Casimir force in $O(n)$ systems with a diffuse interface

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We study the behavior of the Casimir force in $O(n)$ systems with a diffuse interface and slab geometry $\infty^{d-1}\times L$, where $2<d<4$ is the dimensionality of the system. We consider a system with nearest-neighbor anisotropic interaction constants $J_\parallel$ parallel to the film and $J_\perp$ across it. We argue that in such an anisotropic system the Casimir force, the free energy, and the helicity modulus will differ from those of the corresponding isotropic system, even at the bulk critical temperature, despite that these systems both belong to the same universality class. We suggest a relation between the scaling functions pertinent to the both systems. Explicit exact analytical results for the scaling functions, as a function of the temperature T, of the free energy density, Casimir force, and the helicity modulus are derived for the $n\to\infty$ limit of $O(n)$ models with antiperiodic boundary conditions applied along the finite dimension L of the film. We observe that the Casimir amplitude $\Delta_{\mathrm{Casimir}}(d|J_\perp,J_\parallel)$ of the anisotropic d-dimensional system is related to that of the isotropic system $\Delta_{\mathrm{Casimir}}(d)$ via $\Delta_{\mathrm{Casimir}}(d|J_\perp,J_\parallel)=(J_\perp/J_\parallel)^{(d-1)/2}\Delta_{\mathrm{Casimir}}(d)$. For $d=3$ we derive the exact Casimir amplitude $\Delta_{\mathrm{Casimir}}(3,|J_\perp,J_\parallel)=[\mathrm{Cl}_2(\pi/3)/3-\zeta(3)/(6\pi)](J_\perp/J_\parallel)$, as well as the exact scaling functions of the Casimir force and of the helicity modulus $\Upsilon(T,L)$. We obtain that $\beta_c\Upsilon(T_c,L)=(2/\pi^2)[\mathrm{Cl}_2(\pi/3)/3+7\zeta(3)/(30\pi)](J_\perp/J_\parallel)L^{-1}$, where T_c is the critical temperature of the bulk system. We find that the contributions in the excess free energy due to the existence of a diffuse interface result in a repulsive Casimir force in the whole temperature region.

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I. INTRODUCTION

The excess free energy due to the finite-size contributions to the free energy of a system with a film geometry characterizes a fluctuation-mediated interaction which is termed the Casimir force. In the case of a fluid confined between two parallel walls this force is also sometimes called solvation force or disjoining pressure. The force is named so after the Dutch physicist Hendrik B. G. Casimir who in 1948 [1] noticed that when two metallic perfectly conducting uncharged plates face each other in vacuum at zero temperature the restriction and the modification of the zero-point vacuum fluctuations of the electromagnetic field between the two parallel plates lead to a dependence of the energy of the system on the distance L between the plates and, thus, to a force between them which turns out to be attractive. The above is the so-called classical (actually quantum mechanical) Casimir effect. When the fluctuating medium is not a vacuum, but a thermodynamic system, say fluid, near its bulk critical point T_c one arrives at the so-called thermodynamic Casimir effect that has been predicted by Fisher and de Gennes [2] in 1978 and which has been a subject of intensive theoretical and experimental studies afterwards [3–29].

In the current article we will investigate the behavior of the Casimir force in systems with a diffuse interface. When two phases coexist the borderline between them can either be characterized by some abrupt change of their order parameter, i.e., via a sharp interface, or via a continuum change of the order parameter in a given region of space between them, thus forming a diffuse interface. As a realization of such systems that might possess a diffuse interface one can consider the so-called $O(n)$ models. These models are characterized by an order parameter field with n components and by an interaction energy which is $O(n)$ invariant function of the local dynamic variables (fields). More precisely, one can think about the reaction of $O(n)$ models, with $n\geqslant 2$, to some helical external field which can be characterized in terms of some helicity modulus Υ or, in the case of magnetic materials, of Bloch walls between the domains of the magnet. Heuristically, the helicity modulus is the analog of the interface tension of Ising-like, i.e., $n=1$ systems, for $O(n\geqslant 2)$ symmetric systems. The simplest theoretical model of a system with a diffuse interface is the $O(n\geqslant 2)$ model with antiperiodic boundary conditions and short-ranged interactions. Prominent examples of the $O(n)$ models are the XY ($n=2$) and the Heisenberg ($n=3$) models.

A. The thermodynamic Casimir force

We remind the reader that for an $O(n\geqslant 1)$ model of a d-dimensional system with a temperature T and geometry $\infty^{d-1}\times L$ the thermodynamic Casimir force is defined by [3,5]

$$F_{\mathrm{Casimir}}^{(\tau)}(T,L)=-\frac{\partial f_{\mathrm{ex}}^{(\tau)}(T,L)}{\partial L}, \tag{1.1}$$

where $f_{\mathrm{ex}}^{(\tau)}(T,L)$ is the excess free energy

$$f_{\mathrm{ex}}^{(\tau)}(T,L)=f^{(\tau)}(T,L)-Lf_b(T), \tag{1.2}$$

and the superscript τ denotes the dependence on the boundary conditions. Here $f^{(\tau)}(T,L)$ is the full free energy per unit area of such a system under boundary conditions τ and f_b is the bulk free energy density. It is believed, and the accumulated evidences support it [3–28,30–32], that if the boundary conditions are the same at both surfaces bounding the system, $F_{\rm Casimir}^{(\tau)}$ will be negative. 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. If the boundary conditions are essentially different at both surface planes confining the system (e.g., one of the surfaces prefer the liquid phase of the fluid while the other prefers the gas phase) the Casimir force is expected to be positive in the whole region of the thermodynamic parameters, i.e., then the net force between the plates will be *repulsive*.

Recently it has been shown, however, that the above picture is oversimplified. It has been demonstrated, e.g., that under appropriate conditions smooth crossovers from repulsive to attractive as well as from attractive to repulsive Casimir forces are possible as the thickness L of a film changes [29]. It has been also argued [35] that the Casimir force can be influenced by the anisotropy of the system, even in the case when the anisotropy is weak, i.e., when it does not change the universality class of the bulk system. In the current article we will show that the change of the boundary conditions in an $O(n)$ system with film geometry, from such under which the system does not possess a diffuse interface to such under which an interface is enforced, is enough to transform the force between the plates bounding the film from being attractive to being repulsive. We will allow for anisotropy which reflects the geometry of the system taking the interaction constant along the surface to be different from the one perpendicular to the film. We will show that under such anisotropy, which does not change the universality class, the Casimir force of the anisotropic system differs from that one of the isotropic system and will establish a relation that connects both of them. We will perform our calculations on the example of an exactly solvable model—the mean spherical model. We will consider the behavior of this model under periodic and antiperiodic boundary conditions. We recall that under such boundary conditions, which preserve the translational invariance of the system, the spherical model is equivalent to the $n\to\infty$ limit of the $O(n)$ models [36], and thus retains essential properties pertinent to models with continuous symmetry of the order parameter such as the XY and Heisenberg models.

