

## Exact three-dimensional Casimir force amplitude, $C$ function, and Binder's cumulant ratio: Spherical model results

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The three-dimensional mean spherical model on a hypercubic lattice with a film geometry  $L \times \infty^2$  under periodic boundary conditions is considered in the presence of an external magnetic field  $H$ . The universal Casimir amplitude  $\Delta$  and the Binder's cumulant ratio  $B$  are calculated exactly and found to be  $\Delta = -2\zeta(3)/(5\pi) \approx -0.153051$  and  $B = 2\pi/\{\sqrt{5}\ln^3[(1+\sqrt{5})/2]\}$ . A discussion on the relations between the finite temperature  $C$  function, usually defined for quantum systems, and the excess free energy (due to the finite-size contributions to the free energy of the system) scaling function is presented. It is demonstrated that the  $C$  function of the model equals  $4/5$  at the bulk critical temperature  $T_c$ . It is analytically shown that the excess free energy is a monotonically increasing function of the temperature  $T$  and of the magnetic field  $|H|$  in the vicinity of  $T_c$ . This property is supposed to hold for any classical  $d$ -dimensional  $O(n), n > 2$ , model with a film geometry under periodic boundary conditions when  $d \leq 3$ . An analytical evidence is also presented to confirm that the Casimir force in the system is negative both below and in the vicinity of the bulk critical temperature  $T_c$ . [S1063-651X(98)04508-5]

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### I. INTRODUCTION

The Casimir effect is a phenomenon common to all systems characterized by fluctuating quantities satisfying some conditions on the boundaries of the system (for a general review on the Casimir effect see, e.g., [1,2]). In the statistical mechanical systems the Casimir force is usually characterized by the excess free energy

$$f_{a,b}^{\text{ex}}(T,L) = f_{a,b}(T,L) - Lf_{\text{bulk}}(T), \quad (1)$$

due to the finite size contributions to the free energy of finite systems with a film geometry  $L \times \infty^2$ , where boundary conditions  $a$  and  $b$  are imposed on the surfaces bounding the system across the direction  $L$ . Here  $f_{a,b}(T,L)$  is the full free energy per unit area (and per  $k_B T$ ) of such a system and  $f_{\text{bulk}}$  is the corresponding bulk free energy density. The Casimir force

$$f_{\text{Casimir}}^{a,b}(T,L) = -\frac{\partial f_{a,b}^{\text{ex}}(T,L)}{\partial L} \quad (2)$$

then arises naturally in the thermodynamics of these confined systems.

For  $O(n)$ -symmetric model systems ( $n \geq 1$ ), depending on the boundary condition ( $a,b$ ) and on  $n$ ,  $f_{a,b}^{\text{ex}}(T,L)$  may or may not contain contributions independent of  $L$ . For the Ising-like systems, i.e.,  $n=1$ , these can be the surface free energies  $f_{s,a}(T)$  and  $f_{s,b}(T)$ , and the interface free energy  $f_i(T)$  (for brevity we consider the dependence on the temperature  $T$  only). For the  $O(n), n \geq 2$ , models these will be only the contributions stemming from the surface free energies because the analog of the interface free energy is the helicity modulus  $Y(T)$  and the corresponding contribution is of the order  $Y(T)/L$ . In general at the critical temperature  $T_c$  (of the corresponding bulk, i.e.,  $L = \infty$ , system) the full free energy  $f_{a,b}(T,L)$  has the asymptotic form

$$f_{a,b}(T_c, L) \cong Lf_{\text{bulk}}(T_c) + f_{s,a}(T_c) + f_{s,b}(T_c) + L^{-(d-1)}\Delta_{a,b} + \dots, \quad (3)$$

where  $d$  is the dimensionality of the considered system and  $\Delta_{a,b}$  is the so-called Casimir amplitude. The  $L$  dependence of the Casimir term [the last one in Eq. (3)] follows from the scale invariance of the free energy and has been derived by Fisher and de Gennes [4]. The amplitude  $\Delta_{a,b}$  is *universal*, depending on the bulk universality class and the universality classes of the boundary conditions [2,3]. In the present article we will only consider the case of periodic boundary conditions (which implies that  $f_{s,a} = f_{s,b} = Y \equiv 0$ ). Then, according to the standard finite-size scaling theory (see, e.g., [3] for a general review), near the critical temperature  $T_c$  and in the presence of a small external magnetic field  $h$  the behavior of  $f^{\text{ex}}$  is given by

$$f^{\text{ex}}(t,h,L) = L^{-(d-1)}X^{\text{ex}}(a_t t L^{1/\nu}, a_h h L^{\Delta/\nu}), \quad (4)$$

where  $t = (T - T_c)/T_c$  is the reduced temperature,  $h = H/(k_B T)$ ,  $a_t$  and  $a_h$  are nonuniversal scaling factors,  $X^{\text{ex}}$  is *universal* (usually geometry dependent) scaling function,  $X^{\text{ex}}(0,0) \equiv \Delta_{\text{per}}$ , and  $\nu$  and  $\Delta$  are the corresponding (universal) scaling exponents.

An interesting point of view on the properties of the excess free energy comes from the finite-temperature generalizations of the Zamolodchikov's  $C$  theorem [6] for quantum systems with arbitrary dimensionality due to Netto and Fradkin [7] (see also Zabzin [8]; for a general review on phase transitions in quantum system see, e.g., [9,10]). They define from the free energy a function  $C$  of the coupling constants and the temperature that is a positive and, in the regimes where the quantum fluctuations dominate, a monotonically increasing function of the temperature. The  $C$  function is, in fact, an *analog of the excess free energy* of the system that they consider.

