal{E}_d(s), \quad (104)$$

where

$$\mathcal{E}_d(s) = \frac{1}{8\pi^2} \int_0^\infty dy \left\{ \left(\frac{\pi}{y} \right)^{d/2} - \frac{1}{2} [sK(s^2y)]^{d-1} \left[K\left(\frac{y}{4}\right) - 1 \right] \right\} \quad (105)$$

for box geometry and

$$\mathcal{E}_d(0) = \frac{1}{8\pi^2} \int_0^\infty dy \left(\frac{\pi}{y} \right)^{(d-1)/2} \left\{ \left(\frac{\pi}{y} \right)^{1/2} - \frac{1}{2} \left[K\left(\frac{y}{4}\right) - 1 \right] \right\} \quad (106)$$

for film geometry. By a separate calculation at $T=T_c$ we find from Eq. (93),

$$U(0, L, \tilde{L}) = U_b(0) + T_c \xi_0^{-2} [\mathcal{E}_d(s) L^{2-d} + 2\tilde{b}_d \tilde{a}^{3-d} L^{-1}] + O(\tilde{a}^{2-d/2} L^{-d/2}, e^{-\tilde{L}/\tilde{a}}) \quad (107)$$

in agreement with the scaling parts, Eqs. (105) and (106). We note that $A_{surface}^+$, \mathcal{E}_d and \tilde{b}_d diverge for $d \rightarrow 3$.

2. $d = 3$

For $0 < r_0/\tilde{a}^2 \ll 1$ and for $d=3$ we obtain, from Eqs. (24), (80) and (95)–(100),

$$U(t, L, \tilde{L}) = U_b(t) + [2U_{surface}(t) + T_c \xi_0^{-2} \mathcal{E}(L/\xi, L/\tilde{L})] L^{-1} + O(\tilde{a} L^{-4}) \quad (108)$$

with

$$U_{surface}(t) = \frac{1}{2} T_c \xi_0^{-2} [(8\pi)^{-1} \ln(\xi/\tilde{a}) + 2\tilde{b} - (8\pi)^{-1} + O(\tilde{a}/\xi)], \quad (109)$$

where \tilde{b} is given by Eq. (81). Thus, as a special property of the Gaussian model, there exists a logarithmically divergent surface energy density with an explicit dependence on the lattice spacing \tilde{a} . This could have been anticipated on general grounds because of $1-\alpha-\nu=0$ for $d=3$. (This is parallel to logarithmic terms for systems with periodic boundary conditions at the borderline dimension where the specific heat exponent α vanishes [44].) Thus, Eq. (26) is not applicable and the universal scaling prediction for the singular part $U_s(t, L, \tilde{L})$, Eqs. (20)–(22), must be replaced by

$$U_s(t, L, \tilde{L}, \tilde{a}) = T_c \xi_0^{-2} L^{-1} \tilde{\mathcal{U}}(L/\xi, L/\tilde{L}, \tilde{a}/\xi), \quad (110)$$

where

$$\tilde{\mathcal{U}}(L/\xi, L/\tilde{L}, \tilde{a}/\xi) = \mathcal{U}(L/\xi, L/\tilde{L}) + (8\pi)^{-1} \ln(\xi/\tilde{a}) \quad (111)$$

with the scaling part

$$\mathcal{U}(x,s) = -d\nu Y x + \mathcal{E}(x,s) - (16\pi)^{-1}. \quad (112)$$

We identify the nonsingular part as

$$U_{ns}(t, L, \tilde{L}) = U_b(t) - U_{bs}(t) + T_c \xi_0^{-2} \tilde{b} L^{-1} + O(\tilde{a} L^{-4}). \quad (113)$$

The function $\mathcal{E}(x, s)$ diverges logarithmically for $x \rightarrow 0$. This divergence is canceled by $U_{surface}(t)$, which implies that Eq. (108) has a finite limit for $t \rightarrow 0$ at fixed L and \tilde{L} ,

$$U(0, L, \tilde{L}) = U_b(0) + T_c \xi_0^{-2} \{ -(8\pi)^{-1} L^{-1} \ln(\tilde{a}/L) + [\bar{b}(s) + 2\tilde{b}] L^{-1} \} + O(\tilde{a}^{1/2} L^{-3/2}, e^{-\tilde{L}/\tilde{a}}) \quad (114)$$

with the universal constant

$$\begin{aligned} \bar{b}(s) = & \frac{1}{8\pi^2} \int_A^\infty dy \left\{ (\pi/y)^{3/2} - \frac{1}{2} [sK(s^2y)]^2 [K(y/4) - 1] \right\} \\ & + \frac{1}{8\pi^2} \int_0^A dy \left\{ (\pi/y)^{3/2} - \frac{1}{2} [sK(s^2y)]^2 \right. \\ & \times [K(y/4) - 1] - \frac{\pi}{2y} \left. \right\} + (16\pi)^{-1} \ln A - (16\pi)^{-1} \\ & \times [1 - C_E + 2 \ln(2\pi)]. \end{aligned} \quad (115)$$

Note that $\bar{b}(s)$ is independent of the arbitrary constant A . We have confirmed the validity of Eqs. (114) and (115) for $d = 3$ by calculating $U(0, L, \tilde{L})$ directly from Eq. (93) with $r_0 = 0$. Thus there exists a logarithmic nonscaling L dependence of the energy density at T_c , with an explicit dependence on \tilde{a} . As noted above, we conjecture, however, that the coefficients $(8\pi)^{-1}$ and $-(8\pi)^{-1}$ in Eqs. (109) and (114) are universal, i.e., independent of the lattice structure (see also Sec III G). In Sec. IV we shall see that the logarithms in Eqs. (109) and (114) are the origin of the logarithms appearing in the three-dimensional mean spherical model with free boundary conditions.

3. $3 < d < 4$

For $0 < r_0 \tilde{a}^2 \ll 1$ and for $3 < d < 4$ we obtain, from Eqs. (25) and (87),

$$U_{surface}(t) = U_{surface}(0) - T_c \xi_0^{-2} (d-1) A_{surface}^+ \xi^{3-d} + O(\tilde{a} \xi^{2-d}) \quad (116)$$

with the finite critical value

$$U_{surface}(0) = T_c \xi_0^{-2} \tilde{a}^{3-d} \tilde{B}_d > 0, \quad (117)$$

where $A_{surface}^+ > 0$ and \tilde{B}_d are given by Eqs. (88) and (89). The singular second term $\sim \xi^{3-d}$ yields a divergent slope $\sim t^{(d-5)/2}$ for $t \rightarrow 0+$, thus $U_{surface}(t)$ has a nonuniversal finite cusp at $t=0$ for $3 < d < 5$, in contrast to the $d \leq 3$ case. As a consequence, only the temperature dependent contributions $\sim \xi^{3-d}$ and $\sim \mathcal{E}(L/\xi, L/\tilde{L})$ to the energy density

$$U(t, L, \tilde{L}) = U_{ns}(0, L) - T_c \xi_0^{-2} (d-1) A_{surface}^+ \xi^{3-d} L^{-1} + T_c \xi_0^{-2} \mathcal{E}(L/\xi, L/\tilde{L}) L^{2-d} + O(\tilde{a} L^{1-d}) \quad (118)$$

have a universal scaling form. The nonuniversal critical value $U_{surface}(0)$, Eq. (117), increases for $d \rightarrow 3$. It enters the finite energy density at T_c

$$U_{ns}(0, L, \tilde{L}) = U_b(0) + 2U_{surface}(0)/L + O(\tilde{a} L^{1-d}), \quad (119)$$

which belongs to the nonuniversal nonsingular part of $U(t, L, \tilde{L})$ and which has a nonscaling L dependence $\sim L^{-1}$. This L dependence is non-negligible. This will have significant consequences for the mean spherical model in $d > 3$ dimensions to be discussed in Sec. IV.

E. Specific heat

Equations (29) and (93) yield the specific heat (divided by k_B)

$$\begin{aligned} C(t, L) = & \frac{T^2 a_0^2}{2T_c^2} L^{-1} \tilde{L}^{1-d} \sum_{\mathbf{k}, p} (r_0 + J_{\mathbf{k}, d-1} + J_p)^{-2} \\ & - \frac{T a_0}{T_c} L^{-1} \tilde{L}^{1-d} \sum_{\mathbf{k}, p} (r_0 + J_{\mathbf{k}, d-1} + J_p)^{-1}. \end{aligned} \quad (120)$$

From the first term of Eq. (120) we find full agreement with the finite-size scaling prediction, Eq. (30), in $2 < d < 4$ dimensions with $2/\nu = 4$, $\alpha/\nu = 4 - d$. Specifically we find, for large L/\tilde{a} and ξ/\tilde{a} at fixed $L/\xi \geq 0$ and fixed \tilde{L}/L , the universal scaling function for $x \geq 0$

$$C(x, s) = \frac{1}{64\pi^4} \int_0^\infty dy y [sK(s^2y)]^{d-1} \left[K\left(\frac{y}{4}\right) - 1 \right] e^{-yx^2/4\pi^2} \quad (121)$$

for box geometry and

$$C(x, 0) = \frac{1}{32\pi^4} \int_0^\infty dy y \left(\frac{\pi}{y}\right)^{(d-1)/2} e^{-x^2y/4\pi^2} \sum_{n=1}^\infty e^{-n^2y/4} \quad (122)$$

for film geometry. The evaluation of the second term of Eq. (120) can be taken directly from Sec. III D for the energy density and yields only subleading corrections to the first term of Eq. (120). For $T > T_c$, Eqs. (121) and (122) can be decomposed as

$$\begin{aligned} \mathcal{C}(x,s) = & -\frac{1}{4}d(d-2)Yx^{d-4} + A_{C,surface}^+ x^{d-5} \\ & - \frac{1}{32\pi^4} \int_0^\infty dy y \left\{ \left(\frac{\pi}{y} \right)^{d/2} - \frac{1}{2} [sK(s^2y)]^{d-1} \right. \\ & \left. \times \left[K\left(\frac{y}{4}\right) - 1 \right] - \frac{1}{2} \left(\frac{\pi}{y} \right)^{(d-1)/2} \right\} e^{-yx^2/4\pi^2} \end{aligned} \quad (123)$$

and

$$\begin{aligned} \mathcal{C}(x,0) = & -\frac{1}{4}d(d-2)Yx^{d-4} + A_{C,surface}^+ x^{d-5} \\ & - \frac{1}{32\pi^4} \int_0^\infty dy y (\pi/y)^{(d-1)/2} \\ & \times \left[(\pi/y)^{1/2} - \frac{1}{2} K\left(\frac{y}{4}\right) \right] e^{-yx^2/4\pi^2}, \end{aligned} \quad (124)$$

where the bulk part (first term) contains the universal bulk quantity Y , Eq. (59), and where the surface part (second term) has the universal surface amplitude

$$A_{C,surface}^+ = -2^{-d-1} \pi^{(1-d)/2} \Gamma((5-d)/2) \quad (125)$$

$$= \frac{1}{2} (d-1)(3-d) A_{surface}^+ \quad (126)$$

with $A_{surface}^+$ given by Eqs. (76) or (88), in agreement with the predicted structure of the surface specific heat, Eqs. (33) and (35). Equations (124)–(126) can be easily confirmed by calculating the derivative $\partial U/\partial T$ from Eqs. (95)–(100).

Equations (123) and (124) do not yet include the correct exponential part of the large- L behavior at fixed $T > T_c$ which involves the exponential correlation length ξ_1 [7] and which can be derived from Eq. (72).

F. Susceptibility

The thermodynamic quantity of primary interest in the mean spherical model in Sec. IV will be the susceptibility. Important steps in the calculation of its finite-size properties can be performed already on the level of the Gaussian model. For box geometry the susceptibility is defined by

$$\chi(t,L,\tilde{L}) = \frac{\tilde{a}^{2d}}{\tilde{L}^{d-1}L} \sum_{i,j} \langle \varphi_i \varphi_j \rangle. \quad (127)$$

Substituting the representation Eq. (46) into Eq. (127), we find

$$\sum_j \varphi_j = \frac{\tilde{a}^{1-d}}{(L+\tilde{a})\sqrt{2}} \sum_p \hat{\varphi}_{0,p} [1 - (-1)^n] \frac{\sin(p\tilde{a})}{1 - \cos(p\tilde{a})}, \quad (128)$$

$$\chi(t,L,\tilde{L}) = \frac{\tilde{a}^2}{L(L+\tilde{a})^2} \sum_p [1 - (-1)^n] \cot^2(p\tilde{a}/2) \langle \hat{\varphi}_{0,p} \hat{\varphi}_{0,p} \rangle \quad (129)$$

with $n \equiv p(L+\tilde{a})/\pi = 1, 2, \dots, L/\tilde{a}$. From the Gaussian Hamiltonian Eq. (48) we have $\langle \hat{\varphi}_{0,p} \hat{\varphi}_{0,p} \rangle = (L+\tilde{a})(r_0 + J_p)^{-1}$, which leads to

$$\chi(t,L,\tilde{L}) = \frac{\tilde{a}^2}{L(L+\tilde{a})^2} \sum_p [1 - (-1)^n] \frac{\cot^2(p\tilde{a}/2)}{r_0 + J_p}. \quad (130)$$

We note that this expression is independent of the dimension d and of \tilde{L} which is a special property of the Gaussian model. In Appendix B we evaluate Eq. (130) for large L/\tilde{a} . For large ξ/\tilde{a} at fixed ratio $L/\xi \geq 0$, we find the scaling form

$$\chi(t,L,\tilde{L}) = \chi_b f(L/\xi) = L^{\gamma/\nu} \Phi(L/\xi) \quad (131)$$

with $\gamma/\nu = 2$ and the universal scaling function

$$f_\chi(x) = \frac{4}{\pi^2} \int_0^\infty dy (1 - e^{-yx^2/\pi^2}) [K(y) - K(4y)], \quad (132)$$

where $K(z)$ is given by Eq. (70) and

$$\Phi(x) = J_0^{-1} x^{-2} f_\chi(x), \quad (133)$$

with $x = L/\xi$. The leading terms of $f_\chi(x)$ for large x are

$$f_\chi(x) = 1 - 2x^{-1} + O(x^{-2}). \quad (134)$$

For $x \rightarrow 0$ we find $\lim_{x \rightarrow 0} x^{-2} f_\chi(x) = 1/12$, thus the leading L dependence at $T = T_c$ is in accord with the scaling prediction Eq. (42), with $A_\chi \xi_0^{-\gamma/\nu} = J_0^{-1}$ and

$$B_\chi = \frac{1}{12}, \quad (135)$$

independent of the shape factor L/\tilde{L} . In the limit $L \rightarrow \infty$ at fixed $T > T_c$, Eqs. (131)–(134) are valid only up to a non-universal exponential contribution $\sim e^{-L/\xi_1}$ in terms of L/ξ_1 rather than L/ξ [7].