B. Finite-size behavior of systems with a diffuse interface

According to the standard finite-size scaling theory (see, e.g., Refs. [5,37] for a general review) one expects that near the critical temperature T_c (of the corresponding bulk, i.e., $L=\infty$ system) the behavior of $F_{\rm Casimir}^{(a)}$ in a system with sssa film geometry under antiperiodic (a) boundary conditions is given by

$$\beta F_{\rm Casimir}^{(a)}(T,L)=L^{-d}X_{\rm Casimir}^{(a)}(x_t), \tag{1.3}$$

while that one of the excess free energy $f_{\rm ex}^{(a)}$ is

$$\beta f_{\rm ex}^{(a)}(T,L)=L^{-(d-1)}X_f^{(a)}(x_t), \tag{1.4}$$

where $\beta=1/(k_BT)$, $x_t=a_t tL^{1/\nu}$ is the temperature scaling variable with $t=(T-T_c)/T_c$ being the reduced temperature, a_t is a nonuniversal scaling factor, while $X_{\rm Casimir}^{(a)}$ and $X_f^{(a)}$ are *universal* (geometry dependent) scaling functions and ν is the corresponding (universal) scaling exponent that characterizes the temperature divergence of the bulk two-point correlation length ξ when one approaches the bulk critical temperature from above, i.e., $\xi(t\to0^+)\simeq\xi_0^+t^{-\nu}$. The scaling functions $X_{\rm Casimir}^{(a)}$ and $X_f^{(a)}$ are related via

$$X_{\rm Casimir}^{(a)}(x_t)=(d-1)X_f^{(a)}(x_t)-\frac{1}{\nu}x_t\frac{d}{dx_t}X_f^{(a)}(x_t). \tag{1.5}$$

The value of $X_f^{(a)}$ at the critical point is known as the Casimir amplitude $\Delta^{(a)}$, i.e., $\Delta^{(a)}\equiv X_f^{(a)}(x_t=0)$. On its turn, the excess free energy under antiperiodic conditions $f_{\rm ex}^{(a)}$ can be related to the one of the same system under periodic boundary conditions $f_{\rm ex}^{(p)}$ via the finite-size helicity modulus $\Upsilon(T,L)$. The concept of the helicity modulus was introduced by Fisher *et al.* [38]. 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, where $n\geqslant2$, 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, i.e., $n=1$ order parameter (e.g., an Ising model). In other words, the helicity modulus is a measure of the increase of the energy of the system due to the existence of a diffuse interface within it. When in an $O(n)$, $n\geqslant2$, model system such an interface is created by, say, the application of antiperiodic boundary conditions, the *finite-size* helicity modulus can be defined, e.g., as suggested in [39],

$$\Upsilon(T,L)\equiv\frac{2L}{\pi^2}[f_{\rm ex}^{(a)}(T,L)-f_{\rm ex}^{(p)}(T,L)]. \tag{1.6}$$

Obviously, the helicity modulus of the "infinite" system then simply is $\Upsilon(T)\equiv\lim_{L\to\infty}\Upsilon(T,L)$, with $\Upsilon(T)\geqslant0$, which is in a complete agreement with [38]. Thus, inverting the above definitions, one immediately obtains [40]

$$f_{\rm ex}^{(a)}(T,L)=f_{\rm ex}^{(p)}(T,L)+\frac{\pi^2}{2L}\Upsilon(T,L). \tag{1.7}$$

For the behavior of $\Upsilon(T,L)$ near T_c the standard finite-size scaling theory states that

$$\beta\Upsilon(T,L)=L^{-(d-2)}X_\Upsilon(x_t), \tag{1.8}$$

where X_Υ is a universal scaling function. Actually, when $d=3$, a modification of Eq. (1.8) has been suggested in [42] by Privman, who supposed the possibility of appearance of "resonant" logarithmic term due to the mutual influence of the regular and singular contributions in the helicity modulus

$$\beta\Upsilon(T,L)=L^{-1}[\tilde{X}_\Upsilon(x_t)+\omega\ln(L/\sigma_0)]+\Phi(T)L^{-1}+\cdots, \tag{1.9}$$

where ω is an universal amplitude, while $\Phi(T)$ is a regular at T_c function and σ_0 is some characteristic microscopic length scale (e.g., the distance between the molecules of the correlated fluid, or the lattice spacing). The validity of this hypothesis has been checked in [39] on the example of the exactly solvable mean-spherical model with isotropic nearest-neighbor interactions. No logarithmic corrections of the type predicted in Eq. (1.9) have been found. In the current article we will demonstrate that this statement is still valid when the interaction is anisotropic (see below). Let us recall that in the case of superfluids ($n=2$, $d=3$) the helicity modulus Υ is proportional [38] to the superfluid density fraction ϱ, namely $\varrho=(m/\hbar)^2\Upsilon(T)$ with m being the mass of the helium atom, and is directly measurable (for experiments measuring ϱ in thin films of ^{4}He see, e.g., Refs. [43,44]). In fact, Eq. (1.9) was proposed in [42] as an attempt to improve the fit of the experimental data. It turns out, however, that the overall fit of the data is improved only in a very limited way, provided one insists on the bulk value of ν in the scaling variable x_t. The scaling "data collapse" technique works well if one takes ν as an adjustable parameter 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 [43,44].

According to all the accumulated analytical and numerical evidences, see, e.g., Refs. [5,37], and references cited therein, when $x_t \gg 1$ both the excess free energy and the Casimir force under both periodic and antiperiodic boundary conditions in systems with short-ranged interactions is expected to tend to zero in an exponential-in-L way. This is consistent with $\Upsilon(T)\equiv 0$ for $T \geqslant T_c$. When $x_t \to -\infty$ the same quantities tend to zero in a power-law-in-L way. This slow algebraic decay of $f_{\rm ex}$ (and of $F_{\rm Casimir}$) is, of course, associated with the existence of soft modes in the system (spin waves) when $T<T_c$ and in the absence of an ordering external field destroying the $O(n)$ symmetry and suppressing the spin-wave type excitations [45]. This, in turn, will lead to a much greater (in comparison with the Ising-like case) Casimir (solvation) force in $O(n>1)$ models when $T<T_c$. With respect to the Casimir force the last has not only been predicted theoretically, but has been also observed experimentally [12,16] and, relatively recently, confirmed within a Monte Carlo study of the XY model [24,26]. The considered systems do not posses, however, a diffuse interface. When such an interface is present and $T<T_c$, from Eq. (1.7) it is easy to see that

$$F^{(a)}_{\rm Casimir}(T<T_c, L \gg \sigma_0) \simeq \frac{1}{2}\pi^2\Upsilon(T)L^{-2}. \tag{1.10}$$

Since $\Upsilon(T)\geqslant 0$ the last implies that the Casimir force will be *repulsive and much stronger*, of the order of L^{-2}, than in systems with no diffuse interface where it is either of the order of L^{-d}, or smaller.

C. Finite-size behavior of systems with weak anisotropy

Since we consider film geometry, it is natural to allow for an anisotropy of the interactions in the system which reflects this geometry. To that aim we will take the interaction constant in the Hamiltonian along the surface, say $J_\parallel$, to be different from the one perpendicular to the film, say $J_\perp$. Since such anisotropy, known as weak anisotropy, does not change the universality class of the bulk system, one might naively expect that the scaling functions of the *finite* system $X^{(a)}_{\rm Casimir}$, $X^{(a)}_f$, and X_Υ will be the same as for the isotropic system. Recently it has been argued, however, see Refs. [35,49], that this is not true and that one shall expect these functions to be *nonuniversal* and depending on the ratio $J_\perp/J_\parallel$. It has been shown [35,49] that the main reason for this state of affairs is the need of a generalization of the standard hyperuniversality hypothesis [50–55]. According to it, if $\bar{f}_{b,\rm sing}(T)$ is the singular part of the bulk free energy density f_b normalized per k_BT, and $\xi(T)$ is the bulk two-point correlation length in the isotropic system, then one has

