

# Finite-Size Dependence of the Helicity Modulus within the Mean Spherical Model

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The validity of the finite-size scaling prediction about the existence of logarithmic corrections in the helicity modulus  $\Upsilon$  of three-dimensional  $O(n)$ -symmetric order parameter systems in confined geometries is studied for the three-dimensional mean spherical model of geometry  $L^{3-d'} \times \infty^{d'}$ ,  $0 \leq d' < 3$ . For a fully finite geometry the general case of  $d_p \geq 0$  periodic,  $d_a \geq 0$  antiperiodic,  $d_0 \geq 0$  free, and  $d_1 \geq 0$  fixed ( $d_p + d_a + d_0 + d_1 = d$ ,  $d = 3$ ) boundary conditions is considered, whereas for film ( $d' = 2$ ) and cylinder ( $d' = 1$ ) geometries only the case of antiperiodic and/or periodic boundary conditions is investigated. The corresponding expressions for the finite-size scaling function of the helicity modulus and its asymptotics in the vicinity, below, and above the bulk critical temperature  $T_c$  and the shifted critical temperature  $T_{c,L}$  are derived. The obtained results are not in agreement with the hypothesis of the existence of a  $\log(L)$  correction term to the finite-size behavior of the helicity modulus in the finite-size critical region if  $d = 3$ . In the case of film and cylinder geometries there are no logarithmic corrections. In the case of a fully finite geometry a universal logarithmic correction term  $-[(d_0 - d_1)/4\pi + 2^{d_a-1}/\pi^2] \ln L/L$  is obtained only for  $(T_c - T)L \gg \ln L$ .

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## 1. INTRODUCTION

The standard finite-size scaling form for the singular part of the free energy density (per  $k_B T$  and per site) of a hypercubic lattice system with a characteristic finite size  $L$  (where  $L$  is measured in units of an appropriate

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microscopic length, which here is taken to be the lattice spacing) near the critical temperature  $T_c$  (of the corresponding bulk, i.e.,  $L = \infty$ ) system is<sup>(1)</sup>

$$f_{\text{sing}} \approx L^{-d} X(atL^{1/\nu}) \quad (1.1)$$

where  $t = (T - T_c)/T_c$  is the reduced temperature,  $a$  is a nonuniversal scaling factor,  $X$  is a universal (usually geometry-dependent) scaling function, and  $\nu$  is the correlation length scaling exponent. (For brevity we consider the dependence on only one thermodynamic variable.) When nonperiodic boundary conditions are imposed on the system there are also “background” terms, which depend on the shape of the system and which are expected to be of the form

$$f_{\text{bg}} \approx \phi_d(t) + \phi_{d-1}(t)/L + \dots + \phi_0/L^d + o(L^{-d}) \quad (1.2)$$

where the  $\phi_d$  term corresponds to the bulk contribution,  $\phi_{d-1}$  corresponds to the surface one, etc., and the last term in Eq. (1.2) corresponds to the corners (or curvature) of the system. (The functions  $\phi_j$ ,  $j=0, \dots, d$ , are supposed to be regular at  $t=0$ .) It was argued by Privman<sup>(2)</sup> (for reviews see refs. 3 and 4) that when  $d$  is integer, due to the equal exponents of the  $1/L^d$  “scaling” term [given by Eq. (1.1)] and the corresponding contribution from the “background” term [see Eq. (1.2)], one additional so-called “resonant” logarithmic term appears:

$$f_{\text{res}} \approx u \ln L/L^d \quad (1.3)$$

where  $u$  is a universal amplitude. The mechanism of the emergence of this logarithmic term is reminiscent of the one which is anticipated for the appearance of a logarithmic specific heat in the bulk system when the critical exponent  $\alpha$  tends to zero: when  $d$  passes through integer values, “resonant” poles develop in the finite-size scaling function  $X$  and in the amplitude  $\phi_0$ , conspiring so that the logarithmic term in Eq. (1.3) emerges. In fact such logarithmic terms were derived first by conformal invariance arguments<sup>(5)</sup> at  $t=0$  in  $d=2$ . (For a review of the results available in  $d=2$  see Ref. 3.) For  $d > 2$  the above predictions were tested in the framework of a few exactly soluble models, namely in a Gaussian-type model,<sup>(6,7)</sup> in the constrained monomer–dimer model,<sup>(8)</sup> and in the mean spherical model with free<sup>(9)</sup> and fixed<sup>(10)</sup> boundary conditions (for short reviews of the corresponding results see the introductory parts in refs. 8 and 10). Logarithmic corrections were found in the finite-size behavior of the interfacial free energy.<sup>(3,7)</sup> It was shown, for example (for a general review of sizes effects on interfacial properties see ref. 3), that in the capillary-wave Gaussian-type model the singular part (per  $k_B T$ ) of the interfacial free

energy density (where the interface is created by applying controlled surface fields, fixing its mean position) has the form<sup>(7)</sup>

$$f_{\text{singular part}}^{(\text{interface})}(T; L) = f_{d-1}(T) + f_{d-2}(T)/L + \dots - 2^{d-1} \ln L/L^{d-1} + \dots \quad (1.4)$$

at any fixed  $T < T_c$  as  $L \rightarrow \infty$ . As it is shown, a *universal* logarithmic term is again present, even though at any fixed  $T$  the functions  $f_k$  are *not* universal (for more details see ref. 7). An extension of the above ideas to the helicity modulus  $Y$  of  $O(n)$ -vector models with  $n \geq 2$  was proposed by Privman.<sup>(11)</sup> Heuristically, the helicity modulus is the analog of the interface tension for  $O(n)$ -symmetric systems; for a short discussion on possible formal definitions of  $Y$  in finite systems, see Section 2 below. In the framework of the hyperuniversal finite-size scaling it is expected that for  $d_l < d < d_u$  (where  $d_l = 2$  and  $d_u = 4$  are the lower and the upper critical dimensions for this class of systems, respectively) in a finite system with characteristic dimension  $L$  the singular part (as  $L \rightarrow \infty$ ) of the helicity modulus [due to the hyperscaling the critical exponent of  $Y$  describing its temperature dependence is equal to  $(d-2)v^{(12)}$ ] has the form

$$Y_{\text{singular part}}(T; L) \approx L^{2-d} Y(atL^{1/v}) \quad (1.5)$$

where  $Y$  is a universal scaling function. The corresponding background term is expected to be of the general form given by Eq. (1.2) (with  $\phi_d \equiv 0$ ) and so, when  $d$  passes through  $d = 3$ , one resonant logarithmic term could appear, i.e., one could expect<sup>(11)</sup>

$$Y_{d=3}(T; L) = L^{-1} [\tilde{Y}(atL^{1/v}) + \omega \ln L] + \tilde{\phi}_2(t)/L + \phi_1(t)/L^2 + \dots \quad (1.6)$$

Here the new scaling function  $\tilde{Y}$  and the amplitude  $\omega$  are supposed to be universal, whereas the metric factor  $a$  is nonuniversal. To derive Eq. (1.6), the same mechanism (as for the free energy density) of the emergence of the logarithmic contributions is supposed to work here, i.e., as  $d \rightarrow 3$ , poles develop in  $\phi_2(t)$  and in the scaling function  $Y$  conspiring to yield the new logarithmic term at  $d = 3$ . Since the  $L$  dependence has to drop out in the thermodynamic limit, we immediately obtain the leading asymptotic term of the scaling function  $\tilde{Y}$  for large negative arguments,

$$\tilde{Y}(x \rightarrow -\infty) \simeq y_{-\infty} |x|^v \quad (1.7)$$

where  $y_{-\infty}$  is a universal amplitude. Actually, in the original formulation due to Privman<sup>(11)</sup> it is supposed that

$$\tilde{Y}(x \rightarrow -\infty) = y_{-\infty} |x|^v - v\omega \ln |x| + O(1) \quad (1.8)$$

and so, when  $t < 0$  and  $tL^{1/\nu} \rightarrow -\infty$ ,

$$Y \simeq y_{-\infty} a^\nu |t|^\nu - \frac{\nu\omega \ln |t| + O(1)}{L} \quad (1.9)$$

Expressions similar to (1.8) and (1.9) are supposed to hold when  $t > 0$  and  $L \rightarrow \infty$ , but with  $y_\infty = 0$ . We would like to mention that only the presence of the first term on the right-hand side of Eq. (1.8) is necessary in order to keep the agreement with the thermodynamic behavior of  $Y$  when  $t \rightarrow 0^-$ . The next two terms follow from the tacit assumption that the behavior of  $Y$  away from  $T_c$  will be given by the expression similar to that on the right-hand side of Eq. (1.2) [but, of course, with  $\phi_d(t) = 0$  for  $t > 0$ ], i.e., no logarithmic term will present away from  $T_c$ . As we have seen above, this is not true for the interfacial free energy<sup>(7)</sup> ( $t < 0$ ) and a precaution to treat the case of systems with “soft” modes and below  $T_c$  more carefully was first stated in ref. 2.