G. Continuum approximation with Dirichlet boundary conditions

As a first step towards the φ^4 field theory with Dirichlet boundary conditions at finite cutoff Λ in a confined geometry, we briefly consider the continuum version of the Gaussian model. The comparison with the lattice version will serve to distinguish universal contributions from nonuniversal contributions.

The Gaussian continuum Hamiltonian for the scalar field $\varphi(\mathbf{x}) = \varphi(\mathbf{y}, z)$ reads

$$H_{field} = \int d^d x \left[\frac{r_0}{2} \varphi^2 + \frac{1}{2} (\nabla \varphi)^2 \right]. \quad (136)$$

This corresponds to the replacements $2J \rightarrow 1$ and $J_{\mathbf{k},d-1} \rightarrow \mathbf{k}^2, J_p \rightarrow p^2$ in Eqs. (48)–(50), (52), (56), and (57). The wave numbers of the Fourier components of the field $\varphi(\mathbf{x})$ are assumed to have a finite sharp cutoff Λ . Although there exists no real system with a sharp cutoff the sharp-cutoff procedure is of significant *conceptual* relevance as it may signal important physical effects in real systems with sub-leading long-range interactions [7,8,45].

As a consequence of the sharp-cutoff procedure, the bulk correlation function $G(\mathbf{x}) = \langle \varphi(\mathbf{x})\varphi(0) \rangle$ has an oscillatory power-law decay above T_c . For the anisotropic cutoff $|q_i| \leq \Lambda, i=1, \dots, d$ we find the anisotropic nonexponential large-distance behavior

$$G(\mathbf{x}) = 2^d \Lambda^{d-2} (d + \xi^{-2} \Lambda^{-2})^{-1} \prod_{i=1}^d \frac{\sin(\Lambda x_i)}{\Lambda x_i} + O(e^{-|\mathbf{x}|/\xi}), \quad (137)$$

in contrast to the exponential decay of the lattice correlation function, Eq. (64). Thus the sharp cutoff induces long-range correlations, as expected [7,8,45]. For an isotropic sharp cutoff $|\mathbf{q}| \leq \Lambda$, see Ref. [8].

The bulk free energy density above T_c is for $2 < d < 4$ and for $0 < d < 2$

$$f_{b,field} = Y \xi^{-d} + f_{0,field} \quad (138)$$

with the regular part

$$f_{0,field} = \Lambda^d [\hat{c}_1 + r_0 \Lambda^{-2} \hat{c}_2 + r_0^2 \Lambda^{-4} \hat{c}_3 + \dots]. \quad (139)$$

The constants \hat{c}_1 , \hat{c}_2 , and \hat{c}_3 diverge for $d \rightarrow 0, d \rightarrow 2$ and $d \rightarrow 4$, respectively, where $f_{b,field}$ attains a logarithmic dependence on $r_0 \Lambda^{-2}$.

In the following, we assume a $L \times \infty^{d-1}$ film geometry, with Dirichlet boundary conditions $\varphi(\mathbf{y}, 0) = \varphi(\mathbf{y}, L) = 0$ at the top and bottom surfaces. The continuum version of Eq. (53) is

$$f_{field}(t, L) = -\frac{1}{2} \Lambda^d \ln \pi + \frac{1}{2} L^{-1} \times \sum_p \int_{\mathbf{k}} \ln[(r_0 + \mathbf{k}^2 + p^2) \Lambda^{-2}]. \quad (140)$$

The sum \sum_p runs over wave numbers $p = \pi n/L, n = 1, 2, \dots$, in the range $0 < p < \Lambda$, and the components k_i are restricted to $|k_i| \leq \Lambda, i = 1, 2, \dots, d-1$. For large $L\Lambda$ at fixed $L/\xi \geq 0$, we find, for $2 < d < 4$

$$f_{field}(t, L) = f_{b,field} + 2\hat{f}_{surface}(t)L^{-1} + \hat{f}_2(r_0 \Lambda^{-2}) \Lambda^{d-2} L^{-2} + \mathcal{G}(L/\xi) L^{-d} + O(\Lambda^{d-4} L^{-4}), \quad (141)$$

where

$$\hat{f}_{surface}(t) = \frac{\Lambda^{d-1}}{8} \int_0^\infty dy y^{-1} (1 - e^{-y}) S(y)^{d-1} \times \exp(-y r_0 \Lambda^{-2}) \quad (142)$$

and

$$\hat{f}_2(r_0 \Lambda^{-2}) = \frac{\pi}{12} \int_0^\infty dy e^{-y} S(y)^{d-1} \exp(-y r_0 \Lambda^{-2}) \quad (143)$$

with

$$S(y) = \frac{1}{2\pi} \int_{-1}^1 dq \exp(-q^2 y). \quad (144)$$

For the universal function $\mathcal{G}(L/\xi)$ see Eq. (71).

In order to exhibit the universal and nonuniversal contributions to $\hat{f}_{surface}(t)$, we need to distinguish the cases $2 < d < 3, 3 < d < 4$. For $2 < d < 3$ we find, from Eq. (142),

$$\hat{f}_{surface}(t) = \hat{f}_{surface}(0) + A_{surface}^+ \xi^{1-d} - \hat{b}_d r_0 \Lambda^{d-3} + O(r_0^2 \Lambda^{d-5}) \quad (145)$$

with the nonuniversal constant

$$\hat{b}_d = \frac{1}{8} \int_0^\infty dy [(1 - e^{-y}) S(y)^{d-1} - (2\pi)^{1-d} (\pi/y)^{(d-1)/2}]. \quad (146)$$

The universal amplitude $A_{surface}^+ < 0$ is given by Eq. (76). For $d=3$, we find a logarithmic nonscaling term similar to that of Eq. (80)

$$\hat{f}_{surface}(t) = \hat{f}_{surface}(0) - (16\pi)^{-1} \xi^{-2} \ln(\Lambda \xi) - \hat{b} r_0 + O(\Lambda^{-2} \xi^{-4}) \quad (147)$$

with the universal prefactor $(16\pi)^{-1}$ and with the nonuniversal constant

$$\hat{b} = \frac{1}{32\pi} + \frac{1}{8} \int_0^\infty dy \{(1 - e^{-y}) [S(y)^2 - (4\pi y)^{-1}]\}. \quad (148)$$

For $3 < d < 4$, we find

$$\hat{f}_{surface}(t) = \hat{f}_{surface}(0) - \hat{B}_d r_0 \Lambda^{d-3} + A_{surface}^+ \xi^{1-d} + O(\Lambda^{-2} \xi^{-4}) \quad (149)$$

with the universal amplitude $A_{surface}^+ > 0$, Eq. (88), and with the nonuniversal constant

$$\hat{B}_d = \frac{1}{8} \int_0^\infty dy S(y)^{d-1} (1 - e^{-y}) > 0. \quad (150)$$

As expected, $f_{field}(t, L)$ and $\hat{f}_{surface}(t)$ contain the same universal parts as the corresponding functions of the lattice model. The nonuniversal constants \hat{b}_d , \hat{b} , and \hat{B}_d , however, differ from the corresponding constants \tilde{b}_d , \tilde{b} , and \tilde{B}_d of the lattice model. For $d \rightarrow 3$, \hat{b}_d , and \hat{B}_d are divergent.

As an additional effect of the sharp cutoff, there exists the nonuniversal contribution L^{-2} to the free energy in Eq. (141). For $d > 2$, this term is non-negligible compared to the universal scaling term $\sim L^{-d}$, but it has a regular dependence on $r_0 \sim t$ and therefore can be considered to belong to the nonsingular part $f_{ns}(t, L)$ of the free energy density. Nevertheless, it yields a leading nonuniversal contribution $\sim \Lambda^{d-2} L^{-2}$ to the Casimir force at T_c , similar to that for periodic boundary conditions discussed in Ref. [8].

We briefly summarize the results for the energy density $U_{field}(t, L)$ as derived from Eqs. (141)–(150). For $2 < d < 3$, we obtain

$$\begin{aligned} U_{field}(t, L) = & U_{b,field}(t) + T_c \xi_0^{-2} [(1-d)A_{surface}^+ \xi^{3-d} \\ & + \Lambda^{d-3} \hat{b}_d] L^{-1} + T_c \xi_0^{-2} \mathcal{E}(L/\xi) L^{2-d} \\ & + O(\Lambda^{d-2} L^{-2}). \end{aligned} \quad (151)$$

The singular part is in full agreement with the finite-size scaling structure. For $d=3$, the energy density reads for large $L\Lambda$ at fixed $t > 0$,

$$\begin{aligned} U_{field}(t, L) = & U_{b,field}(t) + [2\hat{U}_{surface}(t) + T_c \xi^{-2} \mathcal{E}(L/\xi)] L^{-1} \\ & + O(\Lambda L^{-2}) \end{aligned} \quad (152)$$

with

$$\begin{aligned} \hat{U}_{surface}(t) = & \frac{1}{2} T_c \xi_0^{-2} [(8\pi)^{-1} \ln(\Lambda \xi) + 2\hat{b} - (8\pi)^{-1} \\ & + O(\Lambda^{-1} \xi^{-1})]. \end{aligned} \quad (153)$$

In the limit $t \rightarrow 0$, at fixed L , we obtain

$$\begin{aligned} U_{field}(0, L) = & U_{b,field}(0) + T_c \xi_0^{-2} [(8\pi)^{-1} L^{-1} \ln(\Lambda L) \\ & + (\bar{b} + 2\hat{b}) L^{-1} + O(\Lambda^{-1/2} L^{-3/2})] \end{aligned} \quad (154)$$

with the universal constant \bar{b} , Eq. (115), and the nonuniversal constant \hat{b} , Eq. (148). The logarithmic nonscaling behavior in Eqs. (153) and (154) is parallel to that in Eqs. (109) and (114) of the lattice model in Sec. III D. The prefactors $(8\pi)^{-1}$ in Eqs. (153) and (154) are the same as in Eqs. (109) and (114) of the lattice model and are expected to be universal.

For $3 < d < 4$, Eqs. (116)–(119) remain valid if $\tilde{a}^{3-d} \tilde{B}_d$ is replaced by $\Lambda^{d-3} \hat{B}_d$. Thus the surface energy density is

$$\begin{aligned} \hat{U}_{surface}(t) = & \hat{U}_{surface}(0) - T_c \xi_0^{-2} (d-1) A_{surface}^+ \xi^{3-d} \\ & + O(\Lambda^{-1} \xi^{2-d}) \end{aligned} \quad (155)$$

with a finite critical value

$$\hat{U}_{surface}(0) = T_c \xi_0^{-2} \Lambda^{d-3} \hat{B}_d > 0. \quad (156)$$

The singular part $\sim \xi^{3-d}$ is in agreement with finite-size scaling but is subleading compared to the regular part, as expected from the lattice model.

For completeness, we note that the specific heat and the susceptibility of the Gaussian continuum model with free boundary conditions are in full agreement with finite-size scaling for $2 < d < 4$, with the same scaling functions as those in Secs. III E and III F for the lattice model, as expected.

H. Dimensional regularization

The method of dimensional regularization has been employed in all previous analytic calculations of finite-size and surface effects within the φ^4 theory with Dirichlet boundary conditions. This method neglects the cutoff and lattice effects. This is justified provided that the leading terms are universal. This is the case, however, only for $d < d^*$, where d^* is a certain *upper* borderline dimension. In the present context of the Gaussian model with Dirichlet boundary conditions, there exist the following upper borderline dimensions: $d^*=0$ for the bulk free energy density f_b , $d^*=1$ for the surface free energy $f_{surface}$, $d^*=2$ for the bulk energy density U_b , $d^*=3$ for the surface energy density $U_{surface}$, $d^*=4$ for the bulk specific heat C_b and bulk susceptibility χ_b , and $d^*=5$ for the surface specific heat $C_{surface}$ and surface susceptibility $\chi_{surface}$. The method of dimensional regularization correctly accounts for the leading universal parts only for $d < d^*$ (where the cutoff and lattice effects are negligible corrections) and provides an analytic continuation to $d > d^*$. It does not correctly describe, however, the cutoff- and lattice-dependent terms for $d \geq d^*$. The upper borderline dimension $d^*=3$ for the Gaussian surface energy density will play an important role for the three-dimensional mean spherical model in Sec. IV.