$$\lim_{T\to T_c^+} \bar{f}_{b,\rm sing}(T)[\xi(T)]^d = Q, \tag{1.11}$$

where Q is a universal constant that characterizes the corresponding universality class. If now $\bar{f}_{b,\rm sing}(T|J_\perp,J_\parallel)$ is the corresponding free energy in the anisotropic film system with $\xi_\parallel(t\to 0^+)=\xi^+_{\parallel,0}t^{-\nu}$ being the correlation length along the system surface and $\xi_\perp(t\to 0^+)=\xi^+_{\perp,0}t^{-\nu}$ the one perpendicular to it, then the generalized hyperuniversality hypothesis states that

$$\lim_{T\to T_c^+} \bar{f}_{b,\rm sing}(T|J_\perp,J_\parallel)[\xi_\parallel(T)]^{d-1}\xi_\perp(T) = Q, \tag{1.12}$$

with Q being the same universal quantity as in the isotropic case. Note that in Eq. (1.12) T_c is the critical temperature of the anisotropic system which, in general, differs from that one of the isotropic system, see Eq. (1.11). Next, the hypothesis involves two different correlation lengths, characterized by two different correlation length amplitudes, while the standard hypothesis deals with only one correlation length. It is worthwhile to recall that the validity of Eq. (1.11) is one of the main prerequisites for arguing the validity of the scaling hypothesis (1.4) by Privman and Fisher [56]. It is, however, possible to relate the scaling functions of the normalized free energy densities of the anisotropic to that one of the isotropic system. Indeed, choosing the isotropic system to be such that its correlation length is equal to, say, $\xi_\perp$ and considering in Eqs. (1.11) and (1.12) the limits $T\to T_c$ to the corresponding critical temperatures of the anisotropic and isotropic systems, one obtains that

$$\bar{f}_{b,\rm sing}(T|J_\perp,J_\parallel) \simeq \left[\frac{\xi_\perp(T)}{\xi_\parallel(T)}\right]^{d-1}\bar{f}_{b,\rm sing}(T), \quad T\to T_c^+, \tag{1.13}$$

and, thus one arrives at

$$X^{(a)}_f(x_t|J_\perp,J_\parallel) = \left[\frac{\xi_{\perp,0}}{\xi_{\parallel,0}}\right]^{d-1} X^{(a)}_f(x_t), \tag{1.14}$$

where $\xi_{\parallel,0}$ and $\xi_{\perp,0}$ are the correlation length amplitudes in the anisotropic system, while $X^{(a)}_f(x_t)$ is the universal scaling function of the isotropic one. We expect x_t to be of the form $x_t=a_t(\mathbf{b})tL^{1/\nu}$. The last implies that all the effect of the anisotropy of the type considered can be incorporated in the factor $(\xi_{\perp,0}/\xi_{\parallel,0})^{d-1}$ in front of the scaling function on the right-hand side of Eq. (1.14) and in the nonuniversal factor a_t that enters in the definition of the temperature scaling variable x_t, provided the reduced temperature t is measured with respect to the critical temperature T_c shifted by the anisotropy. Of course, despite of the arguments presented aimed to justify these relations, Eqs. (1.13) and (1.14) shall be considered only as plausible hypotheses whose validity has to be verified [57]. Note that, if valid, Eq. (1.14) implies a relation of the Casimir amplitudes in the anisotropic and isotropic systems

$$\Delta_{\text{Casimir}}(d|J_\perp,J_\|)=(\xi_{\perp,0}/\xi_{\|,0})^{d-1}\Delta_{\text{Casimir}}(d). \qquad (1.15)$$

It is worthwhile to mention that despite Eqs. (1.14) and (1.15) written in terms of systems with antiperiodic boundary conditions, no specific properties of systems with such boundary conditions have been used in arguing their validity. We required only the validity of Eqs. (1.11) and (1.12) which concern bulk systems, i.e., they are independent of any possible boundary conditions applied on the finite system. Thus, we expect that Eqs. (1.14) and (1.15) hold for general boundary conditions τ imposed on the pair of isotropic and anisotropic systems involved in these equations.

In the current article on the example of the exactly solvable mean spherical model with $2<d<4$ we will demonstrate that in the anisotropic system with a diffuse interface the scaling functions $X_{\text{Casimir}}^{(a)}$, $X_f^{(a)}$, and X_Υ indeed depend, in addition on the scaling variable x_t, on the ratio $J_\perp/J_\|$. This will lead, e.g., to nonuniversality of the Casimir amplitudes in such systems which are, however, simply related to the ones of the isotropic system via the relation (1.15). We will determine the explicit form of the scaling function of the free energy, Casimir force, and of the finite-size helicity modulus. For the case $d=3$ in the isotropic system we will find the universal values of these quantities at the critical point T_c of the bulk system. We will also consider the case when the nearest-neighbor interaction $J_\|$ along the film might be different from the one in orthogonal direction $J_\perp$.

The structure of the article is as follows. In Sec. II we define the model under consideration and provide some basic expressions needed for its treatment. The results for the finite-size behavior of the free energy and of the Casimir force are presented in Sec. III, in Sec. III A we present our general results for $2<d<4$, while in Sec. III B the explicit results for the important case of $d=3$ are given. Our findings about the behavior of the helicity modulus are contained in Sec. IV. The article closes with a discussion and concluding remarks given in Sec. V. Some technical details and results needed in the main text are derived in Appendixes A and B.

II. THE SPHERICAL MODEL

As stated above, we will study the finite-size behavior of an anisotropic system with a diffuse interface on the example of a spherical model embedded on a d-dimensional hypercubic lattice $\mathcal{L}\in\mathbb{Z}^d$, where $\mathcal{L}=L_1\times L_2\times\cdots L_d$. Let $L_i=N_i a_i$, $i=1,\cdots,d$, where N_i is the number of spins and a_i is the lattice constant along the axis i with $\mathbf{e}_i$ being a unit vector along that axis, i.e., $\mathbf{e}_i\cdot\mathbf{e}_j=\delta_{ij}$. With each lattice site $\mathbf{r}$ one associates a real-valued spin variable $S_\mathbf{r}$ which obeys the constraint

$$\frac{1}{\mathcal{N}}\sum_{\mathbf{r}\in\mathcal{L}}\langle S_\mathbf{r}^2\rangle=1, \qquad (2.1)$$

where $\mathcal{N}=N_1N_2\cdots N_d$ is the total number of spins in the system. The average in Eq. (2.1) is with respect to the Hamiltonian of the model

$$\beta\mathcal{H}=-\frac{1}{2}\beta\sum_{\mathbf{r},\mathbf{r}'}S_\mathbf{r}J(\mathbf{r},\mathbf{r}')S_{\mathbf{r}'}+s\sum_\mathbf{r}S_\mathbf{r}^2, \qquad (2.2)$$

where s is the so-called "spherical field" whose value is such that the constraint (2.1) is fulfilled. In the current article we will consider only the case of nearest-neighbor interactions, i.e., we take $J(\mathbf{r},\mathbf{r}')=J(|\mathbf{r}-\mathbf{r}'|)=J_i$, if $\mathbf{r}-\mathbf{r}'=\pm a_i\mathbf{e}_i$, $i=1,\cdots,d$, and $J(\mathbf{r},\mathbf{r}')=0$ otherwise. Explicitly, one has $J(\mathbf{r},\mathbf{r}')=\sum_{i=1}^d J_i[\delta(\mathbf{r}-\mathbf{r}'-a_i\mathbf{e}_i)+\delta(\mathbf{r}-\mathbf{r}'+a_i\mathbf{e}_i)]$. Let periodic boundary conditions be applied along directions $\mathbf{e}_i$, $i=1,\cdots(d-1)$, while antiperiodic boundary conditions, responsible for the creation of a diffuse interface within the system, are applied along $\mathbf{e}_d$. Generalizing the results of [5,7,39,59,60] pertinent to an isotropic model for the here considered anisotropic case, it can be shown that the free energy of the model (per unit spin) is given by [61]

$$\beta f^{(a)}(\beta,\mathbf{N}|d,\mathbf{J})=-\frac{1}{2}\ln\pi+\sup_{s>\hat{J}_{\max}^{(a)}}\left\{-s+\frac{1}{2\mathcal{N}}\sum_{\mathbf{k}\in\text{BZ}_1}\ln\left[s-\frac{1}{2}\beta\hat{J}^{(a)}(\mathbf{k})\right]\right\}, \qquad (2.3)$$

where $\mathbf{N}=(N_1,N_2,\cdots N_d)$, $\mathbf{J}=(J_1,J_2,\cdots,J_d)$, $\hat{J}^{(a)}(\mathbf{k})$ is the Fourier transform of the interaction $\mathbf{J}$, i.e.,

$$\hat{J}^{(a)}(\mathbf{k})=\sum_\mathbf{r}J(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}, \qquad (2.4)$$