Finally, we would like to mention that in the case of superfluids ( $n=2, d=3$ ) the helicity modulus  $Y$  is proportional<sup>(12)</sup> to the superfluid density fraction  $\rho$  [ $\rho = (m/\hbar)^2 Y(T)$ , where  $m$  is the mass of the helium atom] and is directly measurable (for experiments measuring  $\rho$  for  $^4\text{He}$  in confined geometries see refs. 13 and 14). In fact, the new finite-size corrections to the behavior of the helicity modulus were proposed by Privman in an attempt to improve the fit of the experimental data.<sup>(11)</sup> But it turns out that the overall fit of the data is improved only in a limited way,<sup>(11)</sup> provided one insists on the bulk value of  $\nu$  in the scaling combination  $atL^{1/\nu}$  (the scaling “data collapse” technique works well if one takes  $\nu$  as an adjustable parameter which is not necessarily equal to the correlation length exponent). It also should be emphasized that one could expect additional complexity in the behavior of the finite-size scaling function of the helicity modulus in the case of superfluid transitions in a film geometry; nevertheless, the analysis of the experimental data shows no clear singularities or a jump in the finite-size scaling function.<sup>(13,14)</sup>

Summarizing, it seems desirable to investigate in more detail the finite-size behavior of the helicity modulus. The author is not aware of any theoretical check of the new finite-size scaling predictions about the existence of the logarithmic term in the behavior of the helicity modulus. This work is an attempt to elucidate the situation in the framework of an exactly soluble model, namely in the mean spherical model.

The paper is organized as follows. In Section 2 we give a definition of the helicity modulus in a finite system under different boundary conditions and in Section 3 we present convenient starting expressions for its investigation in the framework of the mean spherical model. The method

of analysis of the helicity modulus and of the mean spherical constraint for a large, but finite system in two critical regimes, as well as below and above the critical temperature, is described in Section 4. The results for the asymptotic behavior of the solution of the mean spherical constraint, for the scaling function of  $Y$ , and for the corresponding logarithmic corrections are obtained in Section 5. The paper closes with a discussion in Section 6.

## 2. DEFINITION OF THE HELICITY MODULUS IN A FINITE SYSTEM

The concept of the helicity modulus was introduced by Fisher *et al.*<sup>(12)</sup> Fundamentally, the helicity modulus is a measure of the response of the system to a helical or “phase-twisting” field. Alternatively, for an isotropic system with  $n$ -component order parameter ( $n \geq 2$ ), one can consider the helicity modulus to be the analogy of the surface tension or interfacial free energy between two phases in a system with a scalar ( $n = 1$ ) order parameter (e.g., an Ising model).

Let us consider a  $d$ -dimensional  $O(n)$ -symmetric order parameter system with a geometry  $L_1 \times L_2 \times \dots \times L_d$  and boundary conditions  $\tau_i$  imposed across the direction  $L_i$  ( $i = 1, \dots, d$ ). Then, following ref. 12, we can rewrite the usual definition of  $Y$  in the form

$$\frac{1}{2} \beta Y(T) = \lim_{L_1 \rightarrow \infty} \frac{L_1^2}{\pi^2} \left\{ \lim_{L_2 \rightarrow \infty} \dots \lim_{L_d \rightarrow \infty} [f_{\tau_a}(T; \mathbf{L}) - f_{\tau_p}(T; \mathbf{L})] \right\} \quad (2.1)$$

where  $\beta = (k_B T)^{-1}$ ,  $\mathbf{L} \equiv (L_1, \dots, L_d)$ ,  $f_{\tau}(T; \mathbf{L})$  is the free energy density of the system with boundary conditions  $\tau \equiv \{\tau_1, \dots, \tau_d\}$ , and  $\tau_a$  and  $\tau_p$  are sets of boundary conditions, which differ from each other *only* in that the periodic boundary conditions applied across the direction  $L_1$  in  $\tau_p$  are replaced with antiperiodic ones in  $\tau_a$ . Keeping the meaning of the helicity modulus as a quantity associated with the free energy increase due to the order parameter orientational gradients,<sup>(11)</sup> it seems reasonable to define the helicity modulus in a finite system  $Y_{\tau'}(T; \mathbf{L})$  using the following straightforward extension of the “bulk” definition given by Eq. (2.1):

$$Y_{\tau'}(T; \mathbf{L}) = \frac{2L_1^2}{\beta\pi^2} [f_{\tau_a}(T; \mathbf{L}) - f_{\tau_p}(T; \mathbf{L})] \quad (2.2)$$

where  $\tau' \equiv \tau \setminus \{\tau_1\}$ .

Note that even in the defining equation (2.1) of  $Y(T)$  [where  $Y(T)$  is supposed to be independent of the boundary conditions  $\tau'$ ] the properties of the free energy density of two finite systems (with periodic and

antiperiodic boundary conditions across one of the axes) are essentially used. The definition given by Eq. (2.1) has been employed to calculate the helicity modulus for the spherical model<sup>(15)</sup> and for the ideal Bose gas.<sup>(16)</sup> Using  $(+, -)$  and  $(+, +)$  boundary conditions instead of antiperiodic and periodic ones [or, of course,  $(+, -)$  and  $(-, -)$ ], an alternative definition of  $\Upsilon$  is possible (see ref. 12 for more details). Then its extension to a finite system [in a way similar to the one used in (2.2)] will lead to another definition  $\tilde{\Upsilon}_{\tau}(T; \mathbf{L})$  of the helicity modulus in finite systems. While for  $\Upsilon(T)$  it is believed that it will not depend on the boundary conditions, using any of these definitions, for the corresponding finite-size quantities  $\Upsilon_{\tau}(T; \mathbf{L})$  and  $\tilde{\Upsilon}_{\tau}(T; \mathbf{L})$  this obviously will not be true. Furthermore, it is not clear *a priori* that  $\Upsilon_{\tau}(T; \mathbf{L})$  and  $\tilde{\Upsilon}_{\tau}(T; \mathbf{L})$  will have (if at all) the same logarithmic corrections. Note, for example, that if the boundary conditions of the  $(+, +)$  type are imposed in one direction of the system with otherwise free or fixed boundary conditions, this system will have corners, which are another possible source of logarithmic corrections<sup>(2)</sup> [the logarithmic corrections stemming from corners of the corresponding system with  $(+, -)$  boundary conditions may then well differ from those ones of the “ $(+, +)$ ” system and so additional logarithmic corrections due to corners could appear in  $\tilde{\Upsilon}_{\tau}(T; \mathbf{L})$ ]. Finally, it should be emphasized that while antiperiodic boundary conditions will create a diffuse interface whose mean position is not fixed (“floating periodic diffuse interface”), the  $(+, -)$  ones will fix it in the middle of the direction across which they are imposed. As is shown in ref. 7, for the interfacial free energy the universal constant multiplying the logarithmic correction terms could depend also on such features of the system.

So, different extensions of the “bulk” definition (2.1) of the helicity modulus are possible. Generally speaking they will lead to different finite-size corrections. It seems that (2.2) represent one reasonable variant of such a definition.

In what follows we will use the expression (2.2) as a definition of the helicity modulus in a finite system. According to this definition, the helicity modulus in a finite system is a measure of the increase of the free energy of an  $O(n)$  system due to the order parameter orientational gradient created by antiperiodic boundary conditions.

### 3. THE MODEL

We consider the ferromagnetic mean spherical model (see, e.g., refs. 15 and 17) on a fully finite  $d$ -dimensional hypercubic lattice  $A_d \in \mathbb{Z}^d$  of  $|A|$  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 (in the absence of an external field)

$$\beta \mathcal{H}_A^\tau(\{\sigma_i\}_{i \in A}) = -\frac{1}{2}K \sum_{i,j \in A} J_{ij}^\tau \sigma_i \sigma_j + s \sum_{i \in A} \sigma_i^2 \quad (3.1)$$

Here  $\sigma_i \in \mathbb{R}$ ,  $i \in A_d$  [ $\sigma_i \equiv \sigma(\mathbf{r}_i)$ ] is a variable, describing the spin on lattice site  $i$  (at  $\mathbf{r}_i$ ),  $s$  is the spherical field,  $K$  is a dimensionless coupling, and  $J_{ij}^\tau$  is a matrix with dimensionless elements, so that  $(K/\beta) J_{ij}^\tau$  is the exchange energy between the spins at sites  $i$  and  $j$  (of course,  $J_{ij}^\tau = J_{ji}^\tau$ ). The dependence on the boundary condition is denoted by a superscript  $\tau$ .