We begin with the analytic expression for the bulk free energy density of the Gaussian model in d dimensions within the dimensional regularization scheme [26],

$$f_{b,dim}(t) = -2^{-d-1} \pi^{-d/2} \Gamma(-d/2) \xi^{-d}. \quad (157)$$

According to Eqs. (58)–(60), $f_{b,dim}(t)$ indeed agrees with the singular part $f_{bs}(t)$ of the bulk free energy f_b in $2 < d < 4$ and $0 < d < 2$ dimensions. The neglected terms are just those of the regular part f_0 . The latter is ultraviolet divergent for $d \geq 0$ dimensions according to Eqs. (61) and (139). Near $d=2$, the right-hand side of Eq. (157) has a pole $\sim (d-2)^{-1}$ and therefore does not capture the logarithmic temperature dependence of $f_{bs}(t)$ in $d=2$ dimensions.

Next we consider the size-dependent free energy density of the Gaussian model $f_{dim}(t, L)$ for film geometry within the dimensional regularization scheme. We find, for general d ,

$$f_{dim}(t, L) = f_{b,dim}(t) + 2A_{surface}^+ \xi^{1-d} L^{-1} + \mathcal{G}(L/\xi) L^{-d}, \quad (158)$$

where $A_{surface}^+$ and $\mathcal{G}(L/\xi)$ are given by Eqs. (76) and (71), respectively. An alternative representation is given in Eq. (6.3) of Ref. [26]. Equation (158) indeed agrees with the singular part $f_s(t, L)$ calculated in Sec. III for $2 < d < 3$ and for $3 < d < 4$. For $d=3$, however, the singular part depends explicitly on the cutoff or the lattice spacing according to

Eq. (147) or (86). This is reflected in the dimensionally regularized result Eq. (158) only as a pole term $\sim(d-3)^{-1}$ arising from $A_{surface}^+$. Thus Eq. (158) does not correctly describe the leading singular temperature dependence $\sim t \ln t$ of the surface free energy of the Gaussian continuum and lattice model in three dimensions according to Eqs. (86) and (147).

Finally, we consider the dimensionally regularized result for the size-dependent energy density above T_c ,

$$U_{dim}(t, L) = U_{b, dim}(t) + T_c \xi_0^{-2} [(1-d) A_{surface}^+ \xi_0^{3-d} L^{-1} + \mathcal{E}(L/\xi) L^{2-d}]. \quad (159)$$

For $T \rightarrow T_c$ this yields

$$U_{dim}(0, L) = T_c \xi_0^{-2} \mathcal{E}_d L^{2-d} \quad (160)$$

as confirmed by a direct calculation at $T = T_c$. We see that these expressions fail at $d=3$ where $A_{surface}^+$ and \mathcal{E}_d do not exist because of pole terms $\sim(d-3)^{-1}$ as noted already by Dohm [36]. Equation (159) does not capture the logarithmic divergence $\sim \ln t$ of the surface energy density for $T \rightarrow T_c$ at $d=3$ according to Eqs. (109) and (153), and in Eq. (160) the leading size dependence $\sim L^{-1} \ln L$ of $U(0, L)$ for $L \rightarrow \infty$ at $d=3$ is lacking, compare Eqs. (114) and (154).

Also for $d > 3$, Eqs. (159) and (160) are not satisfactory since they contain only terms that are subleading compared to the finite energy density at T_c , Eq. (119). The latter term that exhibits a *nonscaling* L dependence is missing in Eqs. (159) and (160).

As far as the φ^4 field theory is concerned, it is not clear at present whether these shortcomings are only an artifact restricted to the Gaussian approximation (corresponding to one-loop order of the φ^4 theory) or there exist further shortcomings at two-loop order. For this reason we do not consider universal finite-size scaling to be firmly established for nonperiodic boundary conditions since the earlier field-theoretic results of Refs. [24–30] are based on a perturbation approach using Gaussian propagators within the dimensional regularization scheme. On the other hand, we note that the singular parts of both the specific heat and the susceptibility are correctly described for the Gaussian model in $2 < d < 4$ dimensions by means of dimensional regularization.

IV. Mean spherical model with free boundary conditions

Again we consider N scalar spin variables S_i , $-\infty \leq S_i \leq \infty$, on the lattice points \mathbf{x}_i of a simple-cubic lattice with a lattice spacing \tilde{a} in a finite rectangular $L \times \tilde{L}^{d-1}$ box of volume $V = L \tilde{L}^{d-1} = N \tilde{a}^d$. We assume the statistical weight $\propto e^{-\beta H}$ with

$$H = \tilde{a}^d \left\{ -\frac{J}{\tilde{a}^2} \sum_{\langle ij \rangle} S_i S_j + \mu \sum_i S_i^2 \right\} \quad (161)$$

with a nearest-neighbor coupling $J > 0$. The ‘‘spherical field’’ $\mu(T, L, \tilde{L}, \tilde{a})$ is determined as a function of $\beta = (k_B T)^{-1}$ and of L, \tilde{L}, \tilde{a} through the constraint

$$\tilde{a}^{d-2} \sum_i \langle S_i^2 \rangle = N = (L/\tilde{a})(\tilde{L}/\tilde{a})^{d-1}. \quad (162)$$

For $\tilde{a} = 1$, Eqs. (161) and (162) yield the standard formulation of the mean spherical model [16]. Keeping \tilde{a} as an independent nonuniversal parameter will facilitate the distinction between nonuniversal and universal contributions.

In the following, we assume the same boundary conditions as for the Gaussian model of Sec. III. Thus the spin variables S_j can be represented as

$$S_j = \tilde{L}^{-(d-1)} (L + \tilde{a})^{-1} \sum_{\mathbf{k}, p} \hat{S}_{\mathbf{k}, p} \exp(i\mathbf{k} \cdot \mathbf{y}_j) \sqrt{2} \sin(pz_j), \quad (163)$$

and the diagonalized Hamiltonian reads

$$H = \frac{1}{2} \tilde{L}^{-(d-1)} (L + \tilde{a})^{-1} \sum_{\mathbf{k}, p} (\tilde{\mu} + J_{\mathbf{k}, d-1} + J_p) \hat{S}_{\mathbf{k}, p} \hat{S}_{-\mathbf{k}, p} \quad (164)$$

with the shifted spherical field

$$\tilde{\mu} = 2\mu - 2J_0 d \tilde{a}^{-2} \quad (165)$$

with $J_0 = 2J$. For $J_{\mathbf{k}, d-1}$ and J_p see Eqs. (49) and (50). The parameter $\tilde{\mu}(T, L, \tilde{L}, \tilde{a})$ is determined implicitly as a function of d, T, L, \tilde{L} , and \tilde{a} through the constraint equation (162), which now reads

$$\tilde{a}^{d-2} \tilde{L}^{1-d} L^{-1} \sum_{\mathbf{k}, p} (\tilde{\mu} + J_{\mathbf{k}, d-1} + J_p)^{-1} = \beta. \quad (166)$$

The susceptibility for $T \geq T_{c, d}$ is

$$\chi(T, L, \tilde{L}, \tilde{a}) = \beta \frac{\tilde{a}^{2d}}{\tilde{L}^{d-1} L} \sum_{i, j} \langle S_i S_j \rangle \quad (167)$$

$$= \beta \frac{\tilde{a}^2}{L(L + \tilde{a})^2} \sum_p [1 - (-1)^n] \times \cot^2(p\tilde{a}/2) \langle \hat{S}_{\mathbf{0}, p} \hat{S}_{\mathbf{0}, p} \rangle \quad (168)$$

$$= \frac{\tilde{a}^2}{L(L + \tilde{a})} \sum_p [1 - (-1)^n] \times \frac{\cot^2(p\tilde{a}/2)}{\tilde{\mu}(T, L, \tilde{L}, \tilde{a}) + J_p} \quad (169)$$

with $n \equiv p(L + \tilde{a})/\pi = 1, 2, \dots, L/\tilde{a}$ which is parallel to Eqs. (127)–(130) for the Gaussian model. A significant difference, however, is the dependence of χ on d, T, L, \tilde{L} , and \tilde{a} through $\tilde{\mu}(T, L, \tilde{L}, \tilde{a})$.

A. Bulk properties

First we recall some of the bulk properties. The bulk susceptibility at finite wave vector \mathbf{q} above $T_{c,d}$ is defined by

$$\chi_b(\mathbf{q}) = \lim_{V \rightarrow \infty} \beta \frac{\tilde{a}^{2d}}{V} \sum_{i,j} \langle S_i S_j \rangle e^{-i\mathbf{q} \cdot (\mathbf{x}_i - \mathbf{x}_j)}. \quad (170)$$

The Gaussian structure of H , Eq. (164), implies [32]

$$\chi_b(\mathbf{q})^{-1} = \tilde{\mu}_b + J_{\mathbf{q},d}, \quad (171)$$

where

$$\tilde{\mu}_b = \tilde{\mu}(T, \infty, \infty, \tilde{a}) = \chi_b(\mathbf{0})^{-1} \equiv \chi_b^{-1} \quad (172)$$

is determined implicitly by

$$\tilde{a}^{d-2} \beta^{-1} \int_{\mathbf{q}} (\tilde{\mu}_b + J_{\mathbf{q},d})^{-1} = 1. \quad (173)$$

Equation (173) is the bulk version of the constraint equation (166). The square of the second-moment bulk correlation length is determined by the susceptibility according to [32]

$$\xi^2 = \chi_b(\mathbf{0}) \frac{\partial}{\partial q^2} [\chi_b(\mathbf{q})^{-1}]_{\mathbf{q}=\mathbf{0}} = J_0 \chi_b. \quad (174)$$

Setting $\chi_b^{-1} = \tilde{\mu}_b = 0$ yields the bulk critical temperature $T_{c,d}$

$$\frac{1}{k_B T_{c,d}} = \beta_{c,d} = \tilde{a}^{d-2} \int_{\mathbf{q}} J_{\mathbf{q},d}^{-1}. \quad (175)$$

We note that $T_{c,d}$ is nonzero for $d > 2$ and $\lim_{d \rightarrow 2+} T_{c,d} = 0$. It is well known that the bulk critical behavior of the mean spherical model belongs to the universality class of the n -vector model in the large- n limit [46], thus the vanishing of $T_{c,d}$ at $d=2$ is expected from the Mermin-Wagner theorem [37].

In order to elucidate the role played by the borderline dimension $d=3$ for the confined system we extend our analysis to *continuous* dimensions in the range $2 < d < 4$. Equations (173) and (175) can be combined as

$$\tilde{a}^{2-d} (\beta_{c,d} - \beta) = \chi_b^{-1} \int_{\mathbf{q}} [J_{\mathbf{q},d} (J_{\mathbf{q},d} + \chi_b^{-1})]^{-1}. \quad (176)$$

This leads to the asymptotic critical behavior above $T_{c,d}$ for $2 < d < 4$,

$$\chi_b = A_\chi t^{-\gamma}, \quad \xi = \xi_0 t^{-\nu}, \quad t = \frac{T - T_{c,d}}{T_{c,d}}, \quad (177)$$

where

$$\gamma = 2/(d-2), \quad \nu = (d-2)^{-1} \quad (178)$$

and

$$\alpha = 2 - d\nu = (d-4)/(d-2). \quad (179)$$

We note that these critical exponents can be considered as the Fisher-renormalized [47] Gaussian critical exponents

$$\gamma = \frac{\gamma_{Gauss}}{1 - \alpha_{Gauss}}, \quad \nu = \frac{\nu_{Gauss}}{1 - \alpha_{Gauss}}, \quad (180)$$

and

$$\alpha = \frac{-\alpha_{Gauss}}{1 - \alpha_{Gauss}}, \quad (181)$$

as expected from the general theory of constrained systems [47], with the Gaussian exponents of Sec. III

$$\gamma_{Gauss} = 1, \quad \nu_{Gauss} = 1/2, \quad \alpha_{Gauss} = (4-d)/2. \quad (182)$$

The amplitudes are $A_\chi = \xi_0^2/J_0$ and

$$\xi_0 = \tilde{a} [A_d / (\beta_{c,d} J_0 \varepsilon)]^{1/(d-2)} \quad (183)$$

with $\varepsilon = 4-d$ and the geometrical factor A_d , Eq. (60). The factor $A_\chi \xi_0^{-\gamma/\nu}$ in Eqs. (2) and (42) becomes simply $A_\chi \xi_0^{-\gamma/\nu} = J_0^{-1}$.

For completeness, we note that at the lower critical dimension $d=2$, the asymptotic behavior of χ_b and ξ for $T \rightarrow T_{c,2}=0$ is exponential [48] and is derived from Eqs. (173) and (174) as

$$\xi = c \tilde{a} \exp(2\pi\beta J_0), \quad (184)$$

$$\chi_b = c^2 \tilde{a}^2 J_0^{-1} \exp(4\pi\beta J_0) \quad (185)$$

with

$$c = 0.03125. \quad (186)$$

The validity of universal finite-size scaling to be derived in Sec. IV C below for $2 < d < 3$ is expected to hold also for $d=2$ above $T_{c,2}=0$ in terms of the correlation length Eq. (184).