Before passing to a discussion of some details it seems necessary to comment on the well known point that for temperature driven phase transitions with  $T_c > 0$  the quantum fluctuations are unimportant near the temperature critical point. Therefore, it seems that the properties of the system around one quantum critical point (with respect to a given quantum parameter, say,  $g$ ) at  $T=0$  cannot tell us anything about the properties of this system around its temperature critical point  $T_c > 0$ . In fact the dimensional crossover rule helps to make a bridge between these phenomena. According to this rule the critical singularities (with respect to  $g$ ,  $T=0$ ) of a  $d$ -dimensional quantum system are *formally* equivalent to those of a  $d+z$  classical one ( $z$  is the dynamical critical exponent) and critical temperature  $T_c > 0$ . On that idea are actually based the investigations of the low-temperature effects in quantum systems (see, e.g., [11–14]), i.e., one considers an *effective system* with  $d$  infinite space and  $z$  finite “temperature” (“imaginary-time”) dimensions  $L_T \sim [\hbar/(k_B T)]^{1/z}$  with periodic boundary conditions, and applies the methods of the finite-size scaling theory (in what follows we will set  $\hbar = k_B = 1$ ). An exact lattice realization of these ideas is presented in [15].

Since the generalizations of the Zamolodchikov’s  $C$  theorem are formulated for quantum systems with  $z=1$ , in the remainder we will focus our attention on such class of systems only. For these systems Netto and Fradkin define [7] the dimensionless function

$$C(\beta, g, a) = -\beta^{d+1} \tilde{n}(d) \lim_{V \rightarrow \infty} V^{-1} [F_V(\beta, g, a) - E_0(g, a)], \quad (5)$$

where  $E_0$  is the zero-temperature energy, i.e., the energy of the “infinite” system,  $V$  is the volume ( $V \rightarrow \infty$ , but  $N/V$  is fixed, where  $N$  is the number of particles),  $\tilde{n}(d)$  is a positive real quantity,  $\beta = 1/T$ ,  $F_V$  is the full free energy of the “finite” system (where the only “finite” dimension is the “temperature” one, i.e., the “geometry” of the system is  $\infty^d \times L_T$ ) and  $a$  is the characteristic length scale of the lattice.

The real positive quantity  $\tilde{n}(d)$  is supposed to be of the form  $v^d/n(d)$ , where  $n(d)$  is a positive real number (which depends only on the dimensionality of the system) and  $v$  is the characteristic velocity (e.g., the velocity of the quasiparticles) in the system. Obviously, the exact choice of  $n(d)$  does not effect the monotonicity properties of the  $C$  function. In [7] the definitions  $n(d) = \Gamma[(d+1)/2] \zeta(d+1) / \pi^{(d+1)/2}$  for bosons and  $n(d) = \Gamma[(d+1)/2] \zeta(d+1) (2 - 2^{1-d}) / \pi^{(d+1)/2}$  for fermions have been proposed.

In accordance with the dimensional crossover rule the statement that  $C$  is a positive and a monotonically increasing function of the temperature can be “translated” in a statement that the function  $-X^{\text{ex}}$  of the corresponding classical system is positive and a monotonically increasing function of  $L^{-1}$ ; see Eqs. (1) and (4) (of course, the last is equivalent to a statement that  $X^{\text{ex}}$  is a negative and a monotonically increasing function of  $L$ ). In [7,8] it is shown that the monotonicity of the  $C$  function is related to the absence of long range order in the systems under consideration. The existence of long range order destroys the general validity of the

monotonicity. Within the classical systems no long-range order exists above their bulk critical point. So, we expect the statement formulated for  $X^{\text{ex}}$  to be generally valid above  $T_c$  for any classical system. Supposing that this is true and recalling that in the vicinity of  $T_c$   $X^{\text{ex}}$  is a function of the scaling variables  $x_1 = a_t t L^{1/\nu}$  and  $x_2 = a_h h L^{\Delta/\nu}$ , which both are monotonically increasing functions of  $L$ , we come to the conclusion that *in the vicinity of its critical temperature ( $T \geq T_c$ ) the excess free energy of a given system is a monotonically increasing function of any of its scaling parameters when the other one is kept fixed*. Since  $x_1$  and  $x_2$  are monotonically increasing functions of the temperature and the magnetic field, respectively, the last implies that  $X^{\text{ex}}$ , *in the vicinity of  $T_c$ , is a monotonically increasing function of  $t$  ( $t > 0$ ) and  $h$  too*. It is possible to present some arguments to support that *the above statement can be extended to the region  $t < 0$  for  $O(n), n \geq 2$ , systems* in contrast with the Ising-like systems. The reasoning for the difference in the expected behavior of the excess free energy in  $O(n)$  and Ising-type models is closely related to the well known differences in the behavior of the correlation length  $\xi_\infty(T)$  in these models: in the Ising model  $\xi_\infty(T) < \infty$  both below and above the bulk critical temperature, whereas in  $O(n)$ ,  $n \geq 2$ , models below  $T_c$  and in the absence of an external field ( $h=0$ ), due to the existence of soft modes in the system (spin waves),  $\xi_\infty(T)$  is identically infinite. On that basis one expects that, away from  $T_c$ ,  $X^{\text{ex}}$  will tend to zero exponentially fast in  $L$  (see, e.g., [3]) for the Ising-type models, and, therefore, being of the order of  $L^{-(d-1)}$  around  $T_c$ ,  $X^{\text{ex}}$  cannot be a monotonic function of its scaling parameters in the vicinity of  $T_c$ . In  $O(n)$ ,  $n \geq 2$ , models the finite size corrections should be essential not only in the vicinity but also below  $T_c$  [5]. In other words, we expect the monotonicity in the behavior of the correlation length in  $O(n)$ ,  $n \geq 2$ , models around  $T_c$  to be mirrored by a corresponding monotonic behavior of the excess free energy. If an external field is applied ( $h \neq 0$ ) then  $\xi_\infty(T, h) < \infty$  and, of course, we expect that  $X^{\text{ex}} \rightarrow 0$  exponentially fast with  $L$  again, similarly to the Ising-like systems behavior. But, since  $X^{\text{ex}} < 0$ , for any fixed  $t < 0$  the last implies that  $X^{\text{ex}}$  will be a monotonically increasing function of the magnetic field in the under critical vicinity of  $T_c$  too.