In the mean spherical ensemble the partition function is given by

$$Z_d^{(\tau)}(K, s; \mathbf{L}) = \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} \prod_{i \in A} d\sigma_i \exp[-\beta \mathcal{H}_A^\tau(\{\sigma_i\}_{i \in A})] \quad (3.2)$$

Then the canonical free energy [in units of  $(k_B T)^{-1}$ ]  $F_d^{(\tau)}(K; \mathbf{L})$  is defined by the Legendre transformation

$$F_d^{(\tau)}(K; \mathbf{L}) = \sup_s [-\ln Z_d^{(\tau)}(K, s; \mathbf{L}) - s |\mathbf{A}|] \quad (3.3)$$

Let us now suppose that periodic boundary conditions are applied in the "first"  $d_p$  directions  $L_i, i = 1, \dots, d_p$  ( $d_p \geq 0$ ), antiperiodic ones in the next  $d_a$  directions  $L_i, i = d_p + 1, \dots, d_p + d_a$  ( $d_a \geq 0$ ), free in the following  $d_0$  directions  $L_i, i = d_p + d_a + 1, \dots, d_p + d_a + d_0$  ( $d_0 \geq 0$ ), and fixed in the remainder  $d_1$  ( $d_1 = d - d_p - d_a - d_0, d_1 \geq 0$ ) directions. Under the considered set of boundary conditions and for nearest neighbor interaction ( $J_{ij}^\tau = 1$  if  $i$  and  $j$  are nearest neighbors under the applied set of boundary conditions, and zero otherwise) the eigenvalues  $\tilde{J}^{(\tau)}(\mathbf{k})$  of the matrix  $J_{ij}^\tau$  are well known (see, e.g., ref. 7)

$$\begin{aligned} \tilde{J}^{(\tau)}(\mathbf{k}) &\equiv \tilde{J}(\mathbf{k} | d_p, d_a, d_0, d_1) \\ &= 2 \sum_{i=1}^{d_p} \cos\left(\frac{2\pi k_i}{L_i}\right) + 2 \sum_{i=d_p+1}^{d_p+d_a} \cos\left(\frac{\pi(2k_i+1)}{L_i}\right) \\ &\quad + 2 \sum_{i=d_p+d_a+1}^{d_p+d_a+d_0} \cos\left(\frac{\pi k_i}{L_i}\right) + 2 \sum_{i=d_p+d_a+d_0+1}^{d_p+d_a+d_0+d_1=d} \cos\left(\frac{\pi(k_i+1)}{L_i+1}\right) \end{aligned} \quad (3.4)$$

where  $\mathbf{k} \equiv (k_1, \dots, k_d)$ ;  $k_i = 0, \dots, L_i - 1$ ;  $i = 1, \dots, d$ .

It is convenient to replace the spherical field  $s$  by another field  $\lambda^{(\tau)}$ , defined as

$$\lambda^{(\tau)} = 2s/K - \tilde{J}_{\max}^{(\tau)} \quad (3.5)$$

where  $\tilde{J}_{\max}^{(\tau)} = \max_{\mathbf{k}} \tilde{J}^{(\tau)}(\mathbf{k})$ . As it is clear from (3.4), due to the presence of antiperiodic boundary conditions the maximal eigenvalue of the matrix  $J_{ij}^{\tau}$  is  $2^{d_a}$ -fold degenerate.

Performing now the integration in (3.3), we obtain

$$\begin{aligned} \frac{1}{|A|} F_A^{(\tau)}(K) &\equiv f_A^{(\tau)}(K) \\ &= \sup_{\lambda^{(\tau)}} \left\{ \frac{1}{2|A|} \sum_{\mathbf{k}} \ln[\lambda^{(\tau)} + \Delta^{(\tau)}(\mathbf{k})] - \frac{1}{2} \lambda^{(\tau)} K \right\} \\ &\quad + \frac{1}{2} \left[ \frac{\ln K}{2\pi} - K \tilde{J}_{\max}^{(\tau)} \right] \end{aligned} \quad (3.6)$$

where  $f_A^{(\tau)}(K)$  is the free energy density and  $\Delta^{(\tau)}(\mathbf{k}) = \tilde{J}_{\max}^{(\tau)} - \tilde{J}^{(\tau)}(\mathbf{k})$ . Using the identity

$$\ln(a+b) = \ln a + \int_0^{\infty} \frac{dx}{x} \exp(-ax) [1 - \exp(-bx)], \quad a > 0, \quad b > -a \quad (3.7)$$

we can rewrite Eq. (3.6) (after some manipulations) in the equivalent form

$$\begin{aligned} f_A^{(\tau)}(K) &= \sup_{\lambda^{(\tau)}} \left( \frac{1}{2} \int_0^{\infty} \frac{dx}{x} \left\{ \exp(-x) - \exp(-\lambda^{(\tau)} x) \frac{1}{|A|} \sum_{\mathbf{k}} \exp[-\Delta^{(\tau)}(\mathbf{k}) x] \right\} \right. \\ &\quad \left. - \frac{1}{2} \lambda^{(\tau)} K \right) + \frac{1}{2} \left[ \frac{\ln K}{2\pi} - K \tilde{J}_{\max}^{(\tau)} \right] \end{aligned} \quad (3.8)$$

In the remainder, if not stated otherwise, we will consider only the case of a system with a fully finite hypercubic geometry, i.e., when  $L_i = L$ ,  $i = 1, \dots, d$ . From Eq. (3.8), for such a system, we get the following representation for the free energy density:

$$\begin{aligned} f_A^{(\tau)}(K) &\equiv f_L(K | d_p, d_a, d_0, d_1) \\ &= \sup_{\lambda^{(\tau)}} \left( \frac{1}{2} \int_0^{\infty} \frac{dx}{x} \left\{ \exp(-x) - \frac{1}{|A|} \exp(-\lambda^{(\tau)} x) [S_L^p(x)]^{d_p} \right. \right. \\ &\quad \left. \times [S_L^a(x)]^{d_a} [S_L^0(x)]^{d_0} [S_L^1(x)]^{d_1} \right\} - \frac{1}{2} \lambda^{(\tau)} K \Big) \\ &\quad + \frac{1}{2} \left[ \frac{\ln K}{2\pi} - 2K \left( d_p + d_a \cos \frac{\pi}{L} + d_0 + d_1 \cos \frac{\pi}{L+1} \right) \right] \end{aligned} \quad (3.9)$$

where

$$S_L^p(x) = \sum_{k=0}^{L-1} \exp \left[ -2x \left( 1 - \cos \frac{2\pi k}{L} \right) \right] \quad (3.10)$$



$$S_L^a(x) = \sum_{k=0}^{L-1} \exp \left[ -2x \left( \cos \frac{\pi}{L} - \cos \frac{\pi(2k+1)}{L} \right) \right] \tag{3.11}$$

$$S_L^0(x) = \sum_{k=0}^{L-1} \exp \left[ -2x \left( 1 - \cos \frac{\pi k}{L} \right) \right] \tag{3.12}$$

$$S_L^1(x) = \sum_{k=0}^{L-1} \exp \left[ -2x \left( \cos \frac{\pi}{L+1} - \cos \frac{\pi(k+1)}{L+1} \right) \right] \tag{3.13}$$

It is easy to show that the above lattice sums fulfill the following relationships:

$$S_L^a(x) = \exp 2x \left( 1 - \cos \frac{\pi}{L} \right) [S_{2L}^p(x) - S_L^p(x)] \tag{3.14}$$

and

$$S_L^1(x) = \exp 2x \left( 1 - \cos \frac{\pi}{L+1} \right) [S_{L+1}^0(x) - 1] \tag{3.15}$$

The supremum on the right-hand side of Eq. (3.9) is attained at a value  $\lambda^{(\tau)} = \lambda(K; L | d_p, d_a, d_0, d_1)$ , which is determined by

$$\frac{1}{|A|} \int_0^\infty dx \exp(-\lambda^{(\tau)}x) [S_L^p(x)]^{d_p} [S_L^a(x)]^{d_a} [S_L^0(x)]^{d_0} [S_L^1(x)]^{d_1} = K \tag{3.16}$$

Employing now the definition in Eq. (2.1) of the helicity modulus in a finite system, we therefore obtain

$$\begin{aligned} \frac{1}{2} \beta Y^{(\tau)}(K; L) &\equiv \frac{1}{2} \beta Y(K; L | d_p, d_a, d_0, d_1) \\ &= \frac{L^2}{\pi^2} [f_L(K | d_p, d_a, d_0, d_1) - f_L(K | d_p + 1, d_a - 1, d_0, d_1)] \end{aligned} \tag{3.17}$$

which, by using Eq. (3.9), becomes

$$\begin{aligned} &\frac{1}{2} \beta Y(K; L | d_p, d_a, d_0, d_1) \\ &= \frac{L^{-(d-2)}}{2\pi^2} \int_0^\infty \frac{dx}{x} [S_L^p(x)]^{d_p} [S_L^a(x)]^{d_a-1} [S_L^0(x)]^{d_0} [S_L^1(x)]^{d_1} \\ &\quad \times [\exp(-\lambda_p x) S_L^p(x) - \exp(-\lambda_a x) S_L^a(x)] \\ &\quad - \frac{L^2}{2\pi^2} (\lambda_a - \lambda_p) K + K \frac{L^2}{\pi^2} \left( 1 - \cos \frac{\pi}{L} \right) \end{aligned} \tag{3.18}$$

Here  $\lambda_p \equiv \lambda(K; L | d_p + 1, d_a - 1, d_0, d_1)$  and  $\lambda_a \equiv \lambda(K; L | d_p, d_a, d_0, d_1)$  are the solutions of the corresponding equations for the spherical field [Eq. (3.16)] for a system with  $d_p + 1$  periodic and  $d_a - 1$  antiperiodic boundary conditions and for a system with  $d_p$  periodic and  $d_a$  antiperiodic boundary conditions, respectively ( $d_a \geq 1$ ). In accordance with Eq. (3.16) this implies that the first partial derivatives of the right-hand side of Eq. (3.18) with respect to  $\lambda_p$  and  $\lambda_a$  have to be zero.