B. Film critical temperature

For film geometry ($\tilde{L} \rightarrow \infty$), Eqs. (166) and (169) are replaced by

$$\tilde{a}^{d-2} L^{-1} \sum_p \int_{\mathbf{k}} (\tilde{\mu} + J_{\mathbf{k},d-1} + J_p)^{-1} = \beta \quad (187)$$

and

$$\chi(T, L, \infty, \tilde{a}) = \frac{\tilde{a}^2}{L(L+\tilde{a})} \sum_p [1 - (-1)^n] \frac{\cot^2(p\tilde{a}/2)}{\tilde{\mu}(T, L, \infty, \tilde{a}) + J_p}. \quad (188)$$

Unlike the box geometry, the film geometry introduces a considerable complication in that for $d > 3$ the film system of thickness L has its own sharp critical temperature $T_{c,d}(L) > 0$ different from the critical temperature $T_{c,d} \equiv T_{c,d}(\infty)$ of the d -dimensional bulk system. As shown by Barber and

Fisher [16], $T_{c,d}(L) > T_{c,d}(\infty)$ for $d \geq 4$. Here we shall show that this is true also for $3 < d \leq 4$.

The condition for criticality of the film system is $\chi(T, L, \infty, \tilde{a})^{-1} = 0$. This condition is satisfied at a critical value $\tilde{\mu} = \tilde{\mu}_c < 0$, where $\tilde{\mu}_c(L)$ is determined by the vanishing of the denominator of the lowest-mode ($n=1$) term in the sum of Eq. (188),

$$\tilde{\mu}_c(L) = -\frac{2J_0}{\tilde{a}^2} \left(1 - \cos \frac{\pi \tilde{a}}{L + \tilde{a}} \right). \quad (189)$$

We note that $\tilde{\mu}_c(L)$ is independent of d . The leading large L behavior is

$$\tilde{\mu}_c(L) = -J_0 \pi^2 (L + \tilde{a})^{-2} + O(\tilde{a}^2 (L + \tilde{a})^{-4}). \quad (190)$$

According to Eq. (187), the corresponding critical value of $\beta_{c,d}(L) = [k_B T_{c,d}(L)]^{-1}$ is then given by

$$\beta_{c,d}(L) = \frac{\tilde{a}^{d-2}}{L} \sum_p \int_{\mathbf{k}} (\tilde{\mu}_c + J_{\mathbf{k},d-1} + J_p)^{-1}. \quad (191)$$

Separating the lowest-mode ($n=1$) term we obtain for general d

$$\beta_{c,d}(L) = \frac{\tilde{a}^{d-2}}{L} \int_{\mathbf{k}} J_{\mathbf{k},d-1}^{-1} + \frac{\tilde{a}^{d-2}}{L} \sum_{n=2}^{L/\tilde{a}} \int_{\mathbf{k}} (\tilde{\mu}_c + J_{\mathbf{k},d-1} + J_p^{-1}). \quad (192)$$

The first integral in Eq. (192) is directly related to the critical temperature of a $(d-1)$ -dimensional bulk system [compare Eq. (175)] and is infrared divergent for $d \leq 3$; hence $\beta_{c,d}(L) = \infty$ or [16]

$$T_{c,d}(L) = 0 \quad \text{for} \quad d \leq 3 \quad (193)$$

for any finite L , as expected from the Mermin-Wagner theorem [37]. We see that for the film system of finite thickness the dimension $d=3$ plays the role of a *lower critical dimension* $d_l=3$ up to which $T_{c,d}(L)$ vanishes. Thus, at *finite* temperature and in $2 < d \leq 3$ dimensions, there exists only one type of critical behavior for large L near the bulk critical temperature $T_{c,d} > 0$ for the d -dimensional film system of finite thickness.

An analysis of Eq. (191) for $d > 3$ is presented in Appendix B. We find that $T_{c,d}(L)$ is enhanced above $T_{c,d}(\infty)$ for $d > 3$ for sufficiently large $L \gg \tilde{a}$. This enhancement is most naturally expressed in terms of the dimensionless parameter

$$\Delta\beta = J_0 [\beta_{c,d}(\infty) - \beta_{c,d}(L)]. \quad (194)$$

For large $L \gg \tilde{a}$ the result is

$$\Delta\beta = 4\tilde{B}_d \tilde{a}/L - \tilde{C}_d (\tilde{a}/L)^{d-2} + O(\tilde{a}^{d/2} L^{-d/2}) \quad (195)$$

with the nonuniversal amplitude $\tilde{B}_d > 0$, Eq. (89), and the universal amplitude

$$\tilde{C}_d = \frac{1}{8\pi^2} \int_0^\infty dz \left\{ 1 - 2 \left(\frac{\pi}{z} \right)^{1/2} + e^{z/4} \left[K \left(\frac{z}{4} \right) - 1 \right] \right\} \left(\frac{\pi}{z} \right)^{(d-1)/2} \quad (196)$$

with $\tilde{C}_d > 0$. Thus there are competing effects on $T_{c,d}(L)$ from the scaling term $\sim L^{2-d} = L^{1/\nu}$ and the nonscaling term $\sim L^{-1}$. The leading terms of the fractional shift are

$$\frac{T_{c,d}(L) - T_{c,d}(\infty)}{T_{c,d}(\infty)} = a_d \tilde{a}/L - c_d (\tilde{a}/L)^{d-2} + O(\tilde{a}^{d/2} L^{-d/2}) \quad (197)$$

with the positive amplitudes

$$a_d = 4\tilde{B}_d \left\{ \int_0^\infty dy [e^{-2y} I_0(2y)]^d \right\}^{-1}, \quad (198)$$

$$c_d = \tilde{C}_d \left\{ \int_0^\infty dy [e^{-2y} I_0(2y)]^d \right\}^{-1}, \quad (199)$$

where I_0 is given by Eq. (68). The amplitude a_d can be expressed in terms of generalized Watson functions, see Eqs. (90) and (74). For $d=4$, a_4 agrees with the corresponding amplitude of Barber and Fisher [16].

We see that the positive shift of $T_{c,d}(L)$ for $d > 3$ is proportional to the same amplitude $\tilde{B}_d > 0$ that determines the finite cusp of the Gaussian surface energy density, Eq. (115). Thus the nonscaling Gaussian cusp and the nonscaling enhancement of $T_{c,d}(L)$ for film geometry are closely connected. In the following section we shall find that the Gaussian cusp is also responsible for nonscaling finite-size effects on the susceptibility for both box and film geometry in the mean spherical model for $d > 3$.

C. Constraint equation and susceptibility

The crucial question is whether and for which dimension d the susceptibility, Eq. (169), attains the universal scaling form of Eq. (36) for large L, \tilde{L}, ξ at fixed \tilde{a} . This requires one to first analyze the size dependence of $\tilde{\mu}$ implied by Eq. (166). Up to a constant factor, the left-hand side of Eq. (166) has the same form as the right-hand side of Eq. (94) for the Gaussian energy density, thus the constraint equation (166) can be rewritten as

$$E(\tilde{\mu}, L, \tilde{L}, \tilde{a}) = \beta \tilde{a}^{2-d}, \quad (200)$$

where $E(r_0, L, \tilde{L}, \tilde{a})$ is defined by Eq. (94). It is clear that any nonscaling L dependence of the Gaussian function $E(\tilde{\mu}, L, \tilde{L}, \tilde{a})$ will cause a nonscaling form of the L dependence of $\tilde{\mu}$, which, through Eq. (169), will in turn cause a corresponding nonscaling L dependence of the susceptibility. This mechanism explains the existence of a borderline dimension $d=3$ between a scaling ($d < 3$) and a nonscaling ($d \geq 3$) regime in the mean spherical model as a consequence of the size dependence of the energy density of the Gaussian model, for both box and film geometry. More specifically, we can anticipate nonscaling power laws for $d > 3$ arising from

the nonscaling size dependence of the finite cusp of $U_{surface} \sim E_{surface}$ according to Eqs. (116)–(119).

It turns out that the most natural parameter is not $\tilde{\mu}$ but rather the shifted parameter

$$\Delta\mu = J_0^{-1}[\tilde{\mu} - \tilde{\mu}_c(L)], \quad (201)$$

where $\tilde{\mu}_c(L)$ is given by Eq. (189). We note that $\Delta\mu > 0$ for box geometry for any finite L . In Appendix B we derive the following expression for the large- L behavior of the susceptibility, Eq. (169), at fixed $\Delta\mu L^2 > 0$,

$$\begin{aligned} \chi &= \frac{4}{J_0 \pi^2} L^2 \int_0^\infty dy \frac{1 - \exp[-(\Delta\mu L^2 - \pi^2)y/\pi^2]}{\Delta\mu L^2 - \pi^2} \\ &\times [K(y) - K(4y)], \end{aligned} \quad (202)$$

where $K(z)$ is defined by Eq. (70). Equation (202) is valid for general d .

In Appendix D we analyze Eq. (200) for large L/\tilde{a} at fixed shape factor $\tilde{s} = (L + \tilde{a})/\tilde{L} > 0$ near the bulk critical temperature. For small $t = (T - T_{c,d})/T_{c,d} \geq 0$, we find for $2 < d < 4$

$$\begin{aligned} (\Delta\mu L^2)^{(d-2)/2} &= t(L/\xi_0)^{d-2} - \varepsilon(2A_d)^{-1}(L/\tilde{a})^{d-3} \\ &\times E_{surface}(\Delta\mu \tilde{a}^2) \\ &+ 2\varepsilon A_d^{-1} \tilde{\mathcal{E}}_d((\Delta\mu)^{1/2} L, \tilde{s}), \end{aligned} \quad (203)$$

where $E_{surface}(z)$ is given by the Gaussian surface function, Eq. (97). The universal finite-size part reads for box geometry

$$\begin{aligned} \tilde{\mathcal{E}}_d(x, \tilde{s}) &= \frac{1}{16\pi^2} \int_0^\infty dy \left\{ \left(\frac{\pi}{y}\right)^{(d-1)/2} - 2\left(\frac{\pi}{y}\right)^{d/2} \right. \\ &\left. + e^{y/4} \left[K\left(\frac{y}{4}\right) - 1 \right] [\tilde{s}K(\tilde{s}^2 y)]^{d-1} \right\} e^{-yx^2/4\pi^2}. \end{aligned} \quad (204)$$

We note that the term $K(y/4) - 1 = 2\sum_{n=1}^\infty \exp(-n^2 y/4)$ comes from the modes with the free boundary conditions (the z direction), whereas the term $\tilde{s}K(\tilde{s}^2 y) = \tilde{s}\sum_{m=-\infty}^\infty \exp(-\tilde{s}^2 m^2 y)$ comes from the modes with the periodic boundary conditions ($d-1$ horizontal directions). For film geometry ($\tilde{s} = 0$) the latter term is reduced to $(\pi/y)^{1/2}$, and the universal finite-size part becomes

$$\begin{aligned} \tilde{\mathcal{E}}_d(x, 0) &= \frac{1}{16\pi^2} \int_0^\infty dy \left(\frac{\pi}{y}\right)^{(d-1)/2} \left\{ 1 - 2\left(\frac{\pi}{y}\right)^{1/2} \right. \\ &\left. + e^{y/4} \left[K\left(\frac{y}{4}\right) - 1 \right] \right\} e^{-yx^2/4\pi^2}. \end{aligned} \quad (205)$$

Equations (203)–(205) determine $\Delta\mu$ implicitly near $T_{c,d}$ for large L as a function of t, L, \tilde{L} and \tilde{a} . In the absence of the \tilde{a} dependent term $\sim E_{surface}$, Eq. (203) would yield a uni-

versal scaling form for $\Delta\mu L^2$. According to Eq. (202), this would then imply a universal scaling form for the susceptibility. From the analysis of the Gaussian model in Sec. III, we know, however, that different scaling and nonscaling terms arise from $E_{surface}$ depending on whether $2 < d < 3$, $d = 3$, or $3 < d < 4$.