The statements presented above should be considered, of course, only as a *plausible hypothesis*, which has to be checked in order to probe the region of its validity. For example, it is under question if the monotonicity property of  $X^{\text{ex}}$  will still hold if the finite system undergoes a phase transitions of its own. It is reasonable to believe that the hypothesis holds for any  $O(n)$ ,  $n \geq 2$ , system with  $d \leq 3$  (then in the finite system with short range interaction there will be no “real” phase transition).

In the present article we will show, within the three-dimensional mean spherical model, that *in the vicinity of  $T_c$  the excess free energy scaling function  $X^{\text{ex}}$  is, indeed, a monotonically increasing function of any of its scaling parameters ( $x_1$  and  $x_2$ ) when the other one is kept fixed*. The last implies that  $X^{\text{ex}}$  is a monotonically increasing function of  $t$ ,  $h$ , and  $L$  above  $T_c$ , and a monotonically increasing, with respect to  $t$  and  $h$ , but a monotonically decreasing, with respect to  $L$ , function below  $T_c$ .

Let us turn now to the behavior of  $f_{\text{Casimir}}$ . From Eqs. (2) and (4) it immediately follows that [5]

$$f_{\text{Casimir}}(t, h, L) = L^{-d} X_{\text{Casimir}}(x_1, x_2), \quad (6)$$

where the Casimir force scaling function is

$$X_{\text{Casimir}}(x_1, x_2) = (d-1)X^{\text{ex}}(x_1, x_2) - \frac{1}{\nu} x_1 \frac{\partial}{\partial x_1} X^{\text{ex}}(x_1, x_2) - \frac{\Delta}{\nu} x_2 \frac{\partial}{\partial x_2} X^{\text{ex}}(x_1, x_2). \quad (7)$$

Note that  $X_{\text{Casimir}}$  is again a *universal* function of  $x_1$  and  $x_2$ . We recall that for finite-size systems this means that  $X_{\text{Casimir}}$  will be the same for all systems of the same universality class *and* geometry and boundary conditions. It is believed that if  $a \equiv b$  the Casimir force will be negative (see, e.g., [16,17]; strictly speaking, for an Ising-like system this is supposed to be true above the wetting transition temperature  $T_w$  [16–19]). In the case of a fluid confined between identical walls this implies that then the net force between the plates will be attractive for large separations. One of the goals of the present article is to prove analytically this general expectation, i.e., that  $X_{\text{Casimir}}(x_1, x_2) < 0$  for any  $(x_1, x_2) \in \mathbf{R}^2$ , on the example of one exactly solvable model. We will also show that if  $T < T_c$  and  $H = 0$  the Casimir force is a monotonically increasing function of the temperature. We believe that these properties are valid for any  $O(n), n \geq 2$ , model.

The full temperature dependence of the Casimir force has been investigated exactly in two-dimensional Ising strips by Evans and Stecki [16], whereas the upper critical temperature dependence of the force in  $O(n)$  systems has been considered by Krech and Dietrich [20] by means of the field-theoretical renormalization group theory in  $4 - \epsilon$  dimensions. (For the Ising-like case they have derived also some results for  $T < T_c$ .) The only example where an exact expression for the Casimir force as a function of both the temperature and the magnetic field is available is that of the three-dimensional mean spherical model [5]. By numerical evaluation of the expressions derived there it has been shown that the force is negative, i.e., it is consistent with an attraction of the plates confining the system. The most results available at the moment are for the Casimir amplitudes  $\Delta_{a,b}$ . For two-dimensional systems at  $T = T_c$  by using conformal-field theory methods the amplitudes are exactly known for a large class of two-dimensional models [2,24,25]. In addition to the ‘‘flat geometries’’ recently some results about the Casimir amplitudes between spherical particles in a critical fluid have been derived too [26]. For  $d = 3$  the results for the Casimir amplitudes available in the Ising-like case have been obtained by Migdal-Kadanoff renormalization-group calculations [21], by some interpolation of the exact values for  $d = 2$  and  $d = 4$  [20], and, relatively recently, by Monte Carlo methods [22,23]. For  $n \geq 2$  the only existing results are obtained by the  $\epsilon$ -expansion technique, where the calculations are performed up to the first order in  $\epsilon$  [20].