Equations (3.9)–(3.18) provide the basis of our further analysis.

#### 4. THE METHOD

From the mathematical point of view the main problem which has to be solved is the evaluation of the integral on the right-hand side of Eq. (3.18) for  $L \gg 1$ . To achieve this we will employ the method first proposed by Shapiro and Rudnick,<sup>(18)</sup> who used it to investigate the finite-size properties of a fully finite  $d$ -dimensional spherical model with periodic boundary conditions. So, we divide the integral over  $x$  in Eq. (3.18) into two integrals—the first one from 0 to  $L^2$  [let us denote it by  $P(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1)$ ], i.e.,

$$\begin{aligned} P(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1) & \\ \equiv \frac{L^{-(d-2)}}{2\pi^2} \int_0^{L^2} \frac{dx}{x} [S_L^p(x)]^{d_p} [S_L^a(x)]^{d_a-1} [S_L^0(x)]^{d_0} & \\ \times [S_L^1(x)]^{d_1} [\exp(-\lambda_p x) S_L^p(x) - \exp(-\lambda_a x) S_L^a(x)] & \quad (4.1) \end{aligned}$$

and the second one from  $L^2$  to  $\infty$  [it will be denoted by  $Q(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1)$ ], i.e.,

$$\begin{aligned} Q(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1) & \\ \equiv \frac{L^{-(d-2)}}{2\pi^2} \int_{L^2}^{\infty} \frac{dx}{x} [S_L^p(x)]^{d_p} [S_L^a(x)]^{d_a-1} [S_L^0(x)]^{d_0} & \\ \times [S_L^{11}(x)]^{d_1} [\exp(-\lambda_p x) S_L^p(x) - \exp(-\lambda_a x) S_L^a(x)] & \quad (4.2) \end{aligned}$$

First we evaluate the integral in Eq. (4.2). For  $L$  sufficiently large, due to the rapid convergence of the sums (3.10)–(3.13) we can use the quadratic approximation of  $\cos z$  around  $z = 0$ . Proceeding in this way, we obtain the following asymptotic behavior of the lattice sums  $S_L^p(x)$  and  $S_L^0(x)$  (more technical details can be found in ref. 10):

$$S_L^p(x) = 1 + 2R_1 \left( \frac{4\pi^2}{L^2} x \right) - Lv(x) + \mathcal{O}(\exp(-\text{const} \cdot x)) \quad (4.3)$$

and

$$S_L^0(x) = 1 + R_1 \left( \frac{\pi^2}{L^2} x \right) - Lv(x) + \mathcal{O}(\exp(-\text{const} \cdot x)) \quad (4.4)$$

where

$$R_1(x) = \sum_{q=1}^{\infty} \exp(-xq^2) \quad (4.5)$$

and

$$v(x) = (4\pi x)^{-1/2} [1 - \text{erf}(\pi x^{1/2})] \quad (4.6)$$

The corresponding expressions for  $S_L^a(x)$  and  $S_L^1(x)$  follow from Eqs. (4.3) and (4.4) and from the exact relations given by Eqs. (3.14) and (3.15). For convenience and in order to introduce some notations we give the final results below:

$$S_L^a(x) = 2 + 2R_4 \left( \frac{\pi^2}{L^2} x \right) - Lv(x) + \mathcal{O}(\exp(-\text{const} \cdot x)) \quad (4.7)$$

and

$$S_L^1(x) = 1 + R_2 \left( \frac{\pi^2 x}{(L+1)^2} \right) - Lv(x) + \mathcal{O}(\exp(-\text{const} \cdot x)) \quad (4.8)$$

where

$$R_2(x) = \sum_{q=2}^{\infty} \exp[-x(q^2 - 1)] \quad (4.9)$$

and

$$R_4(x) = \sum_{q=1}^{\infty} \exp[-4xq(q+1)] \quad (4.10)$$

Now, inserting the asymptotic expressions in Eqs. (4.3), (4.4), (4.7), and (4.8) into Eq. (4.2) and changing the integration variable, we get

$$\begin{aligned} & Q(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1) \\ &= 2^{d_a-2} \frac{L^{-(d-2)}}{\pi^2} \int_1^{\infty} \frac{dx}{x} \{ 1 + 2R_1(4\pi^2 x)^{d_p} [1 + R_4(\pi^2 x)]^{d_a-1} \\ & \quad \times [1 + R_1(\pi^2 x)]^{d_0} [1 + R_2(\pi^2 x)]^{d_1} \} \\ & \quad \times \{ \exp(-y_p x) [1 + 2R_1(4\pi^2 x)] - 2 \exp(-y_a x) [1 + R_4(\pi^2 x)] \} \\ & \quad + \mathcal{O}(\exp(-\text{const} \cdot L^2); L^{-(d-1)} \exp(-y_p); L^{-(d-1)} \exp(-y_a)) \end{aligned} \quad (4.11)$$

which can be rewritten in the following form, which is more convenient for further investigations:

$$\begin{aligned} Q(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1) &= 2^{d_a-2} \frac{L^{-(d-2)}}{\pi^2} [-\text{Ei}(-y_p) + 2 \text{Ei}(-y_a)] \\ &+ \frac{L^{-(d-2)}}{\pi^2} [g(y_a | d_p, d_a, d_0, d_1) - g(y_p | d_p + 1, d_a - 1, d_0, d_1)] \\ &+ \mathcal{O}(\exp(-\text{const} \cdot L^2; L^{-(d-1)} \exp(-y_p); L^{-(d-1)} \exp(-y_a)) \end{aligned} \tag{4.12}$$

where

$$y_p \equiv \lambda_p L^2 \tag{4.13}$$

$$y_a \equiv \lambda_a L^2 \tag{4.14}$$

Ei(x) is the exponential-integral function<sup>(19)</sup> and

$$\begin{aligned} g(y | d_p, d_a, d_0, d_1) &= -2^{d_a-1} \int_1^\infty \frac{dx}{x} \exp(-yx) \{ [1 + 2R_1(4\pi^2x)]^{d_p} [1 + R_1(\pi^2x)]^{d_0} \\ &\times [1 + R_2(\pi^2x)]^{d_1} [1 + R_4(\pi^2x)]^{d_a - 1} \} \end{aligned} \tag{4.15}$$

It is clear from Eq. (4.15) that  $g(y|\cdot)$  is an analytic function in  $y$ ; its asymptotic behavior for  $y \gg 1$  is  $g(y|\cdot) \sim \exp(-\text{const} \cdot y)$ .

Let us now consider Eq. (4.1). In this case the appropriate asymptotic behavior of the lattice sums  $S_L^p(x)$  and  $S_L^0(x)$  can be obtained by using a technique similar to the one employed by Shapiro and Rudnick<sup>(18)</sup> [see Eq. (42) in ref. 18]. The corresponding results are (see also ref. 10):

$$S_L^p(x) \simeq Le^{-2x} I_0(2x) + \frac{L}{(\pi x)^{1/2}} R_p \left( \frac{L^2}{x} \right) \tag{4.16}$$

and

$$S_L^0(x) \simeq Le^{-2x} I_0(2x) + \frac{L}{(\pi x)^{1/2}} R_1 \left( \frac{L^2}{x} \right) + \frac{1}{2} (1 - e^{-4x}) \tag{4.17}$$

where  $R_p(x) \equiv R_1(x/4)$ . The expressions for  $S_L^a(x)$  and  $S_L^1(x)$  follow from the above and the exact relationships given in Eqs. (3.14) and (3.15):

$$S_L^a(x) \simeq e^{2x} \left( 1 - \cos \frac{\pi}{L} \right) \left[ Le^{-2x} I_0(2x) + \frac{L}{(\pi x)^{1/2}} R_a \left( \frac{L^2}{x} \right) \right] \tag{4.18}$$

and

$$\begin{aligned}
 S_L^1(x) &\simeq e^{2x} \left( 1 - \cos \frac{\pi}{L+1} \right) \\
 &\times \left[ (L+1) e^{-2x} I_0(2x) + \frac{L+1}{(\pi x)^{1/2}} R_1 \left( \frac{(L+1)^2}{x} \right) \right. \\
 &\left. - \frac{1}{2} (1 + e^{-4x}) \right] \tag{4.19}
 \end{aligned}$$

where  $R_a(x) = 2R_1(x) - R_1(x/4)$ . Now we have to evaluate the contributions in Eq. (4.1) stemming from the different products of terms which enter into the right-hand sides of Eqs. (4.16)–(4.19). The following observations greatly simplify our task. First, due to the exponential convergence for  $x \ll L^2$  of the “ $R$ ”-functions [i.e., of  $R_p$ ,  $R_a$ , and  $R_1$  in Eqs. (4.16)–(4.19)], in all products which contain at least one  $R$ -function and  $I_0(x)$ , we can use the asymptotic form of  $I_0(x)$  for  $x \gg 1$ . Second, in all products which in addition to at least one  $R$ -function also contain terms  $[1 - \exp(-4x)]/2$  and/or  $[1 + \exp(-4x)]/2$ , we can neglect the term  $\exp(-4x)$ , because it will produce contributions exponentially small in  $L$ . Proceeding in this way, we obtain