$\hat{J}_{\max}^{(a)}=\max_\mathbf{k}\hat{J}^{(a)}(\mathbf{k})$, and the wave vector $\mathbf{k}=(k_1,k_2,\cdots,k_d)\in\text{BZ}_1$, with BZ_1 being the first Brillouin zone, has components $k_i=2\pi n_i/L_i$, where $n_i=0,\cdots,N_i-1$, and $i=1,\cdots,(d-1)$, while $k_d=2\pi(n_d+1/2)/L_d$ with $n_d=0,\cdots,N_d-1$. Thus, explicitly one has

$$\hat{J}^{(a)}(\mathbf{k})=2\sum_{i=1}^{d-1}J_i\cos\left(\frac{2\pi n_i}{N_i}\right)+2J_d\cos\left(\frac{\pi(2n_d+1)}{N_d}\right), \qquad (2.5)$$

and $\hat{J}_{\max}^{(a)}=2\sum_{i=1}^{d-1}J_i+2J_d\cos(\pi/N_d)\equiv\hat{J}_0-2J_d[1-\cos(\pi/N_d)]$, with $\hat{J}_0=2\sum_{i=1}^d J_i$. Note that the ground state energy $\hat{J}_{\max}^{(a)}$ depends on N_d and is twofold degenerate—it is reached for both $k_1=k_2=\cdots=k_{d-1}=k_d=0$ and $k_1=k_2=\cdots=k_{d-1}=0,k_d=N_d-1$. Equation (2.1) for the spherical field s reads

$$\frac{1}{2\mathcal{N}}\sum_{\mathbf{k}\in\text{BZ}_1}\frac{1}{s-\frac{1}{2}\beta\hat{J}^{(a)}(\mathbf{k})}=1. \qquad (2.6)$$

We will be mainly interested in determination of the Casimir force and the helicity modulus within the considered model in a film geometry. For that aim let us take $J_1=J_2=\cdots=J_{d-1}=J_\parallel$, $N_1=N_2=\cdots=N_{d-1}=N_\parallel$, $J_d=J_\perp$, $N_d=N_\perp$ and perform the limit $N_\parallel\to\infty$, i.e., consider a system with a film geometry in which all the interactions in directions parallel to the film surface are equal (to $J_\parallel$) but possibly different from the interaction in the direction perpendicular to the surface (which is $J_\perp$). Then, Eqs. (2.3) and (2.6) become

$$\beta f^{(a)}(\beta,N_\perp|d,\mathbf{J}) = \frac{1}{2}\ln\frac{K}{2\pi} - \frac{1}{2}K\frac{\hat{J}^{(a)}_{\max}}{\hat{J}_0} + \sup_{w>0}\left\{U^{(a)}(w,N_\perp|d,\mathbf{J}) - \frac{1}{2}Kw\right\}, \tag{2.7}$$

$$K = \frac{1}{N_\perp}\sum_{k_d}\int_{\mathbf{k}_\parallel\in \mathrm{BZ}_1}^{(d-1)} \frac{1}{w+\omega^{(a)}(\mathbf{k}_\parallel,k_d|d,\mathbf{J})}, \tag{2.8}$$

correspondingly, where $\mathbf{k}=(\mathbf{k}_\parallel,k_d)$ with $\mathbf{k}_\parallel=(k_1,k_2,\cdots,k_{d-1})$, $K=\beta\hat{J}_0$,

$$U^{(a)}(w,N_\perp|d,\mathbf{J}) = \frac{1}{2N_\perp}\sum_{k_d}\int_{\mathbf{k}_\parallel\in \mathrm{BZ}_1}^{(d-1)} \ln[w+\omega^{(a)}(\mathbf{k}_\parallel,k_d|d,\mathbf{J})], \tag{2.9}$$

with

$$\omega^{(a)}(\mathbf{k}|d,\mathbf{J}) = [\hat{J}^{(a)}_{\max} - \hat{J}^{(a)}(\mathbf{k})]/\hat{J}_0 \geqslant 0, \tag{2.10}$$

$$\int_{\mathbf{k}\in \mathrm{BZ}_1}^{(d-1)} \equiv \prod_{i=1}^{d-1}\int_0^{2\pi}\frac{dk_i}{2\pi}, \tag{2.11}$$

and we have replaced the spherical field s by another field w, defined as

$$w = 2s/K - \hat{J}^{(a)}_{\max}/\hat{J}_0. \tag{2.12}$$

Here

$$\hat{J}^{(a)}_{\max} = 2(d-1)J_\parallel + 2J_\perp\cos(\pi/N_\perp) \tag{2.13}$$

is the ground state energy of the finite system under antiperiodic boundary conditions, while

$$\hat{J}_0 = 2(d-1)J_\parallel + 2J_\perp \tag{2.14}$$

is the ground state energy of the infinite one and, thus,

$$\hat{J}^{(a)}_{\max}/\hat{J}_0 = (d-1)b_\parallel + b_\perp\cos(\pi/N_\perp), \tag{2.15}$$

where

$$b_\perp = J_\perp/\sum_{i=1}^{d} J_i \tag{2.16}$$

and

$$b_\parallel = J_\parallel/\sum_{i=1}^{d} J_i \tag{2.17}$$

reflect the asymmetry in the interaction.

Equations (2.7)–(2.12) provide the basis for the investigation of the behavior of the Casimir force within the mean-spherical model in the presence of a diffusive interface in the system.

III. FINITE-SIZE BEHAVIOR OF THE FREE ENERGY AND THE CASIMIR FORCE

A. General results for the case $2<d<4$

From Eq. (2.7) for the excess free energy $\beta f^{(a)}_{\mathrm{ex}}(\beta,N_\perp|d,\mathbf{b})=N_\perp[\beta f^{(a)}(\beta,N_\perp|d,\mathbf{b})-\beta f_b(\beta|d,\mathbf{b})]$ one obtains

$$\beta f^{(a)}_{\mathrm{ex}}(\beta,N_\perp|d,\mathbf{b}) = N_\perp\left[\frac{1}{2}b_\perp K\left(1-\cos\frac{\pi}{N_\perp}\right) - \frac{1}{2}K(w-w_b) + U^{(a)}(w,N_\perp|d,\mathbf{b}) - U_d(w_b|\mathbf{b})\right], \tag{3.1}$$