1. Finite-size scaling in $2 < d < 3$ dimensions

The asymptotic form of $E_{surface}(\Delta\mu \tilde{a}^2)$ for small $\Delta\mu \tilde{a}^2$ reads for $2 < d < 3$,

$$\begin{aligned} E_{surface}(\Delta\mu \tilde{a}^2) &= -4(d-1)A_{surface}^+(\Delta\mu \tilde{a}^2)^{(d-3)/2} + 8\tilde{b}_d \\ &+ O((\Delta\mu \tilde{a}^2)^{(d-2)/2}); \end{aligned} \quad (206)$$

compare Eq. (101). Substituting Eq. (206) into Eq. (203) we see that the dependence on \tilde{a} is canceled. This implies, for a given shape factor $s = L/\tilde{L}$, that $\Delta\mu$ has the universal scaling form

$$\Delta\mu = L^{-2} \mathcal{M}_d(L/\xi, s), \quad (207)$$

where the scaling function $\mathcal{M}_d(x, s)$ is determined implicitly by

$$\begin{aligned} \mathcal{M}_d^{(d-2)/2} &= x^{d-2} + 2\varepsilon A_d^{-1} \tilde{\mathcal{E}}_d(\mathcal{M}_d^{1/2}, s) + 2\varepsilon(d-1) \\ &\times A_d^{-1} A_{surface}^+ \mathcal{M}_d^{(d-3)/2}. \end{aligned} \quad (208)$$

Substituting Eq. (207) into Eq. (202) confirms the finite-size scaling prediction, Eq. (36), with the bulk susceptibility $\chi_b = J_0^{-1} \xi^2$ and the universal finite-size scaling function for $2 < d < 3$

$$\begin{aligned} f_\chi(x, s) &= \frac{4x^2}{\pi^2} \int_0^\infty dy \frac{1 - \exp\{-[M_d(x, s) - \pi^2]y/\pi^2\}}{\mathcal{M}_d(x, s) - \pi^2} \\ &\times [K(y) - K(4y)]. \end{aligned} \quad (209)$$

At $T = T_{c,d}$ this yields the power-law Eq. (42) with $\gamma/\nu = 2$ and with the universal amplitude

$$\begin{aligned} B_\chi(s) &= \frac{4}{\pi^2} \int_0^\infty dy \frac{1 - \exp\{-[M_d(0, s) - \pi^2]y/\pi^2\}}{\mathcal{M}_d(0, s) - \pi^2} \\ &\times [K(y) - K(4y)]. \end{aligned} \quad (210)$$

The scaling results of Eqs. (209) and (210) are applicable also to film geometry ($s = 0$) where $f_\chi(x, 0)$ and $B_\chi(0)$ are finite quantities for $d < 3$. We note, however, that both $B_\chi(s)$ and $B_\chi(0)$ diverge for $d \rightarrow 3$. Specifically, for $d \rightarrow 3$ we find from Eq. (210) for box geometry at fixed $s > 0$

$$B_\chi(s) \sim 2\pi^{-3} s^{-2} (3-d)^{-1}, \quad (211)$$

whereas for film geometry

$$B_\chi(0) \sim 2\pi^{-4} (3/2)^{2(3-d)}. \quad (212)$$

The different types of divergences are the consequence of a mode continuum for film geometry and signal different forms of violations of finite-size scaling at $d=3$ for the box and film geometry, as will be confirmed in Sec. IV C 2 below.

At fixed $t>0$ we find from Eqs. (207)–(209) the leading large- L behavior for both box and film geometry,

$$\begin{aligned} \tilde{\mu}^{1/2} = & J_0^{1/2} \xi^{-1} [1 + 2\epsilon(d-1)(d-2)^{-1} A_d^{-1} A_{surface}^+ \xi/L \\ & + O(\xi^2/L^2)], \end{aligned} \quad (213)$$

and

$$\begin{aligned} \chi = & \chi_b \{1 - [4\epsilon(d-1)(d-2)^{-1} A_d^{-1} A_{surface}^+ + 2] \xi/L \\ & + O(\xi^2/L^2)\}, \end{aligned} \quad (214)$$

where $A_{surface}^+ < 0$ is given by Eq. (76). Equation (214) yields the surface susceptibility, Eq. (38), with the scaling surface exponent

$$\gamma_s = \gamma + \nu = 3/(d-2) \quad (215)$$

and the surface amplitude

$$A_{\chi, surface}^+ = -\frac{1}{2} J_0^{-1} \xi_0^3 [4\epsilon(d-1)(d-2)^{-1} A_d^{-1} A_{surface}^+ + 2]. \quad (216)$$

2. Violation of finite-size scaling in $d=3$ dimensions

We recall that at $d=3$ there exists no sharp transition in box geometry and in film geometry of finite thickness other than the bulk transition for $L \rightarrow \infty$ at $T_{c,3} > 0$; thus there is no compelling reason to introduce a shifted reference temperature or to introduce a physical length scale other than the $d=3$ bulk correlation length. At $d=3$, the Gaussian surface function reads [compare Eq. (109)]

$$\begin{aligned} E_{surface}(\Delta\mu\tilde{a}^2) = & -(4\pi)^{-1} \ln(\Delta\mu\tilde{a}^2) + 8[\tilde{b} - (16\pi)^{-1}] \\ & + O(\Delta\mu^{1/2}\tilde{a}). \end{aligned} \quad (217)$$

Substituting Eq. (217) into Eq. (203) yields

$$\begin{aligned} \Delta\mu^{1/2}L = & tL/\xi_0 + \ln(\Delta\mu^{1/2}\tilde{a}) + 1/2 - 8\pi\tilde{b} + 8\pi\tilde{\mathcal{E}}_3(\Delta\mu^{1/2}L, s) \\ & + O(\Delta\mu^{1/2}\tilde{a}) \end{aligned} \quad (218)$$

with $\tilde{\mathcal{E}}_3(x, s)$ given by Eq. (204). Here we have replaced \tilde{s} by $s=L/\tilde{L}$ for large $L/\tilde{a} \gg 1$. Substituting Eq. (218) into Eq. (202) yields the susceptibility. As a consequence of the logarithmic term of $E_{surface}$ in Eq. (217) we now have a logarithmic dependence on \tilde{a} in Eq. (218) that cannot be neglected. One expects that this causes only a logarithmic deviation from finite-size scaling. This will be confirmed for box geometry but not for film geometry where we shall find a power-law violation of finite-size scaling. The origin of this unexpected geometry effect at $d=3$ comes from the different small x behavior of the finite-size part $\tilde{\mathcal{E}}_3(x, s)$ for $s>0$ and for $s=0$.

(a) *Box geometry.* For fixed $s>0$, we find from Eq. (204) the small x behavior

$$\tilde{\mathcal{E}}_3(x, s) = \frac{1}{2} s^2 x^{-2} - \frac{1}{8\pi} \ln x + O(1). \quad (219)$$

Here the first term $\sim x^{-2}$ is the contribution due to the $\mathbf{k} = \mathbf{0}, p = \pi/(L + \tilde{a})$ mode that is the lowest mode of the discrete mode spectrum for box geometry. Equations (218) and (219) yield the leading L dependence at $T = T_{c,3}$

$$\Delta\mu = 4\pi s^2 L^{-2} [\ln(L/\tilde{a})]^{-1} \left[1 + O\left(\frac{1}{\ln(L/\tilde{a})}\right) \right]. \quad (220)$$

Substituting Eq. (220) into Eq. (202) leads to the susceptibility at $T = T_{c,3}$

$$\chi = 2\pi^{-3} J_0^{-1} s^{-2} L^2 \ln(L/\tilde{a}) + O(L^2). \quad (221)$$

At fixed $t>0$ we find from Eq. (218) the leading large- L behavior

$$\begin{aligned} \tilde{\mu}^{1/2} = & J_0^{1/2} \xi^{-1} \{1 - [\ln(\xi/\tilde{a}) + 8\pi\tilde{b} - 2] \xi/L \\ & + O([\ln(\xi/\tilde{a})]^2 \xi^2/L^2)\}. \end{aligned} \quad (222)$$

For the susceptibility, Eq. (202), this implies

$$\begin{aligned} \chi = & \chi_b \{1 + [2\ln(\xi/\tilde{a}) + 16\pi\tilde{b} - 6] \xi/L \\ & + O([\ln(\xi/\tilde{a})]^2 \xi^2/L^2)\}, \end{aligned} \quad (223)$$

which corresponds to the surface susceptibility, at $d=3$,

$$\chi_{surface}(t) = \frac{1}{2} J_0^{-1} \xi^3 [2 \ln(\xi/\tilde{a}) + 16\pi\tilde{b} - 6]. \quad (224)$$

The logarithms in Eqs. (221)–(224) constitute logarithmic deviations from universal finite-size scaling, with an explicit dependence on the nonuniversal lattice constant \tilde{a} . Thus there exists no universal scaling form for box geometry at $d=3$ in the sense of Eq. (36). This is the consequence of the upper borderline dimension $d^*=3$ for the surface energy density of the Gaussian model.

(b) *Film geometry.* A separate analysis is necessary for film geometry in $d=3$ dimensions since Eqs. (220) and (221) do not have finite limits for $s \rightarrow 0$. The susceptibility is again given by Eq. (202), where now $\Delta\mu L^2$ is determined implicitly by

$$\begin{aligned} \Delta\mu^{1/2}L = & tL/\xi_0 + \ln(\Delta\mu^{1/2}\tilde{a}) + 1/2 - 8\pi\tilde{b} \\ & + 8\pi\tilde{\mathcal{E}}_3(\Delta\mu^{1/2}L, 0) \end{aligned} \quad (225)$$

with

$$\begin{aligned} \tilde{\mathcal{E}}_3(x,0) = & \frac{1}{16\pi} \int_0^\infty dy y^{-1} \left\{ 1 - 2 \left(\frac{\pi}{y} \right)^{1/2} \right. \\ & \left. + e^{y/4} \left[K \left(\frac{y}{4} \right) - 1 \right] \right\} e^{-yx^2/4\pi^2}. \end{aligned} \quad (226)$$

We find from Eq. (226) the small- x behavior

$$\tilde{\mathcal{E}}_3(x,0) = -\frac{3}{8\pi} \ln x + \tilde{E}_3 + O(x^2 \ln x), \quad (227)$$

where

$$\begin{aligned} \tilde{E}_3 = & \frac{3}{16\pi} \left[-C_E + \ln \left(\frac{A}{4\pi^2} \right) \right] + \frac{1}{16\pi} \int_0^A dy y^{-1} \left\{ 1 - 2 \left(\frac{\pi}{y} \right)^{1/2} \right. \\ & \left. + e^{y/4} \left[K \left(\frac{y}{4} \right) - 1 \right] \right\} + \frac{1}{8\pi} \int_A^\infty dy y^{-1} \left\{ - \left(\frac{\pi}{y} \right)^{1/2} \right. \\ & \left. + \sum_{n=2}^\infty e^{-(n^2-1)y/4} \right\} \end{aligned} \quad (228)$$

is independent of the arbitrary constant $A > 0$. The absence of a term $\sim x^{-2}$ in Eq. (227) is a consequence of the fact that for film geometry there exists a mode *continuum*, without a discrete lowest mode. At the bulk critical temperature $T = T_{c,3}$, Eqs. (225) and (227) yield the constraint equation in the form

$$\begin{aligned} \Delta\mu^{1/2}L = & \ln(\Delta\mu^{1/2}\tilde{a}) + 1/2 + 8\pi(\tilde{E}_3 - \tilde{b}) - 3 \ln(\Delta\mu^{1/2}L) \\ & + O(\Delta\mu L^2 \ln(\Delta\mu L^2)). \end{aligned} \quad (229)$$

We recall that the first logarithmic term in Eq. (229) is the signature of the (upper) borderline dimension $d^* = 3$ at which the critical exponent $1 - \alpha - \nu$ of the Gaussian surface energy density vanishes, whereas the second logarithmic term in Eq. (229) is the signature of the (lower) borderline dimension $d_l = 3$ at which the film critical temperature $T_{c,3}(L)$ vanishes, in accord with the Mermin-Wagner theorem [37]. Both logarithmic terms can be combined as

$$\ln(\Delta\mu^{1/2}\tilde{a}) - 3 \ln(\Delta\mu^{1/2}L) = \ln(\tilde{a}/L) - \ln(\Delta\mu L^2) \quad (230)$$

and, after substituting into Eq. (229), yield the solution with a power-law (rather than logarithmic) L dependence

$$\Delta\mu = \tilde{A}_\mu \tilde{a} L^{-3} [1 + O(\tilde{a}^{1/2} L^{-1/2})] \quad (231)$$

with the nonuniversal amplitude

$$\tilde{A}_\mu = \exp\{1/2 + 8\pi(\tilde{E}_3 - \tilde{b})\}. \quad (232)$$

Thus $\Delta\mu$ has a nonscaling size dependence at $T = T_{c,3}$. Substituting Eq. (231) into Eq. (202) leads to the susceptibility at $T_{c,3}$

$$\chi = (J_0 \tilde{A}_\mu \tilde{a})^{-1} L^3 [1 + O(\tilde{a}^{1/2} L^{-1/2})], \quad (233)$$

which constitutes a strong power-law violation of the scaling prediction $\chi \sim L^2$, Eq. (42), in contrast with the logarithmic deviation in Eq. (221) for box geometry. The same violation persists in the critical region $\xi L \gtrsim 1$. The unexpected difference between Eqs. (233) and (221) results from the difference between the discrete mode spectrum for box geometry and the mode continuum for film geometry at the lower borderline dimension $d_l = 3$ above which the film critical temperature becomes finite. We emphasize that the existence of this borderline dimension $d_l = 3$, which causes the second logarithmic term in the constraint equation (229), is not restricted to the spherical model. It remains to be seen whether similar geometry-dependent effects exist at $d = 3$ also in other models of $O(n)$ symmetric systems with $n \geq 2$ and with free (or Dirichlet) boundary conditions.

At fixed $T > T_{c,3}$, for film geometry, we find the same leading large- L behavior as already given in Eqs. (222)–(224) for box geometry, with a logarithmic (rather than power-law) violation of finite-size scaling. In summary, it is not possible to write χ in a universal finite-size scaling form, in the sense of Eqs. (1) and (2), in the region $T \geq T_{c,3}$ for film geometry at $d = 3$.