$$\begin{aligned}
 &P(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1) \\
 &= \frac{L^{-(d-2)}}{\pi^2} [\psi(\tilde{y}_a | d_p, d_a, d_0, d_1) - \psi(\tilde{y}_p | d_p + 1, d_0, d_1)] \\
 &\times [1 + \mathcal{O}(d_1 L^{-1}) + \mathcal{O}(L^{-2})] \\
 &+ \frac{L^2}{\pi^2} \sum_{m=0}^{d_0} \sum_{n=0}^{d_1} \sum_{k=0}^n \sum_{p=0}^m \binom{d_0}{m} \binom{d_1}{n} \binom{n}{k} \binom{m}{p} \\
 &\times (-1)^{n+p} (2L)^{-(m+n)} (1 + L^{-1})^{d_1-n} \\
 &\times [f_{d-m-n}(\tilde{\lambda}_a + 4(k+p), L^2) - f_{d-m-n}(\tilde{\lambda}_p + 4(k+p), L^2)] \tag{4.20}
 \end{aligned}$$

where

$$\tilde{\lambda}_p = \lambda_p - 2(d_a - 1) \left( 1 - \cos \frac{\pi}{L} \right) - 2d_1 \left( 1 - \cos \frac{\pi}{L+1} \right) \tag{4.21}$$

$$\tilde{\lambda}_a = \lambda_a - 2d_a \left( 1 - \cos \frac{\pi}{L} \right) - 2d_1 \left( 1 - \cos \frac{\pi}{L+1} \right) \tag{4.22}$$

$$\tilde{y}_p = \tilde{\lambda}_p L^2, \quad \tilde{y}_a = \tilde{\lambda}_a L^2 \tag{4.23}$$

In Eq. (4.20) the functions

$$\begin{aligned} \psi(y|d_p, d_a, d_0, d_1) &= -\frac{1}{2} \pi^{-d/2} \int_0^1 \frac{dx}{x} x^{-d/2} e^{-yx} \\ &\times \left\{ \left[ \frac{1}{2} + R_p \left( \frac{1}{x} \right) \right]^{d_p} \left[ \frac{1}{2} + R_a \left( \frac{1}{x} \right) \right]^{d_a} \left[ \frac{1}{2} + R_1 \left( \frac{1}{x} \right) + \frac{(\pi x)^{1/2}}{2} \right]^{d_0} \right. \\ &\times \left[ \frac{1}{2} + R_1 \left( \frac{1}{x} \right) - \frac{(\pi x)^{1/2}}{2} \right]^{d_1} - 2^{-(d_p + d_a)} \left( \frac{1}{2} + \frac{(\pi x)^{1/2}}{2} \right)^{d_0} \\ &\left. \times \left( \frac{1}{2} - \frac{(\pi x)^{1/2}}{2} \right)^{d_1} \right\} \end{aligned} \tag{4.24}$$

collect all the contributions stemming from products which contain at least one *R*-function, and the remaining ones are given by the *f*-functions

$$f_d(\lambda, x) = \frac{1}{2} \int_0^x \frac{dt}{t} (e^{-t} - e^{-\lambda t}) [e^{-2t} I_0(2t)]^d \tag{4.25}$$

Up to now we have not specified the value of the space dimensions *d*. So, the results obtained above are quite general. Since our main interest is concentrated on the predictions made for the case *d* = 3, in the remainder we will consider only three-dimensional systems.

From Eq. (4.24) it is clear that  $\psi(y|\cdot)$  is an analytic function in *y* and it can be easily shown that its asymptotic behavior for  $y \gg 1$  is given by  $\psi(y|\cdot) \sim y^{(d-1)/4} \exp(-\sqrt{y})$ . The properties of the *f*-functions are derived in the Appendix. Here, for convenience, we will state only the final results:

(i) For  $x \rightarrow \infty, \lambda \rightarrow 0$  with  $\lambda x \rightarrow \infty$  we get

$$f_3(\lambda, x) = f_3 + \frac{1}{2} K_c \lambda - \frac{1}{12\pi} \lambda^{3/2} + \mathcal{O}(\lambda^2, \exp(-\lambda x)) \tag{4.26}$$

$$\begin{aligned} f_2(\lambda, x) &= f_2 + \frac{1}{8\pi} (5 \ln 2 + 1) \lambda - \frac{1}{8\pi} \lambda \ln \lambda \\ &+ \mathcal{O}(\lambda^2 \ln \lambda, \exp(-\lambda x)) \end{aligned} \tag{4.27}$$

$$f_1(\lambda, x) = f_1 + \frac{1}{2} \lambda^{1/2} - \frac{1}{24} \lambda^{3/2} + \mathcal{O}(\lambda^{5/2}, \exp(-\lambda x)) \tag{4.28}$$

where  $f_d \equiv f_d(0, \infty), d = 1, 2, 3,$  are constants.

(ii) For  $\lambda \rightarrow 0$ ,  $x \rightarrow \infty$  with  $\lambda x = \mathcal{O}(1)$ , or  $\lambda x \rightarrow 0$ , we obtain

$$f_3(\lambda, x) = f_3 + \frac{1}{2} K_c \lambda + \frac{1}{2} (4\pi)^{-3/2} \lambda x^{-1/2} \sum_{k=0}^{\infty} \frac{(-1)^k (\lambda x)^k}{(k+1)! (k-1/2)!} + \frac{1}{2} (4\pi)^{-3/2} x^{-3/2} + \mathcal{O}(\lambda^2, \lambda x^{-3/2}, x^{-5/2}) \quad (4.29)$$

$$f_2(\lambda, x) = f_2 + \frac{1}{8\pi} \lambda \ln x + c_2 \lambda + \frac{1}{8\pi} \lambda \sum_{k=1}^{\infty} \frac{(-1)^k (\lambda x)^k}{k(k+1)!} + \frac{1}{8\pi} x^{-1} + \mathcal{O}(\lambda^2 \ln x, x^{-2}) \quad (4.30)$$

$$f_1(\lambda, x) = f_1 + c_1 \lambda + \frac{1}{2} (4\pi)^{-1/2} \lambda x^{1/2} \sum_{k=0}^{\infty} \frac{(-1)^k (\lambda x)^k}{(k+1)! (k+1/2)!} + \frac{1}{2} (4\pi)^{-1/2} x^{-1/2} + \mathcal{O}(\lambda^2, \lambda x^{-1/2}) \quad (4.31)$$

where  $c_1$  and  $c_2$  are constants which will be not specified here.

Now we can turn to the investigation of the finite-size behavior of the helicity modulus given in Eq. (3.18).

## 5. FINITE-SIZE BEHAVIOR OF THE HELICITY MODULUS

According to Eqs. (4.2) and (4.1), the corresponding expression in Eq. (3.18) for the helicity modulus can be written as

$$\begin{aligned} & \frac{1}{2} \beta Y(K; L | d_p, d_a, d_0, d_1) \\ &= P(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1) + Q(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1) \\ & \quad - \frac{L^2}{2\pi^2} (\lambda_a - \lambda_p) K + K \frac{L^2}{\pi^2} \left( 1 - \cos \frac{\pi}{L} \right) \end{aligned} \quad (5.1)$$

First let us consider the case when  $\lambda L^2 = \mathcal{O}(1)$  or  $\lambda L^2 \rightarrow 0$  as  $\lambda \rightarrow 0$  and  $L \rightarrow \infty$ , where  $\lambda$  is either  $\lambda_p$  or  $\lambda_a$ . Note that in this regime also  $\tilde{\lambda} L^2 = \mathcal{O}(1)$  or  $\tilde{\lambda} L^2 \rightarrow 0$  as  $L \rightarrow \infty$  [see Eqs. (4.21) and (4.23)], where  $\tilde{\lambda}$  is equal to  $\tilde{\lambda}_p$  or  $\tilde{\lambda}_a$ . Then the insertion into Eq. (5.1) of the results for the asymptotic behavior of  $P(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1)$  and  $Q(\lambda_a, \lambda_p, L | d_p, d_a, d_0, d_1)$ , given by Eqs. (4.12) and (4.20), respectively, directly leads to the following final expression for the helicity modulus:

$$\begin{aligned}
 & \frac{1}{2} \beta Y(K; L | d_p, d_a, d_0, d_1) \\
 &= \pi^{-2} L^{-1} \left( [\psi(\tilde{y}_a | d_p, d_a, d_0, d_1) - \psi(\tilde{y}_p | d_p + 1, d_a - 1, d_0, d_1)] \right. \\
 & \quad + [g(y_a | d_p, d_a, d_0, d_1) - g(y_p | d_p + 1, d_a - 1, d_0, d_1)] \\
 & \quad + \frac{1}{2} \left\{ [\tilde{f}_3(\tilde{y}_a) - \tilde{f}_3(\tilde{y}_p)] + \frac{1}{2} (d_0 - d_1) [\tilde{f}_2(\tilde{y}_a) - \tilde{f}_2(\tilde{y}_p)] \right. \\
 & \quad \left. + \frac{1}{4} \left[ -d_0 d_1 + \binom{d_1}{2} + \binom{d_0}{2} \right] [\tilde{f}_1(\tilde{y}_a) - \tilde{f}_1(\tilde{y}_p)] \right\} \\
 & \quad + 2^{d_a - 2} [2 \operatorname{Ei}(-y_a) - \operatorname{Ei}(-y_p)] \\
 & \quad + \frac{1}{2} (\tilde{y}_a - \tilde{y}_p) \left[ K_c + \frac{1}{4\pi} (d_0 - d_1) \frac{\ln L}{L} + \frac{\text{const}}{L} - K \right] L \\
 & \quad + \mathcal{O} \left( (d_1 + d_0) \frac{\ln L}{L^2}, L^{-2} \right) \tag{5.2}
 \end{aligned}$$