In the present article the hypotheses for the monotonicity of the excess free energy and that the Casimir force is negative under periodic boundary conditions will be verified ana-

lytically on the example of the three-dimensional mean spherical model. We will present also simple analytical results for the universal values of the Casimir amplitude and the Binder’s cumulant ratio. If one takes the normalization factor of the analog of the  $C$  function in the form for bosons (this will keep the  $C$  function of the critical Gaussian model to be  $C = 1$  for any  $d$ ), it will be shown that the ‘‘ $C$  function of the three dimensional spherical model’’ is  $4/5$  at the critical point. As is well known, the infinite translational invariant spherical model is equivalent to the  $n \rightarrow \infty$  limit of the corresponding  $n$ -component system [27].

The results we are going to present are an extension and continuation of those published in [5]. In the notations and the definitions in the remainder we will closely follow [5]. That is why here we only briefly recall, in Sec. II, the definition of the model and give the final expressions, obtained there, for the excess free energy and the Casimir force, which will be our starting expressions for the aims of the current article. In Sec. III we verify the hypotheses, formulated above, for the excess free energy and the Casimir force. In Sec. IV we derive the exact universal values for the Casimir amplitude and the Binder’s cumulant ratio. The paper closes with concluding remarks given in Sec. V.

## II. THE MODEL

We consider the ferromagnetic mean-spherical model (see, e.g., [28,29] for a general review) on a fully finite  $d$ -dimensional hypercubic lattice  $\Lambda_d$  of  $|\Lambda|$  sites and with block geometry  $L_1 \times L_2 \times \dots \times L_d$ , where  $L_i, i = 1, \dots, d$  are measured in units of the lattice spacing. The Hamiltonian has the form

$$\beta \mathcal{H}_{\Lambda}^{\text{b.c.}}(\{\sigma_i\}_{i \in \Lambda}) = -\frac{1}{2} K \sum_{i,j \in \Lambda} J_{ij}^{\text{b.c.}} \sigma_i \sigma_j + s \sum_{i \in \Lambda} \sigma_i^2 - h \sum_{i \in \Lambda} \sigma_i. \quad (8)$$

Here  $\sigma_i \in IR, i \in \Lambda_d$  [ $\sigma_i \equiv \sigma(\mathbf{r}_i)$ ] is a variable, describing the spin on lattice site  $i$  (at  $\mathbf{r}_i$ ),  $s$  is the spherical field,  $K$  is a dimensionless coupling,  $J_{ij}^{\text{b.c.}}$  is a matrix with dimensionless elements, so that  $(K/\beta)J_{ij}^{\text{b.c.}}$  is the exchange energy between the nearest neighbors (under boundary conditions b.c.) spins at sites  $i$  and  $j$  (of course,  $J_{ij}^{\text{b.c.}} = J_{ji}^{\text{b.c.}}$ ), and  $h$  is the external magnetic field. The dependence on the boundary conditions is denoted by a superscript b.c.

The scaling function of the free energy density of the spherical model has been discussed in detail in the literature for different boundary conditions, dimensionalities, and geometries of the system, for both the cases of short as well as for long range interactions in the Hamiltonian [3,29–32]. By any of the approaches used there one can, of course, derive an expression for the excess free energy scaling function. Here, for  $d = 3$  and under periodic boundary conditions we will take it in the form given in [5]:

$$\begin{aligned}
X^{\text{ex}}(x_1, x_2) = & \frac{1}{2}(4\pi)^{-3/2} \left[ \sum_{k=0}^{\infty} \frac{(-1)^k (y_L^{k+1} - y_\infty^{k+1})}{(k+1)!(k-1/2)} \right. \\
& - \sqrt{4\pi} \int_1^\infty dx x^{-2} [1 + 2R(4\pi^2 x)] \exp[-y_L x] \\
& - 2 \int_0^1 dx x^{-5/2} R(1/4x) \exp[-y_L x] \\
& \left. + \int_1^\infty dx x^{-5/2} \exp(-y_\infty x) \right] + \frac{1}{2} x_2^2 \left( \frac{1}{y_\infty} - \frac{1}{y_L} \right) \\
& + \frac{1}{2} x_1 (y_\infty - y_L), \tag{9}
\end{aligned}$$

where

$$R(x) = \sum_{q=1}^{\infty} \exp[-xq^2], \tag{10}$$

$$x_1 = (K - K_c)L, x_2 = K_c^{-1/2} hL^{5/2} \tag{11}$$

are the scaling variables (note the difference in the definitions of  $x_1$  here and in the Introduction; now  $x_1$  decreases when  $T$  increases),

$$K_c = \int_0^\infty dx [\exp(-2x) I_0(2x)]^3 = 0.25273 \dots \tag{12}$$

is the critical coupling, and  $y_L$  and  $y_\infty$  are the solutions of the spherical field equations that follow from Eq. (9) by requiring the first partial derivatives of the right-hand side of Eq. (9) with respect to  $y_L$  and  $y_\infty$  to be zero.

For the finite-size scaling function of the Casimir force one immediately obtains from Eqs. (6), (7), (9) and the definitions of the scaling variables  $x_1$  and  $x_2$  [5]

$$\begin{aligned}
X_{\text{Casimir}}(x_1, x_2) = & 2X^{\text{ex}}(x_1, x_2) - \frac{5}{2} x_2^2 \left( \frac{1}{y_\infty} - \frac{1}{y_L} \right) \\
& - \frac{1}{2} x_1 (y_\infty - y_L). \tag{13}
\end{aligned}$$

Equations (9)–(13) provide the basis of our further analysis.