where $f_b(\beta|d,\mathbf{b})\equiv\lim_{N_\perp\to\infty} f(\beta,N_\perp|d,\mathbf{b})$, $\mathbf{b}=(b_\parallel,\cdots,b_\parallel,b)$, $w\equiv w(K,N_\perp|d,\mathbf{b})$ is the solution of Eq. (2.8), and $w_b\equiv w_b(K|d,\mathbf{b})$ is the $(N_\perp\to\infty)$ limit of $w_b(K,N_\perp|d,\mathbf{b})$, i.e., $w_b(K|d,\mathbf{b})=\lim_{N_\perp\to\infty} w(K,N_\perp|d,\mathbf{b})$. As it is well known, see e.g., Ref. [5], for $K<K_c=W_d(0|\mathbf{b})$ the spherical filed w_b is solution of the equation

$$K = W_d(w_b|\mathbf{b}), \tag{3.2}$$

where, for $w\geqslant 0$,

$$W_d(w|\mathbf{b}) = \frac{1}{2}\int_{\mathbf{k}\in \mathrm{BZ}_1}^{(d)}\frac{1}{w+\omega(\mathbf{k}|d,\mathbf{b})}, \tag{3.3}$$

is the d-dimensional Watson type integral. When $K\geqslant K_c$ one has $w_b=0$. In Eq. (3.1) $U_d(w|\mathbf{b})=\lim_{N_\perp\to\infty} U^{(a)}(w,N_\perp|d,\mathbf{b})$ which, according to Eq. (2.9), reads

$$U_d(w|\mathbf{b}) = \frac{1}{2}\int_{\mathbf{k}\in \mathrm{BZ}_1}^{(d)}\ln[w+\omega(\mathbf{k}|d,\mathbf{b})]. \tag{3.4}$$

Note that it does not depend on the boundary conditions. Obviously, the only nontrivial $N_\perp$ dependence in $f^{(a)}_{\mathrm{ex}}$ stems from the size dependence of the spherical field w and from the asymptotic behavior of $U^{(a)}(w,N_\perp|d,\mathbf{b})$ on $N_\perp$ for $N_\perp\gg 1$. Let us now study these dependencies in detail.

Using the identity

$$\ln a = \int_0^\infty\frac{dx}{x}(e^{-x}-e^{-ax}) \tag{3.5}$$

one can rewrite Eq. (2.9) into the form

$$U^{(a)}(w,N_\perp|d,\mathbf{b}) = \frac{1}{2}\int_0^\infty\frac{dx}{x}\{e^{-x} - e^{-wx}S^{(a)}_{N_\perp}(xb_\perp)\times[e^{-xb_\parallel}I_0(xb_\parallel)]^{d-1}\}, \tag{3.6}$$

where

$$S_N^{(a)}(z) = \frac{1}{N}\sum_{n=0}^{N-1} \exp\left[-z\left(\cos\frac{\pi}{N} - \cos\frac{\pi(2n+1)}{N}\right)\right] \tag{3.7}$$

and $I_0(z)$ is the modified Bessel function of the first kind [58]. With the help of the identity

$$S_N^{(a)}(z) = \exp\left[z\left(1-\cos\frac{\pi}{N}\right)\right][2S_{2N}^{(p)}(z) - S_N^{(p)}(z)], \tag{3.8}$$

where

$$S_N^{(p)}(z) = \frac{1}{N}\sum_{n=0}^{N-1} \exp\left[-z\left(1-\cos\frac{2\pi n}{N}\right)\right] \tag{3.9}$$

the problem of determining the asymptotic behavior of the sum $S_N^{(a)}(x)$ when $N \gg 1$, which characterizes the *antiperiodic* boundary conditions, can be reduced to the determination of the asymptotic behavior of the sum $S_N^{(p)}(x)$, which is pertinent to systems with *periodic* boundary conditions. It can be shown that [39]

$$S_N^{(a)}(x) \simeq \begin{cases} S_N^{+(a)} = \dfrac{2}{N} + \dfrac{2}{N}R^{(+)}\left(\dfrac{\pi^2}{2N^2}x\right) - v(x/2), & x \geq N^2, \\ S_N^{-(a)} = \exp\left[x\left(1-\cos\dfrac{\pi}{N}\right)\right]\left[e^{-x}I_0(x) + \sqrt{\dfrac{2}{\pi x}}R^{(-)}\left(\dfrac{2N^2}{x}\right)\right], & x \leq N^2, \end{cases} \tag{3.10}$$

with corrections to the right-hand side of the above expressions smaller than the terms retained there; here

$$R^{(+)}(x) = \sum_{n=1}^{\infty} e^{-4n(n+1)x}, \tag{3.11}$$

$$R^{(-)}(x) = 2\sum_{n=1}^{\infty} e^{-n^2 x} - \sum_{n=1}^{\infty} e^{-n^2 x/4}, \tag{3.12}$$

$$v(x) = \frac{1}{\sqrt{4\pi x}}[1-\operatorname{erf}(\pi\sqrt{x})]. \tag{3.13}$$

In addition, with the help of the Poisson identity, one can easily check that the following equivalent representations of functions $R^{(+)}(x)$ and $R^{(-)}(x)$ are valid

$$R^{(+)}(x) = \frac{1}{2}e^{x}\theta_2(0,e^{-4x}) - 1, \tag{3.14}$$

$$R^{(-)}(x) = \sum_{n=1}^{\infty}(-1)^n e^{-n^2 x/4} = \frac{1}{2}[\theta_4(0,e^{-x/4}) - 1], \tag{3.15}$$

where $\theta_2(x)$ and $\theta_4(x)$ are the corresponding elliptic theta functions [58].

If one insists on using only the second asymptote in Eq. (3.10) as the one valid for all x, see, e.g., Ref. [60], then the corresponding result for $U^{(a)}(w,N_\perp|d,\mathbf{b})$ reads

$$U^{(a)}(w,N_\perp|d,\mathbf{b}) = U_d(\tilde{w}|\mathbf{b}) - \frac{N_\perp^{-d}}{(4\pi)^{d/2}}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} \times \int_0^\infty \frac{dx}{x}x^{-d/2}e^{-\tilde{y}x}R^{(-)}\left(\frac{1}{x}\right), \tag{3.16}$$

where

$$\tilde{w} = w - b_\perp\left(1-\cos\frac{\pi}{N_\perp}\right), \tag{3.17}$$

$$\tilde{y} = y - \pi^2, \quad y = (2N_\perp^2/b_\perp)w \tag{3.18}$$

and, see Eq. (3.6),

$$U_d(\tilde{w}|\mathbf{b}) = \frac{1}{2}\int_0^\infty \frac{dx}{x}\{e^{-x} - e^{-\tilde{w}x}[e^{-xb_\perp}I_0(xb_\perp)] \times [e^{-xb_\parallel}I_0(xb_\parallel)]^{d-1}\}. \tag{3.19}$$