Here  $\tilde{f}_i(z)$ ,  $i = 1, 2, 3$ , are analytic functions:

$$\tilde{f}_i(z) = (4\pi)^{-i/2} \sum_{k=0}^{\infty} \frac{(-1)^k z^{k+1}}{(k+1)! (k+1-i/2)}, \quad i = 1, 3 \tag{5.3}$$

$$\tilde{f}_2(z) = (4\pi)^{-1} \sum_{k=1}^{\infty} \frac{(-1)^k z^{k+1}}{(k+1)! k} \tag{5.4}$$

and

$$\text{const} = K_c d_1 - \frac{1}{2} (d_0 + d_1) W_2(4) + (d_0 - d_1) c_2 \tag{5.5}$$

Now we recall that  $\tilde{y}_a$  and  $\tilde{y}_p$  have to satisfy the corresponding spherical field equation (3.16), which can be obtained from Eq. (3.18) requiring the first partial derivatives with respect to  $\lambda_a$  and  $\lambda_p$  from the right-hand side of Eq. (3.18) to be zero. So, from Eq. (5.2), taking into account the defining equations (4.13), (4.14), and (4.21)–(4.23), we obtain the following equations for  $y_a$  and  $y_p$ , respectively:

$$0 = \frac{1}{2} (K_{c,L} - K) L + 2^{d_a - 1} y_a^{-1} \exp(-y_a) + \text{analytic function in } y_a \tag{5.6}$$

for  $y_a$  and

$$0 = \frac{1}{2} (K_{c,L} - K) L + 2^{d_a - 2} y_p^{-1} \exp(-y_p) + \text{analytic function in } y_p \tag{5.7}$$



for  $y_p$ , where we have introduced a shifted critical coupling

$$K_{c,L} = K_c + \frac{1}{4\pi} (d_0 - d_1) \frac{\ln L}{L} \tag{5.8}$$

Therefore, if  $(K_{c,L} - K)L = \mathcal{O}(1)$ , the solutions of Eqs. (5.6) and (5.7) are  $y_a = \mathcal{O}(1)$  and  $y_p = \mathcal{O}(1)$ , which is in agreement with the assumptions under which Eq. (5.2) was derived. Turning to the behavior of the helicity modulus, the results obtained above imply that in the considered regime:

(i)  $Y(K; L | d_p, d_a, d_0, d_1)$  is a function of the single scaling variable  $(K_{c,L} - K)L^{1/\nu}$  ( $\nu=1$  for  $d=3$  in the spherical model<sup>(17)</sup>). The corresponding scaling function is given by the right-hand side of Eq. (5.2), where  $y_a$  and  $y_p$  obey the equation for the spherical field of the system with the considered set of boundary conditions.

(ii) There are no  $\log(L)$  corrections in the finite-size behavior of  $Y(K; L | \cdot)$ .

Let us now consider the temperature region for which  $(K_{c,L} - K)L \rightarrow -\infty$  as  $L \rightarrow \infty$ . From Eqs. (5.6) and (5.7) it follows that  $y_a$  and  $y_p$  then tend to zero:

$$y_a^{-1} = 2^{-d_a}(K - K_{c,L})L + \text{const}_a \tag{5.9}$$

and

$$y_p^{-1} = 2^{-(d_a-1)}(K - K_{c,L})L + \text{const}_p \tag{5.10}$$

where  $\text{const}_a$  and  $\text{const}_p$  are constants depending on the boundary conditions, which will not be specified here. Hence, from Eq. (5.2), we obtain for the helicity modulus

$$\begin{aligned} \beta Y(K; L | d_p, d_a, d_0, d_1) &= (K - K_{c,L}) - \frac{2^{d_a-1}}{\pi^2 L} \ln[(K - K_{c,L})L] \\ &+ \mathcal{O}(L^{-1}) \end{aligned} \tag{5.11}$$

Taking into account that for  $d_0 \geq d_1$  due to  $(K_{c,L} - K)L \rightarrow -\infty$  one has  $(K_c - K)L \rightarrow -\infty$  and  $K - K_c \gg (d_0 - d_1) \ln L / 4\pi L$ , we can rewrite the above equation as

$$\begin{aligned} \beta Y(K; L | d_p, d_a, d_0, d_1) &= (K - K_c) - \left[ \frac{1}{4\pi} (d_0 - d_1) + \frac{2^{d_a-1}}{\pi^2} \right] \frac{\ln L}{L} \\ &- \frac{2^{d_a-1} / \pi^2 \ln(K - K_c) + \mathcal{O}(1)}{L} \end{aligned} \tag{5.12}$$

From this equation it is clear that:

(i) In the limit  $L \rightarrow \infty$  we obtain the well-known expression for the bulk helicity modulus (see, e.g., ref. 15)

$$\beta Y(K) = K - K_c \quad (5.13)$$

which is, as expected, independent of the boundary conditions.

(ii) Below the critical temperature [more precisely, for  $(K - K_c)L \gg \ln L$ ], there are logarithmic corrections in the finite-size behavior of the helicity modulus. These logarithmic contributions have two sources: (a) the lowest eigenvalue modes, which lead to the term  $2^{d_a-1} \ln L/\pi^2 L$ , and (b) the presence of real surfaces in the reference systems [i.e., in the systems whose properties are used in the defining equation (2.2) of the helicity modulus].

It is well known that the three-dimensional spherical model under (in our terminology) fixed boundary conditions is characterized by a logarithmic shift of the critical temperature, which is one of the peculiarities of the model for boundary conditions with real surfaces (see, e.g., refs. 15 and 21). Here we see that the sign of this shift depends on the type of the boundary conditions used to model the free surfaces.

Let us now investigate the case when  $(K_{c,L} - K)L \rightarrow -\infty$  but  $d_0 < d_1$ . Considering the different possibilities, we get:

(i) If, as before,  $K - K_c \gg (d_1 - d_0) \ln L/4\pi L$ , the finite-size behavior of  $Y$  will again be given by Eq. (5.12).

(ii) If  $K - K_c \leq (d_1 - d_0) \ln L/4\pi L$  [note that this covers, for example, the region in which  $(K - K_c)L = \mathcal{O}(1)$ ], instead of Eq. (5.12) we obtain from Eq. (5.11)

$$\beta Y(K; L | d_p, d_a, d_0, d_1) = K - K_c - \frac{2^{d_a-1} \ln[(d_1 - d_0) \ln L] + \mathcal{O}(1)}{L} \quad (5.14)$$

So, if  $d_0 < d_1$ , the appearance of the  $\log(\log(L))$  corrections is possible in the bulk critical region [i.e., for  $L(K - K_c) = \mathcal{O}(1)$ ]. The inspection of the Eq. (5.11) also shows that this can occur if and only if both sources of logarithmic corrections mentioned above are present in the system.

Up to now we have considered the cases when  $(K_{c,L} - K)L = \mathcal{O}(1)$  and when  $(K_{c,L} - K)L \rightarrow -\infty$ . Let us now consider the remaining case  $(K_{c,L} - K)L \rightarrow \infty$ . It is clear that Eqs. (5.6) and (5.7) then have no solutions satisfying the assumptions under which they are derived. This simply means that in this case we have to look for solutions  $y_a$  and  $y_p$  of the type  $y_a \gg 1$  and  $y_p \gg 1$ . Inserting the asymptotic expressions in Eqs. (4.26)–(4.28) into Eq. (4.20) and taking into account the asymptotic behavior of the

functions  $\psi(y|\cdot) \sim y^{(d-1)/4} \exp(-\sqrt{y})$  and  $g(y|\cdot) \sim \exp(-\text{const} \cdot y)$  for  $y \gg 1$ , we obtain from Eqs. (3.18), (4.12), and (4.12) that up to functions which are exponentially small in  $\sqrt{y}$  (where  $y$  is either  $\tilde{y}_a$  or  $\tilde{y}_p$ ), the corresponding expression for  $Y$  is a function symmetric in  $\tilde{y}_a$  and  $\tilde{y}_p$ . This implies that the same is true for the spherical field equations which can be obtained by the vanishing of the first partial derivatives of this expression with respect to  $y_a$  and  $y_p$ . Hence, the difference between  $\tilde{y}_a$  and  $\tilde{y}_p$  will be exponentially small. Turning now to the finite-size helicity modulus and summarizing the above, we obtain

$$\beta Y(K; L|\cdot) \sim \exp(-\text{const} \cdot \sqrt{y}) \quad (5.15)$$

where  $y$  is the solution of one of the equations of the spherical field. Finally we have to determine the leading-order solution of this equation. Proceeding as explained above, we derive the following explicit form of the equation for the spherical field:

$$(K_{c,L} - K) L - \frac{1}{4\pi} \tilde{y}^{1/2} - \frac{1}{8\pi} (d_0 - d_1) \ln \tilde{y} + \mathcal{O}(1) = 0 \quad (5.16)$$

Substituting the leading-order solution of the above equation into Eq. (5.15), we finally get

$$\beta Y(K; L|d_a, d_p, d_0, d_1) \sim \exp[-\text{const} \cdot (K_{c,L} - K) L] \quad (5.17)$$

Hence, (i) for all temperatures  $T > T_c$  (i.e.,  $K < K_c$ ) the helicity modulus tends to zero exponentially; (ii) in the critical region  $(K_c - K) L = \mathcal{O}(1)$  of the bulk critical point  $K_c$  [but when  $(K_{c,L} - K) L \rightarrow \infty$ , and so  $d_0 > d_1$ ] this approach is algebraic in  $L$ .