### III. VERIFICATION OF THE HYPOTHESES

We will prove analytically that the finite-size scaling function of the excess free energy, given by Eq. (9), is a monotonically increasing function of any of its scaling parameters  $x_1$  and  $x_2$  when the other one is kept fixed. First, by using the identity

$$\sum_{k=0}^{\infty} \frac{(-1)^k y^{k+1}}{(k+1)!(k-1/2)} = -\frac{4\sqrt{\pi}}{3} y^{3/2} - \frac{2}{3} y \int_1^\infty x^{-3/2} \exp(-x) dx - \frac{2}{3} [1 - \exp(-y)], \tag{14}$$

the Jacobi identity for the  $R$  function [see Eq. (10)]

$$R(4\pi^2 x) = \frac{1}{2} \left\{ \frac{1}{\sqrt{4\pi x}} \left[ 1 + 2R\left(\frac{1}{4x}\right) \right] - 1 \right\}, \tag{15}$$

and taking into account that

$$\int_0^\infty \frac{dx}{x^{5/2}} R\left(\frac{1}{4x}\right) \exp(-xy) = 4\sqrt{\pi} \{ \sqrt{y} \text{Li}_2[\exp(-\sqrt{y})] + \text{Li}_3[\exp(-\sqrt{y})] \}, \tag{16}$$

after some elementary manipulations we obtain from Eq. (9)

$$X^{\text{ex}}(x_1, x_2) = -\frac{1}{2\pi} \left[ \frac{1}{6} (y_L^{3/2} - y_\infty^{3/2}) + \sqrt{y_L} \text{Li}_2[\exp(-\sqrt{y_L})] + \text{Li}_3[\exp(-\sqrt{y_L})] \right] + \frac{1}{2} x_2^2 \left( \frac{1}{y_\infty} - \frac{1}{y_L} \right) + \frac{1}{2} x_1 (y_\infty - y_L), \tag{17}$$

where  $\text{Li}_p(z)$  are the polylogarithm functions. The main advantage of the above representation of  $X^{\text{ex}}$  is the existence of some nontrivial identities [33,34] for the polylogarithm functions (see next section) that allow the universal constant  $\Delta = X^{\text{ex}}(0,0)$  to be expressed in a simple closed form.

The spherical field equations for  $y_L$  and  $y_\infty$  can be now rewritten in the well known and very simple forms [see, e.g., for  $h=0$ , Eq. (86) in [30]]

$$x_1 = \frac{x_2^2}{y_L^2} - \frac{1}{2\pi} \ln \left[ 2 \sinh \left( \frac{1}{2} \sqrt{y_L} \right) \right], \tag{18}$$

and

$$x_1 = \frac{x_2^2}{y_\infty^2} - \frac{1}{4\pi} \sqrt{y_\infty}, \tag{19}$$

where the first equation is for the finite and the second one for the infinite system, respectively. In order to obtain Eq. (18) use has been made of the facts that  $d\text{Li}_p(x)/dx = \text{Li}_{p-1}(x)/x$  and  $\text{Li}_1(x) = -\ln(1-x)$ . Let us denote by  $g_L(x_2, y_L)$  the right-hand side of Eq. (18) and by  $g_\infty(x_2, y_\infty)$  the right-hand side of Eq. (19). Then, it is easy to see that

$$g_L(x_2, y) = g_\infty(x_2, y) - \frac{1}{2\pi} \ln[1 - \exp(-\sqrt{y})]. \quad (20)$$

From the above equation and having in mind that in Eqs. (18) and (19)  $y_L > 0, y \geq 0$  we conclude that

$$g_L(x_2, y) > g_\infty(x_2, y). \quad (21)$$

It is also elementary to verify that  $g_L(x_2, y_L)$  and  $g_\infty(x_2, y_\infty)$  are monotonically decreasing functions of  $y_L$  and  $y_\infty$ , respectively. Let now  $y_\infty(x_1, x_2)$  be the solution of Eq. (19) for given  $x_1$  and  $x_2$ . Then, from Eq. (21), the fact that  $g_L(x_2, y)$  is a monotonically decreasing function of  $y$ , and that for the solution  $y_L(x_1, x_2)$  of Eq. (18) one should have  $g_L(x_2, y_L) = g_\infty(x_2, y_\infty)$ , we obtain

$$y_L(x_1, x_2) > y_\infty(x_1, x_2). \quad (22)$$

We are now ready to deal with the monotonicity properties of the excess free energy scaling function. From Eq. (17) and having in mind the spherical field equations (18) and (19) we derive

$$\frac{\partial X^{\text{ex}}}{\partial x_1} = -\frac{1}{2}(y_L - y_\infty) \quad (23)$$

and

$$\frac{\partial X^{\text{ex}}}{\partial x_2} = -x_2 \left( \frac{1}{y_L} - \frac{1}{y_\infty} \right). \quad (24)$$

From these expressions and Eq. (22), taking into account the definitions of the scaling variables (11), we obtain that the excess free energy scaling function is a monotonically increasing function of both the temperature  $T$  and the magnetic field  $|H|$ . As a function of the finite size  $L$  of the system the scaling function is monotonically increasing above and decreasing below  $T_c$ . These properties of the scaling function as a function of the scaling variables  $x_1$  and  $x_2$  are illustrated in Fig. 1. One clearly sees that for any fixed  $x_2$  the scaling function is a monotonically decreasing function of  $x_1$ , and, for any fixed  $x_1$  a monotonically increasing function of  $|x_2|$ . Finally, it is worth mentioning that, for  $x_2 = 0$  from Eqs. (17) and (22), it immediately follows that  $X^{\text{ex}} < 0$ . From Fig. 1 one observes that this is true also for  $x_2 \neq 0$ .