(c) *Comparison with Barber and Fisher.* The susceptibility of the mean spherical model in film geometry with free boundary conditions was calculated by Barber and Fisher [16] using a different mathematical technique. For $d = 3$ they introduced a “quasicritical temperature shift” and found that, for large $n \equiv L/\tilde{a}$, there exists a scaling representation in terms of a scaled temperature variable $n\Delta\tilde{K}$

$$\chi_{BF} = \frac{n^2}{2J} X(n\Delta\tilde{K}), \quad (234)$$

with a shifted inverse temperature deviation from the $d = 3$ bulk critical temperature $T_{c,3}$

$$\Delta\tilde{K} = \frac{J}{k_B T_{c,3}} - \frac{J}{k_B T} - \frac{1}{8\pi n} \ln n + \tilde{C}_{BF}/n, \quad (235)$$

$$\tilde{C}_{BF} = \frac{1}{2} \left[W_3(0) - \frac{1}{2} W_2(4) - \frac{7 \ln 2}{16\pi} \right]. \quad (236)$$

The scaling function was represented parametrically via

$$X(z) = y^{-2} [1 - (2/y) \tanh(y/2)], \quad (237)$$

$$8\pi z = \ln[(\sinh y)/y] \quad (238)$$

and was plotted for $z > 0$ in Fig. 4 of Ref. [16]. For finite $L/\tilde{a} \gg 1$ and at $\Delta\tilde{K} = 0$, Eq. (235) defines a “quasicritical” [16] temperature $\tilde{T}(L) > T_{c,3}$, where

$$\frac{J}{k_B \tilde{T}(L)} = \frac{J}{k_B T_{c,3}} - \frac{\tilde{a}}{8\pi L} \ln \left(\frac{L}{\tilde{a}} \right) + \tilde{C}_{BF} \tilde{a}/L. \quad (239)$$

We note that all thermodynamic quantities are smooth functions of T near $\tilde{T}(L)$ and that there exists no *physical* criterion for defining $\tilde{T}(L)$. The analysis of the susceptibility in

terms of $\Delta\hat{K}$ in Ref. [16] was restricted to $\Delta\hat{K}\geq 0$ and did not include the region $T_{c,3}\leq T<\tilde{T}(L)$, $\xi/L\gg 1$ which is of principal interest for testing the scaling predictions of Eqs. (1) and (2).

Our dimensionless susceptibility χ/\tilde{a}^2 corresponds to χ_{BF} . Our explicit result for χ/\tilde{a}^2 , however, is at variance with that of Barber and Fisher since Eqs. (202), (225), and (226) cannot be reduced to the simple form of Eqs. (234)–(238). Our result differs from that of Ref. [16] both in the region $T_{c,3}\leq T<\tilde{T}(L)$ and in the region $T\geq\tilde{T}(L)$. A unique analytic comparison between χ/\tilde{a}^2 and χ_{BF} can be made in the region $L/\xi\gg 1$ at fixed T above $\tilde{T}(L)$. Substituting into χ_{BF} the large- z representation according to Eq. (9.17) of Ref. [16]

$$X(z) = (8\pi z)^{-2} - 2(8\pi z)^{-3} \ln(16\pi e z) + O(z^{-4} \ln z) \quad (240)$$

and rewriting the resulting expression in terms of the bulk susceptibility χ_{BF}^{bulk} and the asymptotic bulk correlation length [compare our Eqs. (177), (183)]

$$\xi = \frac{\tilde{a}}{8\pi} \frac{k_B T_{c,3}}{J} t^{-1}, \quad (241)$$

we find

$$\chi_{BF} = \chi_{BF}^{bulk} \left\{ 1 + \left[2 \ln \left(\frac{\xi}{\tilde{a}} \right) + C_{BF} \right] \frac{\xi}{L} + O \left(\frac{\xi^2}{L^2} \right) \right\} \quad (242)$$

with

$$C_{BF} = -2 + \frac{3}{2} \ln 2 + 16\pi \left[\frac{1}{4} W_2(4) - \frac{1}{2} W_3(0) \right]. \quad (243)$$

While the leading logarithmic term $\sim [\ln(\xi/\tilde{a})]\xi/L$ of Eq. (242) agrees with ours in Eq. (223), the leading correction term $\sim \xi/L$ differs from ours. We note that our constant \tilde{b} , Eq. (82), does contain the last two terms of C_{BF} , but the additional integral expressions in Eq. (82) are missing in C_{BF} , Eq. (243). Our integral expressions come from the finite part of $W_{d-1}(0)$ for $d\rightarrow 3$, after subtracting the pole term $\sim (d-3)^{-1}$, see Eq. (91). We believe that our result for \tilde{b} is correct since it has been obtained both by a calculation directly at $d=3$ and by a calculation at $d\neq 3$, taking the limits $d\rightarrow 3+$ and $d\rightarrow 3-$. A further analytic comparison between our χ/\tilde{a}^2 and χ_{BF} can be made directly at $T = \tilde{T}(L)$, where χ_{BF} is simply given by $\chi_{BF} = (n^2/2J)X(0)$ with $X(0) = 1/12$ according to Eq. (9.18) of Ref. [16]. Our result at $T = \tilde{T}(L)$ depends on \tilde{b} and differs from the simple result for χ_{BF} . Thus we doubt the correctness of the previous result [16] for χ_{BF} for free boundary conditions at $d = 3$.

3. Violation of finite-size scaling in $3 < d < 4$ dimensions

From Eqs. (96), (116), and (117) we have the Gaussian surface function for $d > 3$,

$$E_{surface}(\Delta\mu\tilde{a}^2) = 8\tilde{a}^{3-d}\tilde{B}_d - 4(d-1) \times A_{surface}^+(\Delta\mu\tilde{a}^2)^{(d-3)/2} + O((\Delta\mu\tilde{a}^2)^{(d-2)/2}), \quad (244)$$

where $A_{surface}^+ > 0$ and \tilde{B}_d are given by Eqs. (88) and (89). Substituting Eq. (244) into Eq. (203) yields

$$(\Delta\mu L^2)^{(d-2)/2} = t(L/\xi_0)^{d-2} + 2\varepsilon(d-1) \times A_d^{-1} A_{surface}^+(\Delta\mu L^2)^{(d-3)/2} - 4\varepsilon A_d^{-1} \tilde{B}_d(L/\tilde{a})^{d-3} + 2\varepsilon A_d^{-1} \tilde{E}_d(\Delta\mu^{1/2} L, s). \quad (245)$$

We see that the finite value of $E_{surface}(0) \sim \tilde{B}_d > 0$ causes a non-negligible term $\sim (L/\tilde{a})^{d-3}$ in Eq. (245) that depends on the lattice spacing \tilde{a} . This will imply power-law violations of finite-size scaling for box geometry.

At fixed $s = L/\tilde{L} > 0$, Eq. (245) yields the L dependence at $T = T_{c,d}$, for $3 < d < 4$,

$$\Delta\mu = \frac{1}{2} \tilde{a}^{d-3} \tilde{B}_d^{-1} s^{d-1} L^{1-d} [1 + O(\tilde{a}^{d-3} L^{3-d})]. \quad (246)$$

For the susceptibility at $T = T_{c,d}$, this implies

$$\chi = 4J_0^{-1} \tilde{a}^{3-d} \tilde{B}_d s^{1-d} L^{d-1} [1 + O(\tilde{a}^{d-3} L^{3-d})], \quad (247)$$

in contrast to the scaling prediction $\chi \sim L^2$, Eq. (42).

At fixed $T > T_{c,d}$ we find from Eq. (245) the leading large- L behavior

$$\tilde{\mu}^{1/2} = J_0^{1/2} \xi^{-1} [1 - \tilde{m}_d(\xi/\tilde{a}) \xi/L + O((\xi/\tilde{a})^{d-3} \xi^2/L^2)] \quad (248)$$

with the nonuniversal function for $3 < d < 4$

$$\tilde{m}_d(\xi/\tilde{a}) = 2\varepsilon(d-2)^{-1} A_d^{-1} [2\tilde{B}_d(\xi/\tilde{a})^{d-3} - (d-1)A_{surface}^+]. \quad (249)$$

Substituting Eqs. (248) and (249) into Eq. (202) yields the susceptibility

$$\chi = \chi_b \{ 1 + [2\tilde{m}_d(\xi/\tilde{a}) - 2] \xi/L + O((\xi/\tilde{a})^{d-3} \xi^2/L^2) \}. \quad (250)$$

The corresponding surface susceptibility is, for $\xi \gg \tilde{a}$ and for $3 < d < 4$,

$$\chi_{surface} = \frac{1}{2} J_0^{-1} [2\tilde{m}_d(\xi/\tilde{a}) - 2] \xi^3 \sim \xi^d \sim t^{-d/(d-2)}. \quad (251)$$

This is in contrast to the scaling prediction $\chi_{surface} \sim \chi_b \xi \sim t^{-3/(d-2)}$, Eqs. (37) and (38).

We see that the amplitudes of the leading nonscaling terms are proportional to \tilde{B}_d , both for the size dependence at $T_{c,d}$, Eq. (247), and for the temperature dependence above $T_{c,d}$, Eqs. (250) and (251). Thus it is the cusp of the Gaussian surface energy density that is the origin of the nonscaling effects in the mean spherical model for $3 < d < 4$ rather than an enhanced transition temperature that does not exist for box geometry.

For film geometry in $3 < d < 4$ dimensions a new analysis of our solution would be necessary since there exists a sharp critical temperature $T_{c,d}(L) > T_{c,d}(\infty)$. Here we only note that the leading size dependence at fixed $T > T_{c,d}(L)$ for film geometry is the same as given in Eqs. (248)–(251) for box geometry. It is expected that a full description of the crossover from the L -dependent film critical behavior near $T_{c,d}(L)$ to the d -dimensional bulk critical behavior near $T_{c,d}(\infty)$ would involve *two* different correlation lengths. Our solution for χ does provide the basis for such an analysis of a dimensional crossover, which, however, is beyond the scope of our present paper.

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APPENDIX A: GAUSSIAN FREE ENERGY DENSITY

In this appendix we derive the asymptotic form, Eq. (66), for the free energy density of the Gaussian lattice model for box geometry. We start from Eq. (52). Using the representation

$$\ln z = \int_0^\infty dy y^{-1} (e^{-y} - e^{-zy}), \quad (\text{A1})$$

we rewrite the L -dependent part

$$\Delta f(t, L, \tilde{L}, \tilde{a}) \equiv f(t, L, \tilde{L}, \tilde{a}) - f_b(t) + \frac{1}{2} \tilde{a}^{-d} (\tilde{L}/\tilde{a})^{1-d} \ln 2 \quad (\text{A2})$$

of the free energy density in the form

$$\Delta f(t, L, \tilde{L}, \tilde{a}) = \frac{1}{2} \tilde{a}^{-d} \int_0^\infty dy y^{-1} e^{-\tilde{r}_0 y} \Phi(L/\tilde{a}, \tilde{L}/\tilde{a}, y) \quad (\text{A3})$$

with $\tilde{r}_0 \equiv r_0 \tilde{a}^2 / (2J)$ and

$$\Phi(L/\tilde{a}, \tilde{L}/\tilde{a}, y) = [S(\infty, y)]^d - [S(\tilde{L}/\tilde{a}, y)]^{d-1} S_D(\tilde{L}/\tilde{a}, y), \quad (\text{A4})$$

where

$$S(\tilde{L}/\tilde{a}, y) = (\tilde{a}/\tilde{L}) \sum_k \exp[-2y(1 - \cos k)], \quad (\text{A5})$$

$$S(\infty, y) = (2\pi)^{-1} \int_{-\pi}^{\pi} dx \exp[-2y(1 - \cos x)], \quad (\text{A6})$$

$$S_D(L/\tilde{a}, y) = (\tilde{a}/L) \sum_p \exp[-2y(1 - \cos p)]. \quad (\text{A7})$$

The sums \sum_k and \sum_p run over dimensionless wave numbers in the range $-\pi \leq k = 2\pi \tilde{a} m / \tilde{L} < \pi$ and $0 < p = \pi \tilde{a} n / (L + \tilde{a}) < \pi$ with integers $m = 0, \pm 1, \pm 2, \dots$ and $n = 1, 2, \dots, L/\tilde{a}$, as is appropriate for periodic and free boundary conditions, respectively. In determining the large- L/\tilde{a} and large- \tilde{L}/\tilde{a} behavior of Δf at fixed finite ratio L/\tilde{L} , it is important to distinguish the regimes $0 \leq y \leq y_0$ and $y \geq y_0$ with

$$y_0 = \frac{L + \tilde{a}}{\tilde{a}} \quad (\text{A8})$$

in the integral representation (A3). Accordingly, we split

$$\Delta f = \frac{1}{2} \tilde{a}^{-d} (\Delta f_1 + \Delta f_2), \quad (\text{A9})$$

where

$$\Delta f_1 = \int_0^{y_0} dy y^{-1} e^{-\tilde{r}_0 y} \Phi(L/\tilde{a}, \tilde{L}/\tilde{a}, y), \quad (\text{A10})$$

$$\Delta f_2 = \int_{y_0}^\infty dy y^{-1} e^{-\tilde{r}_0 y} \Phi(L/\tilde{a}, \tilde{L}/\tilde{a}, y). \quad (\text{A11})$$