Using the representation (3.19) it can be shown [19] that when $\tilde{w}\to 0^+$ one has

$$U_d(\tilde{w}|\mathbf{b}) = U_d(0|\mathbf{b}) + \frac{1}{2}\tilde{w}W_d(0|\mathbf{b}) - \frac{1}{2}\frac{\Gamma(-d/2)}{(2\pi)^{d/2}\prod_{i=1}^{d}\sqrt{b_i}}\tilde{w}^{d/2} + \cdots, \tag{3.20}$$

with the dots representing terms of higher order than those retained in the expression. From Eqs. (3.16) and (3.20), and with the help of the representation (3.15), for the finite-size part $U(w,N_\perp|d,\mathbf{b})$ of the free energy in the limit $\tilde{w}\to 0^+$ and, thus $\tilde{y}\geq 0$, see Eq. (3.18), one obtains

$$\begin{aligned} U^{(a)}(w,N_\perp|d,\mathbf{b}) = {} & U_d(0|\mathbf{b}) + \frac{1}{4}b_\perp\tilde{y}W_d(0|\mathbf{b})N_\perp^{-2} \\ & - N_\perp^{-d}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\tilde{y}^{d/2}\left\{\frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}} + \frac{2}{(2\pi)^{d/2}}\sum_{n=1}^{\infty}(-1)^n\frac{K_{d/2}(n\sqrt{\tilde{y}})}{(n\sqrt{\tilde{y}})^{d/2}}\right\} \\ & + O(N_\perp^{-4}), \end{aligned} \tag{3.21}$$

where $K_\nu(z)$ is the modified Bessel function of the second kind [58]. Then, from Eqs. (3.1), (3.20), and (3.21) for the excess free energy one derives the final result

$$\beta f_{\rm ex}^{(a)}(\beta,N_\perp|d,\mathbf{b}) = N_\perp^{-(d-1)}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\left\{\frac{1}{4}x_t(\tilde{y}-y_b) - \frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}(\tilde{y}^{d/2}-y_b^{d/2}) - \frac{2\tilde{y}^{d/2}}{(2\pi)^{d/2}}\sum_{n=1}^{\infty}(-1)^n\frac{K_{d/2}(n\sqrt{\tilde{y}})}{(n\sqrt{\tilde{y}})^{d/2}}\right\}, \quad (3.22)$$

where x_t is the temperature dependent scaling variable

$$x_t = b_\perp\left(\frac{b_\parallel}{b_\perp}\right)^{(d-1)/2}(K_c-K)N_\perp^{1/\nu}, \quad \nu = 1/(d-2), \quad (3.23)$$

$$y_b = (2N_\perp^2/b_\perp)w_b, \quad (3.24)$$

with w_b being the solution of the bulk spherical field equation (3.2). We recall that both K_c and w_b in Eqs. (3.23) and (3.24) depend on $\mathbf{b}$, i.e., on the anisotropy of the system.

Let us now see what is the correct answer when the complete asymptotic behavior, as given in Eq. (3.10), is used for the determination of the excess free energy.

Using the asymptotes given by Eq. (3.10) one obtains, see Appendix A,

$$U^{(a)}(w,N_\perp|d,\mathbf{b}) = U_d(0|\mathbf{b}) + \frac{1}{4}b_\perp(y-\pi^2)W_d(0|\mathbf{b})N_\perp^{-2} - \frac{1}{2}N_\perp^{-d}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\frac{1}{(4\pi)^{d/2}}\left\{\Gamma(-d/2)y^{d/2} + \pi^2\Gamma(1-d/2)y^{d/2-1} + 2\sqrt{4\pi}\int_0^\infty\frac{dx}{x}x^{-(d-1)/2}e^{-yx}\left[1+R^{(+)}(\pi^2 x) - \frac{1}{2\sqrt{4\pi x}}(1+\pi^2 x)\right]\right\}, \quad (3.25)$$

where $y=(2N_\perp^2/b_\perp)w \geqslant 0$. Then from Eqs. (3.1) and (3.20) for the excess free energy one obtains

$$\beta f_{\rm ex}^{(a)}(\beta,N_\perp|d,\mathbf{b}) = N_\perp^{-(d-1)}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\left\{\frac{1}{4}x_t(y-\pi^2-y_b) - \frac{1}{2}\frac{1}{(4\pi)^{d/2}}[\Gamma(-d/2)(y^{d/2}-y_b^{d/2}) + \pi^2\Gamma(1-d/2)y^{d/2-1}] + I(y,d)\right\}, \quad (3.26)$$

where

$$I(y,d) \equiv -\frac{1}{(4\pi)^{(d-1)/2}}\int_0^\infty dx\, x^{-(d+1)/2}e^{-yx}\times\left[1+R^{(+)}(\pi^2 x) - \frac{1+\pi^2 x}{2\sqrt{4\pi x}}\right]. \quad (3.27)$$

The expression (3.26) has to be compared with Eq. (3.22) that follows when one uses as asymptote of $S_N^{(a)}$, when $N \gg 1$, only the asymptote $S_N^{-(a)}$ from Eq. (3.10) (see, e.g., Ref. [60]). As we see, Eqs. (3.26) and (3.22) differ from each other. However, using the identity

$$1+R^{(+)}(\pi^2 x) = \frac{e^{\pi^2 x}}{\sqrt{4\pi x}}\left[\frac{1}{2}+R^{(-)}\left(\frac{1}{x}\right)\right] \quad (3.28)$$

one can show that when $d<4$ and $y \geqslant \pi^2$,

$$I(y,d) = -\tilde{y}^{d/2}\frac{2}{(2\pi)^{d/2}}\sum_{n=1}^{\infty}(-1)^n\frac{K_{d/2}(n\sqrt{\tilde{y}})}{(n\sqrt{\tilde{y}})^{d/2}} - \frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}\times\left[(\tilde{y}^{d/2}-y^{d/2}) + \pi^2\frac{d}{2}y^{d/2-1}\right] \quad (3.29)$$

and, thus, expression (3.26) is equivalent to (3.22) for $y \geqslant \pi^2$. In the opposite case, when $y<\pi^2$, one can use Eq. (3.26) or, equivalently, the analytical continuation of Eq. (3.22). Therefore, although in the derivation of Eq. (3.22) the incomplete asymptotic behavior of sums involved has been used, which makes this derivation mathematically wrong, and the expansion (3.20) of the bulk quantities has been applied, which is valid only for $y \geqslant \pi^2$, Eq. (3.22) is still valid and can be used for all $y \geqslant 0$ since this equations is equivalent to Eq. (3.26) which is obtained when one follows the proper mathematical procedures.

When $|y-\pi^2|<4\pi^2$ one can provide a representation of the integral $I(y,d)$ in terms of power series which is very convenient for analysis of its behavior for small values of the argument y. The corresponding representation is derived in Appendix B, and reads

$$I(y,d) = \frac{y^{(d-2)/2}}{2(4\pi)^{d/2}}[\pi^2\Gamma(1-d/2) + y\Gamma(-d/2)] - \pi^{(d-1)/2}\sum_{m=0}^{\infty}a_m^{(d)}(\pi^2-y)^m, \quad (3.30)$$

where the coefficients $a_m^{(d)}$ are given by

$$a_m^{(d)} = \frac{(2^{1-d}-2^{-2m})\Gamma\left(m+\frac{1-d}{2}\right)\zeta(2m+1-d)}{\pi^{2m}m!}. \quad (3.31)$$

From Eqs. (1.1), (3.22), and (3.26) for the Casimir force one obtains the following two equivalent representations:

$$\beta F^{(a)}_{\text{Casimir}}(\beta, N_\perp|d, \mathbf{b}) = N_\perp^{-d}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\Bigg\{\frac{1}{4}x_t(\tilde{y}-y_b) - (d-1)\Bigg[\frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}\times(\tilde{y}^{d/2}-y_b^{d/2}) + \tilde{y}^{d/2}\frac{2}{(2\pi)^{d/2}}\times\sum_{n=1}^{\infty}(-1)^n\frac{K_{d/2}(n\sqrt{\tilde{y}})}{(n\sqrt{\tilde{y}})^{d/2}}\Bigg]\Bigg\}, \tag{3.32}$$

in the derivation of which we have used the identity

$$\frac{\partial}{\partial y}[y^\mu K_\mu(ay)] = -ay^\mu K_{\mu-1}(ay), \tag{3.33}$$

and

$$\beta F^{(a)}_{\text{Casimir}}(\beta, N_\perp|d, \mathbf{b}) = N_\perp^{-d}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\Bigg[\frac{1}{4}x_t(y-\pi^2-y_b) - (d-1)\Bigg(\frac{1}{2}\frac{1}{(4\pi)^{d/2}}[\Gamma(-d/2)(y^{d/2} - y_b^{d/2}) + \pi^2\Gamma(1-d/2)y^{d/2-1}] - I(y,d)\Bigg)\Bigg]. \tag{3.34}$$