Note that if  $K < K_c$ , the finite-size corrections to the bulk free energy are of the order of  $L^{-1}$  in the presence of surfaces (i.e., if  $d_0 + d_1 > 0$ ; see, e.g., refs. 15, 21, and 3) and are exponentially small only under periodic and/or antiperiodic boundary conditions (see, e.g., refs. 15, 22, and 23). This, in turn, means that above the critical point all the finite-size corrections to the bulk free energies of both systems (used in the definition of the helicity modulus) are equal to each other up to terms exponentially small in  $L$ .

In the remainder of this section we will consider the behavior of the helicity modulus if only antiperiodic and/or periodic boundary conditions are imposed, i.e., the case  $d_1 = d_0 = 0$ . We consider the geometry  $L^{3-d'} \times \infty^{d'}$ . Taking into account that

$$\lim_{L \rightarrow \infty} \frac{1}{L} S_L^\tau(x) = \exp(-2x) I_0(2x) \quad (5.18)$$

where  $\tau$  denotes any of the boundary conditions under consideration, and using the expression in Eq. (3.9) for the free energy of the system, instead of Eq. (3.18) we obtain the following equation for the helicity modulus of the system:

$$\begin{aligned} & \frac{1}{2} \beta Y^{(d')} (K; L | d_p, d_a) \\ &= \frac{L^{2-d+d'}}{2\pi^2} \int_0^\infty \frac{dx}{x} [e^{-2x} I_0(2x)]^{d'} [S_L^a(x)]^{d_a-1} [S_L^p(x)]^{d_p} \\ & \quad \times [e^{-\lambda_p x} S_L^p(x) - e^{-\lambda_a x} S_L^a(x)] - \frac{L^2}{2\pi^2} K(\tilde{\lambda}_a - \tilde{\lambda}_p) \end{aligned} \quad (5.19)$$

where  $d_p + d_a + d' = 3$  and all the other symbols have the same meaning as before. This relation can be treated further in the same fashion as in the case of a fully finite geometry. Here we skip completely the intermediate calculations and present only the final expression:

$$\begin{aligned} & \frac{1}{2} \beta Y^{(d')} (K; L | d_p, d_a) \\ &= \pi^{-2} L^{-1} \{ [g_{d'}(y_a | d_p, d_a) - g_{d'}(y_p | d_p + 1, d_a - 1)] \\ & \quad + [\psi_{d'}(\tilde{y}_a | d_p, d_a) - \psi_{d'}(\tilde{y}_p | d_p + 1, d_a - 1)] \\ & \quad + 2^{d_a-d'-2} \pi^{-d'/2} [y_p^{d'/2} \Gamma(-d'/2, y_p) - 2y_a^{d'/2} \Gamma(-d'/2, y_a)] \\ & \quad + \frac{1}{2} [(K_c - K) L] (\tilde{y}_a - \tilde{y}_p) + \frac{1}{2} [\tilde{f}_3(\tilde{y}_a) - \tilde{f}_3(\tilde{y}_p)] \} \end{aligned} \quad (5.20)$$

where

$$\begin{aligned} & g_{d'}(y | d_p, d_a) \\ &= - \frac{2^{d_a-d'-1}}{\pi^{d'/2}} \int_1^\infty \frac{dx}{x} x^{-d'/2} \{ [1 + R_4(\pi^2 x)]^{d_a} \\ & \quad \times [1 + 2R_1(4\pi^2 x)]^{d_p} - 1 \} e^{-yx} \end{aligned} \quad (5.21)$$

and

$$\begin{aligned} & \psi_{d'}(y | d_p, d_a) = - (2^{d'+1} \pi^{d/2})^{-1} \int_0^1 \frac{dx}{x} x^{-d/2} \\ & \quad \times \left\{ \left[ \frac{1}{2} + R_a \left( \frac{1}{x} \right) \right]^{d_a} \left[ \frac{1}{2} + R_p \left( \frac{1}{x} \right) \right]^{d_p} - 2^{-(d_a+d_p)} \right\} e^{-yx} \end{aligned} \quad (5.22)$$

Here it is supposed that  $y_a$  and  $y_p$  are of the order of unity or tend to zero. Starting from the equation above and proceeding in the same manner as for the case considered previously, we now obtain:

(i) If  $(K_c - K) L = \mathcal{O}(1)$ , i.e., in the bulk critical region, the behavior of the helicity modulus is given by a function of the scaling variable  $(K_c - K) L \sim (T - T_c) L$  with no  $\log(L)$  finite-size correction terms. This is true for fully finite, film ( $d' = 2$ ) and cylinder geometry ( $d' = 1$ ).

(ii) If  $(K_c - K) L \rightarrow -\infty$ , i.e., below the critical temperature, and up to the leading-order terms, the corresponding equations for the spherical field for  $d' = 1$  and  $d' = 2$  are [for  $d' = 0$  see Eqs. (5.9) and (5.10) with  $K_{c,L}$  replaced from  $K_c$  in them]:

(a) For  $d' = 1$

$$\frac{1}{2}(K - K_c) L = \begin{cases} 2^{d_a-2} y_a^{-1/2} + \mathcal{O}(1) & \text{for } y_a \\ 2^{d_a-3} y_p^{-1/2} + \mathcal{O}(1) & \text{for } y_p \end{cases} \quad (5.23)$$

and (b) for  $d' = 2$

$$\frac{1}{2}(K - K_c) L = \begin{cases} -\frac{1}{4\pi} \ln y_a + \mathcal{O}(1) & \text{for } y_a \\ -\frac{1}{8\pi} \ln y_p + \mathcal{O}(1) & \text{for } y_p \end{cases} \quad (5.24)$$

Substituting the solutions of these equations into Eq. (5.20) yields

$$\frac{1}{2}\beta Y^{(d')}(K; L | d_p, d_a) = K - K_c + \mathcal{O}(1)/L, \quad d' = 1, 2 \quad (5.25)$$

Hence, if in the geometry of the system there is at least one infinite dimension and only antiperiodic and/or periodic boundary conditions are imposed, there are no logarithmic finite-size corrections in the behavior of the helicity modulus, not in the bulk critical region nor below  $T_c$ . For the temperatures above the critical one it is easy to see that the helicity modulus in this case tends to zero exponentially as in the previously considered case of a fully finite geometry.

## 6. DISCUSSION

In the present paper the finite-size behavior of the helicity modulus has been investigated in the framework of the three-dimensional mean spherical model. The helicity modulus in a finite system is defined as a straightforward extension of the corresponding “bulk” definition [see Eq. (2.1)] due to Fisher *et al.*<sup>(12)</sup> It is proportional to the increase of the free energy of an  $O(n)$  finite system due to the order parameter orientational gradients

created when the periodic boundary conditions imposed across one direction of the system are changed to antiperiodic ones [see Eq. (2.2)].

As is well known, the infinite translational-invariant spherical model is equivalent to the  $n \rightarrow \infty$  limit of such an  $n$ -component system,<sup>(24,25)</sup> but the spherical model of a system with free surfaces (or more generally without translational invariance symmetry) is in fact *not* such a limit (to restore the equivalence we have to consider a modification of the spherical model with a distinct spherical field applied to each layer parallel to any of the surfaces<sup>(26)</sup>; unfortunately, this version of the model is rather untractable). Nevertheless, the spherical model with free surfaces was extensively investigated in the context of the theory of finite-size scaling and surface critical phenomena (see for reviews, e.g., ref. 23 and 27). It turns out that the finite-size scaling remains valid in terms of a shifted critical coupling variable  $(K_{c,L} - K)L$ , where  $K_{c,L}$  is given by Eq. (5.8). Thus, as far as we are interested in the finite-size scaling properties of the helicity modulus, it is worthwhile to have, at least for completeness, the corresponding results for a spherical model with surfaces, too.

In the present work two main cases of the geometry of the system and applied boundary conditions have been considered:

(i) The case of a system with fully finite hypercubic geometry with  $d_p \geq 0$  periodic,  $d_a \geq 0$  antiperiodic,  $d_0 \geq 0$  free, and  $d_1 \geq 0$  fixed boundary conditions ( $d_p + d_a + d_0 + d_1 = 3$ ).