First we derive the leading L/\tilde{a} and \tilde{L}/\tilde{a} dependences of Δf_1 . Since $\cos k$ is a periodic function, the sum $S(\tilde{L}/\tilde{a}, y)$ satisfies the Poisson identity [49]

$$S(\tilde{L}/\tilde{a}, y) = \sum_{N=-\infty}^{\infty} (2\pi)^{-1} \int_{-\pi}^{\pi} dk e^{ikN\tilde{L}/\tilde{a}} \times \exp[-2y(1 - \cos k)] \quad (\text{A12})$$

$$= S(\infty, y) + 2e^{-2y} \sum_{N=1}^{\infty} F(N\tilde{L}/\tilde{a}, y) \quad (\text{A13})$$

with

$$F(M, y) = (2\pi)^{-1} \int_{-\pi}^{\pi} dk e^{ikM} \exp(2y \cos k) = I_M(2y), \quad (\text{A14})$$

$$S(\infty, y) = e^{-2y} I_0(2y), \quad (\text{A15})$$

where

$$I_M(z) = \frac{1}{\pi} \int_0^{\pi} d\theta e^{z \cos \theta} \cos(M\theta) \quad (\text{A16})$$

are the Bessel functions of integer order M (see, e.g., 9.6.19 of Ref. [50], see also Eqs. (3.6)–(3.10) of Ref. [7]). For $y < y_0$ at fixed L/\tilde{L} , the large- \tilde{L}/\tilde{a} behavior of $F(N\tilde{L}/\tilde{a}, y)$ for $N \geq 1$ is $F(N\tilde{L}/\tilde{a}, y) \sim O(e^{-\tilde{L}/\tilde{a}})$; thus

$$S(\tilde{L}/\tilde{a}, y) = S(\infty, y) + O(e^{-\tilde{L}/\tilde{a}}). \quad (\text{A17})$$

In order to determine the leading L/\tilde{a} dependence of the sum $S_D(L/\tilde{a}, y)$ for $y < y_0$, we first derive a representation of the one-dimensional integral

$$I(a, b) = \int_a^b f(x) dx \quad (\text{A18})$$

in terms of summations. The derivation is similar to that in Eqs. (A.21)–(A.30) of Ref. [32]. We assume the arbitrary real function $f(x)$ of the real variable x to be well behaved in the interval $a \leq x \leq b$; in particular, we assume that $f(x)$ has a convergent Taylor expansion around any x in this interval. We split the interval $a \leq x \leq b$ into N subintervals of length $\Delta x = (b-a)/N > 0$ between the points $x_i = a + i\Delta x$, $i = 0, 1, \dots, N$, with $x_0 = a, x_N = b$. The integral I can be represented as

$$I(a, b) = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x) dx. \quad (\text{A19})$$

For each interval we expand $f(x)$ into a Taylor series around x_{i+1} (rather than around x_i as in Ref. [32])

$$\begin{aligned} \int_{x_i}^{x_{i+1}} f(x) dx &= \int_{x_i}^{x_{i+1}} \left[f(x_{i+1}) + \sum_{n=1}^{\infty} \frac{1}{n!} f^{(n)}(x_{i+1}) \right. \\ &\quad \left. \times (x - x_{i+1})^n \right] dx \quad (\text{A20}) \\ &= f(x_{i+1})\Delta x + \sum_{n=1}^{\infty} \frac{(-1)^n}{(n+1)!} f^{(n)}(x_{i+1}) \\ &\quad \times (\Delta x)^{n+1}, \quad (\text{A21}) \end{aligned}$$

where $f^{(n)}(x) \equiv d^n f(x)/dx^n$. Thus we obtain

$$\int_a^b f(x) dx = \sum_{i=0}^{N-1} f(x_{i+1})\Delta x + \sum_{n=1}^{\infty} \frac{(-1)^n (\Delta x)^n}{(n+1)!} K_N^{(n)}(a, b), \quad (\text{A22})$$

where

$$K_N^{(n)}(a, b) = \sum_{i=0}^{N-1} f^{(n)}(x_{i+1})\Delta x. \quad (\text{A23})$$

Since $f(x)$ is an arbitrary function, we may also apply Eq. (A22) to the function $f'(x)$ instead of $f(x)$. This yields an expression for $K_N^{(1)}(a, b)$ in terms of higher derivatives,

$$K_N^{(1)}(a, b) = f(b) - f(a) - \sum_{n=1}^{\infty} \frac{(-1)^n (\Delta x)^n}{(n+1)!} K_N^{(n+1)}(a, b), \quad (\text{A24})$$

which can be substituted into the $n=1$ term of Eq. (A22). Successive application of this procedure permits one to express the difference

$$\int_a^b f(x) dx - \sum_{i=0}^{N-1} f(x_{i+1})\Delta x \equiv \tilde{R}_N(a, b) \quad (\text{A25})$$

in terms of the differences of the derivatives at a and b ,

$$\Delta f^{(k)} = f^{(k)}(b) - f^{(k)}(a). \quad (\text{A26})$$

Note that $\tilde{R}_N(a, b)$ differs from $R_N(a, b)$ of Ref. [32]. The result is

$$\tilde{R}_N(a, b) = -\frac{\Delta x}{2} [f(b) - f(a)] - \frac{(\Delta x)^2}{12} \Delta f^{(1)} + O((\Delta x)^4). \quad (\text{A27})$$

The coefficient of the $O((\Delta x)^3)$ term vanishes. Since $\Delta x \sim O(N^{-1})$ this representation is expected to converge rapidly for large N if $\Delta f^{(k)}$ remains sufficiently well behaved for large k . Equation (A27) differs from Eq. (A30) of Ref. [32] by a minus sign in the first term.

We apply Eqs. (A25)–(A27) to the integral

$$S(\infty, y) = \frac{1}{\pi} \int_0^\pi dp \exp[-2y(1 - \cos p)], \quad (\text{A28})$$

where the integration variable p plays the role of x in the integral of Eq. (A25). The sum on the left-hand side of Eq. (A25) now corresponds to

$$\frac{1}{\pi} \sum_{n=1}^N \Delta p \exp\{-2y[1 - \cos(n\Delta p)]\} \equiv \tilde{I}_N(y) \quad (\text{A29})$$

with $\Delta p = \pi/N$. Setting $N = L/\tilde{a}$, we see that

$$\tilde{I}_{L/\tilde{a}}(y) = \frac{L + \tilde{a}}{L} S_D(L/\tilde{a}, y). \quad (\text{A30})$$

We note that the derivative of the integrand of Eq. (A28) with respect to p vanishes at $p=0$ and $p=\pi$. Equations (A25)–(A30) yield the leading large- L/\tilde{a} behavior, for $y < (L + \tilde{a})/\tilde{a}$,

$$\begin{aligned} S_D(L/\tilde{a}, y) &= S(\infty, y) - \frac{\tilde{a}}{2L} [1 + e^{-4y} - 2e^{-2y} I_0(2y)] \\ &\quad + O(\tilde{a}^4/L^4). \quad (\text{A31}) \end{aligned}$$

In order to ensure that the discretization intervals Δp become sufficiently small for large L/\tilde{a} , the restriction $y \leq O(L/\tilde{a})$ was necessary. For this reason, Eq. (A31) is applicable only

to Δf_1 , Eq. (A10), but not to Δf_2 , Eq. (A11). Using Eq. (A17) and substituting Eq. (A31) into Eqs. (A4) and (A10), we arrive at

$$\begin{aligned} \Delta f_1 &= \frac{\tilde{a}}{2L} \int_0^{y_0} dy \{y^{-1} e^{-\tilde{r}_0 y} [S(\infty, y)]\}^{d-1} \\ &\quad \times [1 + e^{-4y} - 2S(\infty, y)] + O(\tilde{a}^4/L^4, e^{-\tilde{L}/\tilde{a}}). \end{aligned} \quad (\text{A32})$$

This can be combined with Δf_2 in the form

$$\begin{aligned} \Delta f_1 + \Delta f_2 &= \frac{\tilde{a}}{2L} \int_0^\infty dy \{y^{-1} e^{-\tilde{r}_0 y} [S(\infty, y)]\}^{d-1} \\ &\quad \times [1 + e^{-4y} - 2S(\infty, y)] + \Delta f_3(L/\tilde{a}, \tilde{L}/\tilde{a}) \\ &\quad + O(\tilde{a}^4/L^4, e^{-\tilde{L}/\tilde{a}}), \end{aligned} \quad (\text{A33})$$

$$\begin{aligned} \Delta f_3 &= \int_{y_0}^\infty dy y^{-1} e^{-\tilde{r}_0 y} \left\{ [S(\infty, y)]^d (1 + \tilde{a}/L) \right. \\ &\quad \left. - [S(\tilde{L}/\tilde{a}, y)]^{d-1} S_D(L/\tilde{a}, y) - \frac{\tilde{a}}{2L} [S(\infty, y)]^{d-1} \right\}. \end{aligned} \quad (\text{A34})$$

The integral term in Eq. (A33) represents the surface contribution of $O(L^{-1})$ to Δf , whereas Δf_3 will yield the finite-size part of $O(L^{-d})$. Since $y > y_0$ in Eq. (A34) is sufficiently large it suffices to use the small k approximation $-2y(1 - \cos k) \approx -k^2 y$ in Eq. (A5), and similarly in Eqs. (A6) and (A7),

$$\begin{aligned} S(\tilde{L}/\tilde{a}, y) &\approx (\tilde{a}/\tilde{L}) \sum_k e^{-k^2 y} \\ &= (\tilde{a}/\tilde{L}) K(4\pi^2 \tilde{a}^2 L^{-2} y) + O(e^{-\pi^2 y}), \end{aligned} \quad (\text{A35})$$

$$\begin{aligned} S(\infty, y) &\approx \pi^{-1} \int_0^\pi dk e^{-k^2 y} = (2\pi)^{-1} (\pi/y)^{1/2} \\ &\quad + O(e^{-\pi^2 y}), \end{aligned} \quad (\text{A36})$$

$$S_D(L/\tilde{a}, y) \approx (\tilde{a}/L) \sum_p e^{-p^2 y} \quad (\text{A37})$$

$$\begin{aligned} &= \frac{1}{2} (\tilde{a}/L) [K(\pi^2 \tilde{a}^2 (L + \tilde{a})^{-2} y) - 1] \\ &\quad + O(e^{-\pi^2 y}), \end{aligned} \quad (\text{A38})$$

where $K(y)$ is given by Eq. (70). Furthermore, it is useful to turn to the integration variable

$$z = 4\pi^2 \tilde{a}^2 y / (L + \tilde{a})^2. \quad (\text{A39})$$

Instead of y_0 , we then have the lower integration limit $z_0 = 4\pi^2 \tilde{a} / (L + \tilde{a}) \rightarrow 0$ for large L/\tilde{a} . This leads to

$$\begin{aligned} \Delta f_3 &= \frac{\tilde{a}^d L^{-1}}{(L + \tilde{a})^{d-1}} \int_0^\infty dz \left(z^{-1} \left\{ \left(\frac{\pi}{z} \right)^{d/2} \right. \right. \\ &\quad \left. \left. - \frac{1}{2} [\tilde{s} K(\tilde{s}^2 z)]^{d-1} [K(z/4) - 1] - \frac{1}{2} \left(\frac{\pi}{z} \right)^{(d-1)/2} \right\} \right. \\ &\quad \left. \times \exp \left[-\frac{r_0 (L + \tilde{a})^2}{8J\pi^2} z \right] \right) [1 + O(\tilde{a}^2/L^2)] \end{aligned} \quad (\text{A40})$$

with the shape factor

$$\tilde{s} = \frac{L + \tilde{a}}{\tilde{L}}. \quad (\text{A41})$$

For $L \gg \tilde{a}$, we finally obtain Eqs. (66)–(69).

The surface free energy, Eq. (67), can be expressed in terms of the generalized Watson function, Eqs. (73) and (74), as follows:

$$\begin{aligned} f_{\text{surface}}(t) &= \frac{\tilde{a}^{1-d}}{8} \int_{r_0 \tilde{a}^2 J_0^{-1}}^\infty dz [W_{d-1}(z) + W_{d-1}(z+4) \\ &\quad - 2W_d(z)]. \end{aligned} \quad (\text{A42})$$

It can be shown that for $d \neq 3$ there exists the following common representation of the coefficients \tilde{b}_d , Eq. (77), and \tilde{B}_d , Eq. (89), of the regular term of f_{surface} linear in r_0 :

$$\begin{aligned} \tilde{b}_d = \tilde{B}_d &= \frac{1}{8} [W_{d-1}(4) - 2W_d(0)] \\ &\quad + \frac{1}{8} \int_0^A dy [e^{-2y} I_0(2y)]^{d-1} + \frac{1}{8} \int_A^\infty \{ [e^{-2y} I_0(2y)]^{d-1} \\ &\quad - (4\pi y)^{(1-d)/2} \} + 2^{-d-1} \pi^{(1-d)/2} (d-3)^{-1} A^{(3-d)/2}. \end{aligned} \quad (\text{A43})$$

This expression is independent of the arbitrary constant $A > 0$. For $d \rightarrow 3+$ and $d \rightarrow 3-$, the first two terms have a finite limit $[W_2(4) - 2W_3(0)]/8$, whereas the last term exhibits a divergence $\sim (d-3)^{-1}$ that originates from $W_{d-1}(0)/8$ for $d \rightarrow 3+$ according to Eq. (91). The same divergence is contained in A_{surface}^+ , see Eqs. (79) and (92).