We turn now to properties of the Casimir force. Our aim is to show that the force is negative under periodic boundary conditions for any values of  $T$  and  $H$ . The finite-size behavior of the Casimir force in the vicinity of the critical point is given by Eq. (6) where the scaling function is given by Eq. (13). For  $T < T_c$  the same expressions are actually valid with the only difference that the definition of the variable  $x_2$  now should be  $x_2 = K^{-1/2}hL^{5/2}$  and  $x_1 \gg 1$ . Here we are not going to discuss if then the above expressions can be simplified further, e.g., being a function of a given combination of  $x_1$

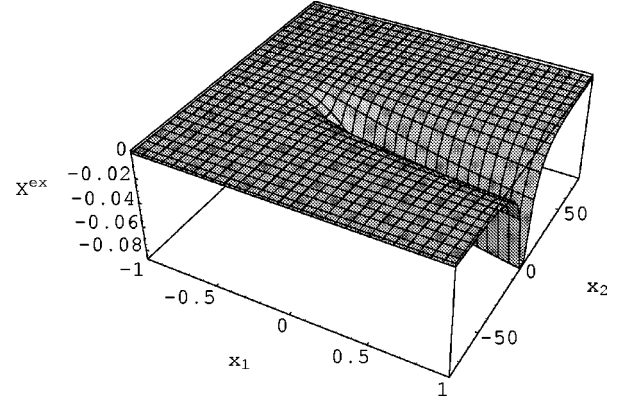


FIG. 1. The universal finite-size scaling function of the excess free energy  $X^{\text{ex}}$  as a function of the scaling variables  $x_1 = L(K - K_c)/K_c$  and  $x_2 = K_c^{-1/2}hL^{5/2}$ . For a better visualization of the properties of  $X^{\text{ex}}$  we have allowed  $h$  to change its sign. Of course,  $X^{\text{ex}}$  is a symmetric function of  $x_2$ .

and  $x_2$ , as is usually the case of first order phase transitions [35]. For  $T$  way above  $T_c$  the Casimir force, as shown in [5], tends to zero exponentially fast with  $L$  in full accordance with the general expectations about its behavior above the critical point. We will not be interested in the explicit form of these exponentially small corrections. Having in mind all these comments, for the behavior of the Casimir force for any  $T$  and  $H$  one obtains explicitly

$$f_{\text{Casimir}}(t, h, L) = L^{-3} \left\{ \frac{3}{2} x_2^2 \left( \frac{1}{y_L} - \frac{1}{y_\infty} \right) - \frac{1}{2} x_1 (y_L - y_\infty) - \frac{1}{\pi} \left[ \frac{1}{6} (y_L^{3/2} - y_\infty^{3/2}) + \sqrt{y_L} \text{Li}_2[\exp(-\sqrt{y_L})] + \text{Li}_3[\exp(-\sqrt{y_L})] \right] \right\}. \quad (25)$$

Since the inequality (22) is still valid, from the above expression it immediately follows that  $f_{\text{Casimir}}(t, h) < 0$ . Numerical evaluation of the behavior of the finite-size scaling function of the Casimir force has been given in [5]. It is in full agreement with our analytical result. Finally we show that for  $T < T_c$  and  $h = 0$ , i.e.,  $x_1 > 0$  and  $x_2 = 0$ , the Casimir force is a monotonically increasing function of the temperature, i.e., a monotonically decreasing function of  $x_1$ . From Eq. (25) and taking into account that  $y_\infty = 0$  when  $T < T_c$  we obtain

$$\frac{d}{dx_1} X_{\text{Casimir}}(x_1, 0) = -\frac{1}{2} y_L + \frac{1}{2} x_1 \frac{dy_L}{dx_1}. \quad (26)$$

From Eq. (18) it is easy to see that  $dy_L/dx_1 < 0$ , and, therefore  $dX_{\text{Casimir}}(x_1, 0)/dx_1 < 0$ , i.e., the Casimir force is an increasing function of  $T$  for  $T < T_c$  and  $h = 0$ .

In this way we have completely verified the hypotheses formulated in the introductory part of the article for the behavior of the excess free energy and the Casimir force.

#### IV. CASIMIR AMPLITUDE, C FUNCTION, AND BINDER'S CUMULANT RATIO

Here we will be interested in the properties of the system at its bulk critical point. This implies  $x_1 = x_2 = 0$  with a solution of the spherical field equations [see Eqs. (19) and (18)]  $y_\infty = 0$  and  $y_L \equiv y_{L,c} = 4 \ln^2[(1 + \sqrt{5})/2]$  (this value of  $y_{L,c}$  is well known and seems to have been derived for the first time in [36]). The problem of determination of the Casimir amplitude reduces now to exact evaluation of the expression

$$X^{\text{ex}}(0,0) = -\frac{1}{2\pi} \left[ \frac{1}{6} y_{L,c}^{3/2} + \sqrt{y_{L,c}} \text{Li}_2[\exp(-\sqrt{y_{L,c}})] + \text{Li}_3[\exp(-\sqrt{y_{L,c}})] \right]. \quad (27)$$