In Eqs. (3.32) and (3.34) the variables y (or $\tilde{y}$) and y_b satisfy the spherical field equations (2.8) and (3.2), respectively. It can be easily shown that these two equations can be rewritten in a scaling form. In the geometry of a film and under antiperiodic boundary condition the equation for $\tilde{y}$ reads

$$-\frac{1}{2}x_t = \frac{\Gamma(1-d/2)}{(4\pi)^{d/2}}\tilde{y}^{d/2-1} + \tilde{y}^{d/2-1}\frac{2}{(2\pi)^{d/2}}\times\sum_{n=1}^{\infty}(-1)^n\frac{K_{d/2-1}(n\sqrt{\tilde{y}})}{(n\sqrt{\tilde{y}})^{d/2-1}}, \tag{3.35}$$

which is equivalent to

$$-\frac{1}{2}x_t = \frac{\Gamma(1-d/2)}{(4\pi)^{d/2}}y^{d/2-1} + \frac{\Gamma(2-d/2)}{2^d\pi^{d/2-2}}y^{d/2-2} + 2\frac{d}{dy}I(y,d), \tag{3.36}$$

while the corresponding equation for y_b is

$$-\frac{1}{2}x_t = \frac{\Gamma(1-d/2)}{(4\pi)^{d/2}}y_b^{d/2-1}. \tag{3.37}$$

Equations (3.23), (3.32), (3.34), (3.35), and (3.37) demonstrate that the Casimir force in a system with an anisotropic interaction can be written in the form

$$\beta F^{(a)}_{\text{Casimir}}(\beta, N_\perp|d, \mathbf{b}) = N_\perp^{-d}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} X_{\text{Casimir}}(x_t), \tag{3.38}$$

where X_{Casimir} is a universal scaling function, provided a suitable definition of the scaling variables, see Eq. (3.23), is used. Note that x_t is of the form $x_t = a_t(\mathbf{b})\, tL^{1/\nu}$ which means that all the effect of the anisotropy of the type considered can be incorporated in the factor $(b_\perp/b_\parallel)^{(d-1)/2} = (J_\perp/J_\parallel)^{(d-1)/2}$ in front of the scaling function on the right-hand side of Eq. (3.38) and in the nonuniversal factor a_t that enters in the definition of the temperature scaling variable x_t, provided the reduced temperature t is measured with respect to the critical temperature T_c shifted by the anisotropy. Note that with respect to the Casimir amplitudes Eq. (3.38) leads to the following relation between the amplitudes in the anisotropic and isotropic systems

$$\Delta_{\text{Casimir}}(d|J_\perp, J_\parallel) = \left(\frac{J_\perp}{J_\parallel}\right)^{(d-1)/2}\Delta_{\text{Casimir}}(d). \tag{3.39}$$

Note also that, because of the universality, the value of the Casimir amplitude in the isotropic system does not depend on $J \equiv J_\perp = J_\parallel$. In order to achieve a conformity with relation (1.15) one needs only to determine the ratio $\xi_\perp/\xi_\parallel$ in the anisotropic system. In fact, this has already been done in [19] with the result that

$$\frac{\xi_\perp}{\xi_\parallel} = \sqrt{\frac{J_\perp}{J_\parallel}}. \tag{3.40}$$

Inserting Eq. (3.40) into Eq. (3.39) one, indeed, immediately obtains Eq. (1.15).

B. Results for the case $d=3$

Since $d=3$ is of special importance we will present some explicit results for this case. With $d=3$, Eqs. (3.32) and (3.34) simplify to

$$\beta F^{(a)}_{\text{Casimir}}(\beta, N_\perp|d=3, \mathbf{b}) = N_\perp^{-3}\left(\frac{b_\perp}{b_\parallel}\right)\Bigg\{\frac{1}{4}x_t(\tilde{y}-y_b) - \frac{1}{6\pi}(\tilde{y}^{3/2}-y_b^{3/2}) - \frac{\sqrt{\tilde{y}}}{\pi}\mathrm{Li}_2(-e^{-\sqrt{\tilde{y}}}) - \frac{1}{\pi}\mathrm{Li}_3(-e^{-\sqrt{\tilde{y}}})\Bigg\}, \tag{3.41}$$

where $\mathrm{Li}_n(z)$ is the polylogarithm [58], and

$$\beta F^{(a)}_{\text{Casimir}}(\beta, N_\perp|d=3, \mathbf{b}) = N_\perp^{-3}\left(\frac{b_\perp}{b_\parallel}\right)\Bigg\{\frac{1}{4}x_t(y-\pi^2-y_b) - \frac{1}{6\pi}(y^{3/2}-y_b^{3/2}) + \frac{\pi}{4}y^{1/2} + 2I(y,3)\Bigg\}, \tag{3.42}$$

respectively. Accordingly, Eqs. (3.35) and (3.36) for $\tilde{y}$ and y become

$$x_t = \frac{1}{2\pi}\sqrt{\tilde{y}} + \frac{1}{\pi}\ln[1+e^{-\sqrt{\tilde{y}}}], \tag{3.43}$$

and

$$x_t = \frac{1}{2\pi}\sqrt{y} - \frac{\pi}{4\sqrt{y}} + \frac{1}{\pi}\int_0^\infty \frac{dx}{x}e^{-yx}\left[1+R^{(+)}(\pi^2 x) - \frac{1+\pi^2 x}{2\sqrt{4\pi x}}\right]. \tag{3.44}$$

Equation (3.43) can be explicitly solved in the form

$$\sqrt{\tilde{y}} = 2\,\mathrm{arccosh}\left[\frac{1}{2}e^{\pi x_t}\right]. \tag{3.45}$$

At $T=T_c$, i.e., when $x_t=0$, this solution simplifies to

$$\sqrt{\tilde{y}} = \pm i\frac{2\pi}{3}. \tag{3.46}$$

As it is well known [5], the scaling form of the solution of Eq. (3.37) for y_b for the infinite system with $d=3$ is

$$\sqrt{y_b} = \begin{cases} 2\pi x_t, & x_t \geq 0, \\ 0, & x_t \leq 0. \end{cases} \tag{3.47}$$

At $T=T_c$ with $y_b=0$, according to Eq. (3.47), and $\tilde{y}$ from Eq. (3.46) one can from Eq. (3.41) obtain the Casimir amplitude in the form

$$\Delta_{\mathrm{Casimir}} = \left(\frac{J_\perp}{J_\parallel}\right)\left[\frac{1}{3}\,\mathrm{Im}[\mathrm{Li}_2(\sqrt[3]{-1})] - \frac{\zeta(3)}{6\pi}\right], \tag{3.48}$$

which, using the relation $\mathrm{Im}[\mathrm{Li}_2(e^{i\theta})]=\mathrm{Cl}_2(\theta)$ between the polylogarithm and the Clausen function (see, e.g., [62]),

$$\mathrm{Cl}_2(\theta) = \sum_{k=1}^\infty \frac{\sin(k\theta)}{k^2}, \tag{3.49}$$

can be written as

$$\Delta_{\mathrm{Casimir}} = \left(\frac{J_\perp}{J_\parallel}\right)\left[\frac{1}{3}\mathrm{Cl}_2\left(\frac{\pi}{3}\right) - \frac{\zeta(3)}{6\pi}\right] \simeq 0.274\,543\left(\frac{J_\perp}{J_\parallel}\right). \tag{3.50}$$