APPENDIX B: SUSCEPTIBILITY

We rewrite Eq. (130) as

$$\chi = \frac{\tilde{a}^2}{L(L + \tilde{a})} \sum_p \{ 2 - [1 + (-1)^n] \} \frac{\cot^2(p\tilde{a}/2)}{r_0 + J_p} \quad (\text{B1})$$

$$\begin{aligned}
&= \frac{2\tilde{a}^4}{J_0 L(L+\tilde{a})} \sum_p \frac{1+\cos p}{(1-\cos p)[\tilde{r}_0+2(1-\cos p)]} \\
&\quad - \frac{2\tilde{a}^4}{J_0 L(L+\tilde{a})} \sum_q \frac{1+\cos q}{(1-\cos q)[\tilde{r}_0+2(1-\cos q)]}
\end{aligned} \tag{B2}$$

with $\tilde{r}_0 = r_0 \tilde{a}^2 / J_0$. The sums \sum_p and \sum_q run over dimensionless wave numbers $p = \pi \tilde{a} n / (L + \tilde{a})$ with integers $n = 1, 2, \dots, L/\tilde{a}$ and $q = 2\pi \tilde{a} m / (L + \tilde{a})$ with integers $m = 1, 2, \dots, L/(2\tilde{a})$ where we have assumed that L/\tilde{a} is an even integer. Using the decomposition

$$\begin{aligned}
&\frac{1+\cos x}{(1-\cos x)[\tilde{r}_0+2(1-\cos x)]} \\
&= -\frac{1}{\tilde{r}_0+2(1-\cos x)} + \frac{4}{\tilde{r}_0} \left[\frac{1}{2(1-\cos x)} \right. \\
&\quad \left. - \frac{1}{\tilde{r}_0+2(1-\cos x)} \right]
\end{aligned} \tag{B3}$$

and applying the representation Eq. (C2), we obtain

$$\chi = \frac{2\tilde{a}^3}{J_0(L+\tilde{a})} \int_0^\infty dy \left[\frac{4}{\tilde{r}_0} (1 - e^{-\tilde{r}_0 y}) - e^{-\tilde{r}_0 y} \right] \Psi(L/\tilde{a}, y) \tag{B4}$$

with

$$\Psi(L/\tilde{a}, y) = S_D(L/\tilde{a}, y) - \frac{1}{2} \bar{S}_D(L/\tilde{a}, y), \tag{B5}$$

where $S_D(L/\tilde{a}, y)$ is given by Eq. (A7) and

$$\bar{S}_D(L/\tilde{a}, y) = \frac{2\tilde{a}}{L} \sum_q \exp[-2y(1-\cos q)]. \tag{B6}$$

We distinguish the regions $0 \leq y \leq y_0 = (L + \tilde{a})/\tilde{a}$ and $y \geq y_0$. The large- L behavior of $S_D(L/\tilde{a}, y)$ in the former region is given by Eq. (A31); the corresponding behavior of \bar{S}_D is

$$\bar{S}_D(L/\tilde{a}, y) = (1 + \tilde{a}/L) S(\infty, y) - \pi \tilde{a} / (L + \tilde{a}) + O(\tilde{a}^3 / L^3), \tag{B7}$$

which follows from the Poisson identity (see, e.g., Eq. (3.6) of Ref. [7]). In the region $y \geq y_0$ we may use approximation (A37) and

$$\begin{aligned}
\bar{S}_D(L/\tilde{a}, y) &\approx (2\tilde{a}/L) \sum_{n=1}^{\infty} \exp[-4\pi^2 \tilde{a}^2 y n^2 / (L + \tilde{a})^2] \\
&\quad + O(e^{-\pi^2 y}).
\end{aligned} \tag{B8}$$

While the contributions of region $y \leq y_0$ are important for the large L behavior of χ at fixed $T > T_c$, the contributions of

region $y \geq y_0$ yield the finite-size scaling behavior of χ in the critical region $L/\tilde{a} \gg 1$, $\xi/\tilde{a} \gg 1$ at fixed ratio $x = L/\xi \geq 0$, including the leading terms of the scaling function for large x , as given by Eqs. (131)–(135) for the Gaussian model.

The derivation of χ from Eq. (169) is parallel to that given above, except that \tilde{r}_0 is to be replaced by

$$\tilde{\mu}/J_0 = \Delta\mu - \pi^2 / (L + \tilde{a})^2 + O(\tilde{a}^2 L^{-4}), \tag{B9}$$

where $\Delta\mu$ is defined by Eq. (201). At fixed $\tilde{M} \equiv \Delta\mu(L + \tilde{a})^2 > 0$, this leads to the large L -behavior

$$\begin{aligned}
\chi &= \frac{4(L+\tilde{a})^3}{J_0 \pi^2 L} \int_0^\infty dy \left\{ \frac{1 - \exp[-(\tilde{M} - \pi^2)y/\pi^2]}{\tilde{M} - \pi^2} \right. \\
&\quad \left. - \frac{\tilde{a}^2}{(L+\tilde{a})^2} \exp[-(\tilde{M} - \pi^2)y/\pi^2] \right\} [K(y) - K(4y)],
\end{aligned} \tag{B10}$$

where $K(z)$ is given by Eq. (70). For $L \gg \tilde{a}$ this yields Eq. (202).

APPENDIX C: FILM CRITICAL TEMPERATURE FOR $D > 3$

In the following, we consider Eq. (191) for $d > 3$. Subtracting

$$\beta_{c,d}(\infty) = \tilde{a}^{d-2} \int_p \int_{\mathbf{k}} (J_{\mathbf{k},d-1} + J_p)^{-1} \tag{C1}$$

and using the representation

$$\frac{1}{z} = \int_0^\infty dy e^{-zy} \tag{C2}$$

for $z > 0$, we obtain

$$2J[\beta_{c,d}(\infty) - \beta_{c,d}(L)] = \int_0^\infty dy \bar{\Phi}(L/\tilde{a}, y), \tag{C3}$$

$$\begin{aligned}
\bar{\Phi}(x, y) &= [S(\infty, y)]^{d-1} \left\{ S(\infty, y) - S_D(x, y) \right. \\
&\quad \left. \times \exp \left[2y \left(1 - \cos \frac{\pi}{1+x} \right) \right] \right\},
\end{aligned} \tag{C4}$$

where $S(\infty, y)$ and $S_D(L/\tilde{a}, y)$ are defined by Eqs. (A6) and (A7) [see also Eq. (A15)]. It is important to distinguish regimes $0 \leq y \leq y_0$ and $y \geq y_0$ with y_0 given by Eq. (A8). Accordingly, we split

$$\int_0^\infty dy \bar{\Phi}(x, y) = \int_0^{y_0} dy \bar{\Phi}(x, y) + \int_{y_0}^\infty dy \bar{\Phi}(x, y) \equiv \bar{\Delta}_1 + \bar{\Delta}_2. \tag{C5}$$

In $\tilde{\Delta}_1$ we use Eq. (A31). A treatment similar to that in Eqs. (A32)–(A39) leads to

$$\tilde{\Delta}_1 + \tilde{\Delta}_2 = 4\tilde{B}_d \frac{\tilde{a}}{L} - \tilde{C}_d \left(\frac{\tilde{a}}{L + \tilde{a}} \right)^{d-2} \left(1 + \frac{\tilde{a}}{L} \right) + O(\tilde{a}^{d/2} L^{-d/2}) \quad (\text{C6})$$

with the nonuniversal amplitude \tilde{B}_d , Eq. (89), and the universal amplitude

$$\tilde{C}_d = \frac{1}{8\pi^2} \int_0^\infty dz \left\{ 1 - 2 \left(\frac{\pi}{z} \right)^{1/2} + e^{z/4} \left[K \left(\frac{z}{4} \right) - 1 \right] \right\} \left(\frac{\pi}{z} \right)^{(d-1)/2} \quad (\text{C7})$$

with $\tilde{C}_d > 0$. The first term $\sim L^{-1}$ in Eq. (C6) has a nonscaling L dependence, whereas the second term $\sim L^{2-d}$ has the scaling L dependence $\sim L^{1/\nu}$. Equations (C3)–(C7) lead to Eq. (195). Rewriting

$$1 + e^{-4y} - 2e^{-2y} I_0(2y) = 2e^{-2y} [\cosh(2y) - I_0(2y)] \quad (\text{C8})$$

and using (see 9.6.39 of Ref. [50])

$$\cosh(z) - I_0(z) = 2I_2(z) + 2I_4(z) + \dots \geq 0, \quad (\text{C9})$$

we see that \tilde{B}_d is *positive* and finite for $d > 3$; thus $T_{c,d}(L) > T_{c,d}(\infty)$ for $L \gg \tilde{a}$. Using the representation

$$2J\beta_{c,d}(\infty) = \int_0^\infty dy [S(\infty, y)]^d, \quad (\text{C10})$$

we obtain the fractional shift of the film critical temperature as given in Eqs. (197)–(199). We have verified that a_d , Eq. (198), agrees with the corresponding amplitude of Barber and Fisher [16] at $d=4$, which was expressed in terms of the generalized Watson function, Eqs. (73) and (74). The amplitude $a_d = 4\tilde{B}_d/W_d(0)$, Eq. (198), diverges for $d \rightarrow 3$. This divergence is canceled by the next term of $O(L^{2-d})$ in Eqs. (C6) and (197).

APPENDIX D: CONSTRAINT EQUATION

We start from the constraint equation (166) for box geometry where we decompose $\tilde{\mu} = J_0 \Delta\mu + \tilde{\mu}_c(L)$ and subtract $\beta_{c,d}$ in the form of Eq. (C1). Furthermore we add and subtract

$$\tilde{\beta}(\Delta\mu) \equiv \tilde{a}^{d-2} \int_{\mathbf{k}} \int_p (J_0 \Delta\mu + J_{\mathbf{k},d-1} + J_p)^{-1}. \quad (\text{D1})$$

This yields

$$\beta_{c,d} - \beta = M_1 + M_2, \quad (\text{D2})$$

$$M_1 = \tilde{\beta}(\Delta\mu) - \tilde{a}^{d-2} \tilde{L}^{1-d} L^{-1} \times \sum_{\mathbf{k},p} (J_0 \Delta\mu + \tilde{\mu}_c + J_{\mathbf{k},d-1} + J_p)^{-1}, \quad (\text{D3})$$

$$M_2 = \tilde{a}^{d-2} \Delta\mu \int_{\mathbf{k}} \int_p (J_0 \Delta\mu + J_{\mathbf{k},d-1} + J_p)^{-1} (J_{\mathbf{k},d-1} + J_p)^{-1}. \quad (\text{D4})$$

Using the representation Eq. (C2) we obtain

$$J_0 M_1 = \int_0^\infty dy \Phi(L/\tilde{a}, \tilde{L}/\tilde{a}, y) \exp(-\Delta\mu \tilde{a}^2 y), \quad (\text{D5})$$

where $\Phi(L/\tilde{a}, \tilde{L}/\tilde{a}, y)$ is given by Eq. (A4). Again we split the integral in Eq. (D5) as $\int_0^\infty = \int_0^{y_0} + \int_{y_0}^\infty \equiv I_1 + I_2$ with $y_0 = (L + \tilde{a})/\tilde{a}$. For large L/\tilde{a} and \tilde{L}/\tilde{a} , we find

$$I_1 = \frac{\tilde{a}}{2L} \int_0^{y_0} dy [1 + e^{-4y} - 2S(\infty, y)] [S(\infty, y)]^{d-1} \times \exp(-\Delta\mu \tilde{a}^2 y) + O(e^{-\tilde{L}/\tilde{a}}, \tilde{a}^{d/2} L^{-d/2}), \quad (\text{D6})$$

$$I_2 = \frac{\tilde{a}}{L} \left(\frac{L + \tilde{a}}{\tilde{a}} \right)^{3-d} \frac{1}{8\pi^2} \int_{z_0}^\infty dz \left\{ e^{z/4} \left[K \left(\frac{z}{4} \right) - 1 \right] [\tilde{s} K(\tilde{s}^2 z)]^{d-1} + \left(\frac{\pi}{z} \right)^{(d-1)/2} - 2 \left(\frac{\pi}{z} \right)^{d/2} \right\} + O(\tilde{a}^{d/2} L^{-d/2}) \quad (\text{D7})$$

with $z_0 = 4\pi^2 \tilde{a}/(L + \tilde{a})$ and $\tilde{s} = (L + \tilde{a})/\tilde{L}$, where $K(z)$ is given by Eq. (70). For large L/\tilde{a} we can let $z_0 \rightarrow 0$ in Eq. (D7). Evaluating the integral in Eq. (D4) for small $\Delta\mu$ yields for $2 < d < 4$,

$$J_0 M_2 = \varepsilon^{-1} A_d (\Delta\mu \tilde{a}^2)^{(d-2)/2} + O(\Delta\mu \tilde{a}^2). \quad (\text{D8})$$

Equations (D2)–(D8) lead to

$$J_0 (\beta_{c,d} - \beta) = \varepsilon^{-1} A_d (\Delta\mu \tilde{a}^2)^{(d-2)/2} - E_{surface}(\Delta\mu \tilde{a}^2) \times (\tilde{a}/2L) + 2\tilde{\mathcal{E}}_d((\Delta\mu)^{1/2}(L + \tilde{a}), \tilde{s}) \times [(L + \tilde{a})/\tilde{a}]^{2-d}, \quad (\text{D9})$$

where $E_{surface}(z)$ and $\tilde{\mathcal{E}}_d(x, s)$ are given by Eqs. (97) and (204). Multiplying Eq. (D9) by $\varepsilon A_d^{-1} (L/\tilde{a})^{d-2}$ and using

$$\varepsilon A_d^{-1} J_0 (\beta_c - \beta) = t(\xi_0/\tilde{a})^{2-d} + O(t^2), \quad (\text{D10})$$

we obtain Eq. (203) for $L \gg \tilde{a}$.

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