(ii) The case of a geometry of the system of the type  $L^{3-d'} \times \infty^{d'}$  with only antiperiodic and/or periodic boundary conditions imposed.

It is shown that in the critical region  $(K - K_{c,L})L = \mathcal{O}(1)$  of the shifted critical point the behavior of the helicity modulus (in both cases) is described by a scaling function [see Eqs. (5.2), (5.6), and (5.7) for case (i) and the corresponding equations (5.20), (5.23), and (5.24) for case (ii)] depending on the scaling variable  $(L_{c,L} - K)L^{1/\nu}$  ( $\nu = 1$  for three-dimensional spherical model), where  $K_{c,L}$  is given by Eq. (5.8) in case (i) and  $K_{c,L} \equiv K_c$  for case (ii). In this temperature region *no* finite-size  $\log(L)$  corrections are found.

In the critical region of the bulk critical point the finite-size behavior of the helicity modulus in case (i) depends on whether  $d_0 \geq d_1$  or  $d_0 < d_1$ : in the former subcase the helicity modulus tends to zero algebraically in  $L$ , whereas in the last case a *universal*  $\log(\log(L))$  leading-order term [see Eq. (5.14)]

$$-\frac{2^{d_a-1} \ln[(d_1 - d_0) \ln L]}{\pi^2 L}$$

has been derived.

Above the critical temperature the helicity modulus in both cases (i) and (ii) tends to zero exponentially in  $L$ .

A *universal, logarithmic* finite-size term [see Eq. (5.12)]

$$- \left[ \frac{1}{4\pi} (d_0 - d_1) + \frac{2^{d_a - 1}}{\pi^2} \right] \frac{\ln L}{L}$$

has been found only *below* the critical temperature (more precisely, when  $K - K_c \gg \ln L/L$ ) and for the case of a system with a fully finite geometry. This term collects logarithmic contributions due to the presence of surfaces in the geometry of the system and other ones which stem from the lowest eigenvalue modes. In the presence of at least one infinite dimension the last logarithmic contributions disappear. It is plausible that due to the presence of surfaces logarithmic terms could appear below  $T_c$  also in a cylinder geometry, but this case has not been investigated here.

As we have seen, the exact results for the spherical model are not in agreement with the finite-size scaling predictions about the existence of an additional  $\log(L)$  correction term in the finite-size dependence of the helicity modulus in the critical region of a three-dimensional  $O(n)$  system.<sup>(3)</sup> It should be emphasized, however, that different definitions of the helicity modulus in a finite system, leading to the same bulk, but different finite-size behavior [including also  $\log(L)$  terms] are possible (for a short discussion of this point see Section 2). The present work elucidates only the consequences if one of these possibilities is employed. Thus the problem needs to be explored further.

## APPENDIX. EXPANSIONS FOR THE FUNCTIONS $f_d(\lambda, x)$

In this appendix we consider the asymptotic expansions for  $\lambda \rightarrow 0$  and  $x \gg 1$  of the functions  $f_d(\lambda, x)$  defined in Eq. (4.25):

$$f_d(\lambda, x) = \frac{1}{2} \int_0^x \frac{dt}{t} (e^{-t} - e^{-\lambda t}) [e^{-2t} I_0(2t)]^d \quad (\text{A.1})$$

First we investigate the case  $\lambda \rightarrow 0$  but  $x\lambda \gg 1$ . From the above definition we immediately obtain

$$\begin{aligned} f_d(\lambda, x) &= \frac{1}{2} \int_0^x \frac{dt}{t} \{ e^{-t} - e^{-\lambda t} [e^{-2t} I_0(2t)]^d \} \\ &\quad - \frac{1}{2} \int_0^x \frac{dt}{t} \{ e^{-t} - e^{-t} [e^{-2t} I_0(2t)]^d \} \\ &= f_d(\lambda) - A_d + \mathcal{O}(\exp(-\lambda x)) \end{aligned} \quad (\text{A.2})$$

where

$$f_d(\lambda) = \frac{1}{2} \int_0^\infty \frac{dt}{t} \{e^{-t} - e^{-\lambda t} [e^{-2t} I_0(2t)]^d\} \quad (\text{A.3})$$

and  $A_d = f_d(1)$  is a constant. Note that [see, e.g., Eq. (52) in ref. 20]

$$\begin{aligned} F_B(K, \lambda) &\equiv \frac{1}{2} \int_0^\infty \frac{dt}{t} \{e^{-t} - e^{-\lambda t} [e^{-2t} I_0(2t)]^d\} + \frac{1}{2} \ln K \\ &= f_d(\lambda) + \frac{1}{2} \ln K \end{aligned} \quad (\text{A.4})$$

is the bulk (per  $k_B T$ ) free energy density (with  $\lambda$  determined from the corresponding bulk spherical constraint) of the  $d$ -dimensional spherical model. Employing the asymptotic expansions of the functions  $F_B(K, \lambda)$  around  $\lambda = 0$ , from Eqs. (A.2) and (A.4) we obtain the required asymptotic representations in Eqs. (4.26)–(4.28) of the functions  $f_d(\lambda, x)$  for the case  $\lambda \rightarrow 0$  with  $\lambda x \gg 1$ .

Let us now consider the remaining case when  $\lambda x = \mathcal{O}(1)$  or  $\lambda x \rightarrow 0$  as  $\lambda \rightarrow 0$  and  $x \rightarrow \infty$ . Starting again from Eq. (A.1), we obtain (for  $d \geq 1$ )

$$\begin{aligned} f_d(\lambda, x) &= \frac{1}{2} \int_0^\infty \frac{dt}{t} (e^{-t} - 1) [e^{-2t} I_0(2t)]^d \\ &\quad - \frac{1}{2} \int_x^\infty \frac{dt}{t} (e^{-t} - 1) [e^{-2t} I_0(2t)]^d + \frac{1}{2} \int_0^x \frac{dt}{t} (1 - e^{-\lambda t}) [e^{-2t} I_0(2t)]^d \\ &= f_d + \frac{1}{2} \int_x^\infty \frac{dt}{t} [e^{-2t} I_0(2t)]^d \\ &\quad + \frac{1}{2} \int_0^\lambda ds \int_0^x dt e^{-st} [e^{-2t} I_0(2t)]^d + \mathcal{O}(\exp(-x)) \\ &= f_d - \frac{1}{2} \int_0^\lambda ds W_d(s, x) + \frac{1}{2} (4\pi x)^{-d/2} + \mathcal{O}(x^{-(1+d/2)}) \end{aligned} \quad (\text{A.5})$$

where

$$f_d = \frac{1}{2} \int_0^\infty \frac{dt}{t} (e^{-t} - 1) [e^{-2t} I_0(2t)]^d \quad (\text{A.6})$$

is a constant and

$$W_d(s, x) = \int_0^x dt e^{-st} [e^{-2t} I_0(2t)]^d \quad (\text{A.7})$$



represents a generalization of the Watson functions [see, e.g., Eq. (A4) in ref. 15]

$$W_d(s) = \int_0^\infty dt e^{-st} [e^{-2t} I_0(2t)]^d \quad (\text{A.8})$$

To proceed further we need to evaluate the functions  $W_d(s, x)$ . First we note that  $sx = \mathcal{O}(1)$  or  $sx \rightarrow 0$  as  $x \rightarrow \infty$  and  $s \in [0, \lambda]$ . Second we divide the integration interval over  $t$  in Eq. (A.7) into two intervals—the first one from 0 to  $a$ , where  $1 \ll a \ll x$  is a large positive constant, and the second one over the remaining part from  $a$  to  $x$ . The integration over  $t$  in the first integral leads to a function which is analytic in  $s$ . In the second integral we use the asymptotic form of the Bessel function<sup>(19)</sup>  $I_0$  for large values of its argument. Proceeding in this way, we obtain

$$W_3(s, x) = W_3(0) + (4\pi)^{-3/2} x^{-1/2} \sum_{k=0}^{\infty} \frac{(-1)^k (xs)^k}{k! (k-1/2)} + \mathcal{O}(x^{-3/2}, s) \quad (\text{A.9})$$

$$W_2(s, x) = \frac{1}{4\pi} \ln x + \frac{1}{4\pi} \sum_{k=1}^{\infty} \frac{(-1)^k (xs)^k}{k! k} + c_2 + \mathcal{O}(x^{-1}, s \ln x) \quad (\text{A.10})$$

$$W_1(s, x) = \frac{1}{(4\pi)^{1/2}} x^{1/2} \sum_{k=0}^{\infty} \frac{(-1)^k (xs)^k}{k! (k+1/2)} + c_1 + \mathcal{O}(x^{-1/2}, s) \quad (\text{A.11})$$

where  $c_1$  and  $c_2$  are constants. Substituting now the above expansions of the functions  $W_d(s, x)$  for  $d=1, 2, 3$  into Eq. (A.5), we obtain the asymptotic representations in Eqs. (4.29)–(4.30) for the functions  $f_d(\lambda, x)$  in the case  $\lambda x = \mathcal{O}(1)$  or  $\lambda x \rightarrow 0$  as  $\lambda \rightarrow 0$  and  $x \rightarrow \infty$ .

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