Denoting by  $\tau$  the ‘‘golden mean,’’ i.e.,  $\tau = (1 + \sqrt{5})/2$ , it is easy to show that

$$\exp(-\sqrt{y_{L,c}}) = \tau^{-2} = 2 - \tau, \quad (28)$$

which reduces the above problem for  $X^{\text{ex}}(0,0)$  to the problem for evaluation of the expression

$$a = \text{Li}_3(2 - \tau) - \ln(2 - \tau) \text{Li}_2(2 - \tau) - \frac{1}{6} \ln^3(2 - \tau). \quad (29)$$

Fortunately, this is exactly the problem solved by Sachdev [34] studying his example of a conformal field theory in three dimensions. By the help of some polylogarithm identities he has shown that  $a = 4\zeta(3)/5$ . Therefore, we obtain for the Casimir amplitude of the three dimensional spherical model under periodic boundary conditions

$$\Delta = -\frac{2\zeta(3)}{5\pi} \approx -0.153\,051. \quad (30)$$

The numerical value of this amplitude has already been reported in [5]. Recalling now that  $-X^{\text{ex}}(0,0)$  corresponds to the analog of the  $C$  function for our model and taking the normalization factor in the form that will keep the  $C$  function of the critical Gaussian model to be  $C = 1$  for any  $d$  (i.e., by taking the normalization in the form for bosons) we conclude that the ‘‘ $C$  function of the spherical model’’ is  $4/5$  (at  $T = T_c$  for  $d = 3$  under periodic boundary conditions).

Let us turn now to a determination of the Binder's cumulant ratio for the considered model. We will use for it the definition of the form [3] (up to a prefactor  $1/3$ )

$$B_L = -L^{-d} \frac{\chi^{(4)}(t, h=0, L)}{3\chi^{(2)}(t, h=0, L)}, \quad (31)$$

where  $\chi^{(n)}$  means the  $n$ th derivative with respect of  $h$  of the free energy density at  $h = 0$  (of course,  $\chi^{(2)} = -\chi$ , where  $\chi$  is the susceptibility of the system). In the vicinity of the critical point this expression can be rewritten in the form

$$B_L(x_1) = -\frac{1}{3} \left\{ \frac{\partial^4 X(x_1, x_2) / \partial x_2^4}{[\partial^2 X(x_1, x_2) / \partial x_2^2]^2} \right\}_{x_2=0}, \quad (32)$$

where  $X(x_1, x_2)$  is the finite-size scaling function of the free energy density. The exact form of this function follows from Eq. (17) just by omitting the terms depending on  $y_\infty$  in it, i.e.,

$$X(x_1, x_2) = -\frac{1}{2\pi} \left[ \frac{1}{6} y_L^{3/2} + \sqrt{y_L} \text{Li}_2[\exp(-\sqrt{y_L})] + \text{Li}_3[\exp(-\sqrt{y_L})] \right] - \frac{1}{2} \frac{x_2^2}{y_L} - \frac{1}{2} x_1 y_L. \quad (33)$$

From the above expression at the critical point it immediately follows that

$$B \equiv B_L(x_1 = 0) = - \left[ 2y_{L,c}^{-1} \left( \frac{\partial y_L}{\partial x_2} \right)^2_{x_1=x_2=0} - \left( \frac{\partial^2 y_L}{\partial x_2^2} \right)_{x_1=x_2=0} \right]. \quad (34)$$

By subsequent differentiation of the spherical field equation for the finite system (18) it is easy to show that at the critical point  $\partial y_L / \partial x_2 = 0$ , whereas

$$\left( \frac{\partial^2 y_L}{\partial x_2^2} \right)_{x_1=x_2=0} = \frac{16\pi}{y_{L,c}^{3/2} \coth(\sqrt{y_{L,c}}/2)}. \quad (35)$$

Combining these results and having in mind that  $y_{L,c} = 4 \ln^2 \tau$  we obtain for the Binder's cumulant ratio at the critical point

$$B = \frac{2\pi}{\sqrt{5} \ln^3 \tau} \approx 25.216\,57. \quad (36)$$

Having the exact solution for the spherical field equation and such a simple form for the free energy density, one can easily determine in an exact manner the behavior of other physically interesting quantities at  $T = T_c$ . For example, it is easy to show that the specific heat is of the form

$$c_L(T_c) = \frac{1}{2} - L^{-1} \frac{16\pi}{\sqrt{5}} K_c^2 \ln \tau, \quad (37)$$

and that the critical finite-size correlation length is ( $\xi_L = L / \sqrt{y_L}$  [32,37])

$$\xi_L(T_c) = \frac{1}{2 \ln \tau} L \quad (38)$$

(for explicit results of the behavior of  $\xi_L$  under other geometries, boundary conditions and long ranges of the spin-spin interactions see [32,37–39]).

#### V. CONCLUDING REMARKS

In the present paper we present a hypothesis that in the vicinity of the bulk critical temperature  $T_c$  of  $O(n)$ ,  $n \geq 2$ ,

systems with a film geometry  $L \times \infty^{d-1}$  the excess free energy (due to the finite size of the system) will be, under periodic boundary conditions, a monotonically increasing function of the temperature and the magnetic field if the finite system does not undergo a real phase transition of its own (i.e., when  $d \leq 3$  for systems with short-range interactions). As a function of the finite size  $L$  of the system the finite size scaling function of the excess free energy is expected to be monotonically increasing above and decreasing below  $T_c$ . This hypothesis, together with the hypothesis that the Casimir force should be negative under periodic boundary conditions have been verified *analytically* on the example of the three-dimensional mean spherical model. It has been shown that the force is negative in the whole region of the thermodynamic parameters. In addition the universal Casimir amplitude  $\Delta_{\text{per}}$  and the Binder's cumulant ratio have been determined exactly in a simple close form and found to be  $\Delta_{\text{per}} = -2\zeta(3)/(5\pi) \approx -0.153\,051$  and  $B = 2\pi/\{\sqrt{5}\ln^3[(1+\sqrt{5})/2]\} \approx 25.216\,57$ . For comparison we give the corresponding result for the Ising universality class,  $\Delta_{\text{per}} = -0.1526 \pm 0.0010$  [23], and  $B = 0.615 \pm 0.003$  [40,41] obtained by Monte Carlo calculations. As we see, the value for the Casimir amplitude for the spherical model is *surprisingly close* (within the error bar) to the value reported above for the Ising model. The vast difference for the cumulant ratio indicates the lack of a real phase transition in the three dimensional spherical model film in comparison with the Ising-like films. Actually, in three-dimensional Ising films the situation is more complicated [42]. If the thickness of the film  $L$  is held constant and the other two linear dimensions  $D$  tend to infinity, the cumulant ratio converges to the two-dimensional Ising value ( $B = 0.615$ ). However, if the ratio  $L/D$  is not too small, there exist crossover problems. In any case the value of  $B$  is between that for the two-dimensional system and that for the three-dimensional system ( $B = 0.47$  [43]). The value of  $B$  for the spherical model shows that the probability distribution at  $T_c$  of the order parameter density is too different from a single Gaussian, where  $B = 0$ , or from a normalized sum of two Gaussians, where  $B = 2/3$ . This, of course, raises the question what then that distribution is, but this question is out of the scope of the current article. The situation recalls the one of Ising strips (no real phase transition in the system) with  $B = 2.46044 \pm 0.00006$  [3,40,44]. The crossover problems in Binder's cumulant ratio can be studied within the spherical model, considering a  $3 + \varepsilon$  dimensional film,  $\varepsilon > 0$  (then in the finite system there will be a real phase transition). This is also an interesting problem, especially if one takes into account that there are almost no exact results for the Binder's cumulant ratio, but it is again out of the scope of the current article.

The results reported in the current investigation are in full agreement with the predictions of the finite-size scaling theory. Equations (17), (18), (19), (25), and (33) give the *universal* finite-size scaling function of the excess free energy, Casimir force, and free energy density. It should be, however, emphasized that in contrast to the Ising-like case the excess free energy, and, therefore, the Casimir force in the absence of an external field tend to zero below  $T_c$  not in

an exponential in  $L$  way. For example, the finite-size scaling functions of the excess free energy and Casimir force tend to a constant below  $T_c$  [see Eq. (31) in [5]]. The explanation of this behavior, which, we believe, is common for all  $O(n), n \geq 2$ , models, is based on the fact that due to the existence of soft modes in the system (spin waves) below  $T_c$  and in the absence of an external field ( $h=0$ )  $\xi_b$  is identically infinite. If an external field is applied ( $h \neq 0$ ) then  $\xi_b < \infty$ , and, of course,  $f^{\text{ex}} \rightarrow 0$  again exponentially fast in  $L$ .

Finally, it is worth mentioning the close parallel that exists between the properties of the  $C$  function defined by Netto and Fradkin [7], see also Zabzin [8], for a  $d$ -dimensional quantum system as a function of the temperature  $T$  and the properties of the excess free energy scaling function  $-X^{\text{ex}}$  of the corresponding classical system as a function of  $L^{-1}$ . If in the finite system a real phase transition does not exist, and if the system is somehow equivalent to the  $O(n), n > 2$ , system we have proposed some arguments that  $-X^{\text{ex}}$  is a monotonically increasing as a function of  $L^{-1}$  above  $T_c$  and decreasing below  $T_c$ . We would expect the same to be true for the  $C$  function of the corresponding quantum system as a function of  $T$  around its quantum critical point. If the classical system is equivalent to some Ising-type model, the same type of arguments we have used for the  $O(n), n > 2$ , models, taking into account the lack of monotonicity of the correlation length in the vicinity of  $T_c$ , lead to the hypothesis that  $-X^{\text{ex}}$  will be a monotonic function of  $L^{-1}$  both below and above  $T_c$ . For the corresponding  $C$  function of a quantum system that has its mapping into a classical Ising system (according to the dimensional crossover rule) this means that  $C$  is a monotonically increasing function of the temperature both below and above its quantum critical point. This is indeed the case plotted in Fig. 2 in [7] for the quantum version of the two-dimensional Ising model. Finally we would like to stress that the relatively simple picture described here should probably change significantly, if the finite system undergoes a phase transition of its own. In that case the upper critical part of the excess free energy scaling function for  $4 - \varepsilon$  Ising model is known [20] (up to a first order in  $\varepsilon, \varepsilon > 0$ ). It shows a *minimum* in  $X^{\text{ex}}$ , as a function of  $T$  *slightly above*  $T_c$ . Unfortunately, no results are available for  $X^{\text{ex}}$  when  $T < T_{c,L}$ , where  $T_{c,L}$  is the shifted critical temperature of the finite system. It is possible to investigate the above problems exactly within the spherical model with  $3 + \varepsilon$  infinite dimensions. We hope to return to this problem later.

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