One can also determine the full temperature dependence of the Casimir force. For that aim, in Fig. 1 we present the scaling function $X_{\mathrm{Casimir}}(x_t)$ of the Casimir force $F_{\mathrm{Casimir}}^{(a)}(\beta,N_\perp|d=3,\mathbf{b})$ as a function of the temperature scaling variable x_t. We observe that $X_{\mathrm{Casimir}}(x_t)>0$ for all x_t, i.e., the Casimir force under antiperiodic boundary conditions is always a repulsive force. Furthermore, from Eqs. (3.41), (3.43), and (3.47) it is easy to check that when $x_t \gg 1$, one has $y, y_b \gg 1$ which lead to the result that the scaling function $X_{\mathrm{Casimir}}(x_t)$ decays exponentially fast to zero, while for $x_t \ll -1$ one has $y \to 0^+$, $y_b=0$ and that

$$X_{\mathrm{Casimir}}(x_t) \underset{x_t\to-\infty}{\approx} -\frac{\pi^2}{4}x_t - \frac{\zeta(3)}{\pi}. \tag{3.51}$$

As we will see below, the last equation, together with Eqs. (3.38) and (4.7), leads to the conclusion that when $T \ll T_c$ the behavior of the Casimir force in systems with a diffuse interface in indeed given by Eq. (1.10).

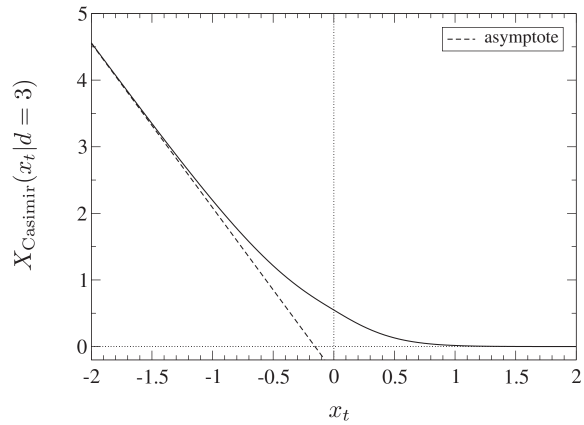

FIG. 1. The scaling function $X_{\mathrm{Casimir}}(x_t)$ of the Casimir force $F_{\mathrm{Casimir}}^{(a)}(\beta,N_\perp|d=3,\mathbf{b})$ for $d=3$. Note that $X_{\mathrm{Casimir}}(x_t)>0$ for all x_t. The asymptotic behavior of $X_{\mathrm{Casimir}}(x_t)$ for $x_t \ll -1$ is given according to Eq. (3.51).

IV. HELICITY MODULUS

A. General results for the case $2<d<4$

When in an $O(n \geq 2)$ system an interface is created by, say, applying antiperiodic boundary conditions, the corresponding helicity modulus characterizing that interface can be defined, e.g., as suggested in [39]

$$\Upsilon(\beta,N_\perp|d,\mathbf{b}) \equiv \frac{2N_\perp}{\pi^2}[f_{\mathrm{ex}}^{(a)}(\beta,N_\perp|d,\mathbf{b}) - f_{\mathrm{ex}}^{(p)}(\beta,N_\perp|d,\mathbf{b})], \tag{4.1}$$

where $f_{\mathrm{ex}}^{(p)}(\beta,N_\perp|d,\mathbf{b})$ is the excess free energy of the system under periodic boundary conditions when no such diffuse interface exists. Obviously, the helicity modulus of the infinite system then simply is $\Upsilon(\beta|d,\mathbf{b}) \equiv \lim_{N_\perp\to\infty}\Upsilon(\beta,N_\perp|d,\mathbf{b})$.

Within the isotropic spherical model the corresponding result for $\Upsilon(\beta|d)$ is known, see, e.g., Ref. [39],

$$\beta\Upsilon(T|d) = \frac{1}{2d}(K-K_c). \tag{4.2}$$

The needed information for $f_{\mathrm{ex}}^{(p)}(\beta,N_\perp|d,\mathbf{b})$ is also available, see, e.g., Ref. [19],

$$\begin{aligned}\beta f_{\mathrm{ex}}^{(p)}(\beta,N_\perp|d,\mathbf{b}) = N_\perp^{-(d-1)}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\Bigg\{&\frac{1}{4}x_t(y_p-y_b) \\ &- \frac{\Gamma(-d/2)}{2(4\pi)^{d/2}}(y_p^{d/2}-y_b^{d/2}) \\ &- y_p^{d/2}\frac{2}{(2\pi)^{d/2}}\sum_{n=1}^\infty \frac{K_{d/2}(n\sqrt{y_p})}{(n\sqrt{y_p})^{d/2}}\Bigg\},\end{aligned} \tag{4.3}$$

where y_p is the solution of the equation

$$-\frac{1}{2}x_t = \frac{\Gamma(1-d/2)}{(4\pi)^{d/2}}y_p^{d/2-1} + y_p^{d/2-1}\frac{2}{(2\pi)^{d/2}}\sum_{n=1}^{\infty}\frac{K_{d/2-1}(n\sqrt{y_p})}{(n\sqrt{y_p})^{d/2-1}}. \tag{4.4}$$

Using Eqs. (3.22) and (4.3), for the finite-size scaling behavior of the helicity modulus we obtain

$$\beta\Upsilon(\beta,N_\perp|d,\mathbf{b}) = N_\perp^{-(d-2)}\left(\frac{J_\perp}{J_\parallel}\right)^{(d-1)/2}X_\Upsilon(x_t), \tag{4.5}$$

where the scaling function of the helicity modulus Υ is

$$X_\Upsilon(x_t) = \frac{2}{\pi^2}\Bigg\{\frac{1}{4}x_t(\tilde{y}-y_p) - \frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}(\tilde{y}^{d/2}-y_p^{d/2}) - \frac{2}{(2\pi)^{d/2}}\Bigg[\tilde{y}^{d/2}\sum_{n=1}^{\infty}(-1)^n\frac{K_{d/2}(n\sqrt{\tilde{y}})}{(n\sqrt{\tilde{y}})^{d/2}} - y_p^{d/2}\sum_{n=1}^{\infty}\frac{K_{d/2}(n\sqrt{y_p})}{(n\sqrt{y_p})^{d/2}}\Bigg]\Bigg\}, \tag{4.6}$$

where $\tilde{y}$ is the solution of Eq. (3.35), y_p is the solution of Eq. (4.4), and x_t is defined in Eq. (3.23). Taking into account that when $T<T_c$ and $N_\perp \gg 1$ one has $y_p \to 0^+$ and $y\to 0^+$, from Eqs. (4.5) and (4.6) one derives, within the spherical model, the behavior of the "bulk" helicity modulus in an anisotropic system,

$$\beta\Upsilon(T|d,\mathbf{b}) = \frac{1}{2}b_\perp(K-K_c). \tag{4.7}$$

Despite the close similarity with Eq. (4.2), note that here K_c is the critical coupling of the anisotropic system, while in Eq. (4.2) it is the corresponding one of the isotropic system.

B. Results for the case $d=3$

Since $d=3$ is of special importance we, similar to what we have done for the Casimir force in systems with a diffuse interface, will present in more details explicit results for the finite-size behavior of the helicity modulus in this case. When $d=3$ Eqs. (4.6) and (4.4) simplify to

$$\beta\Upsilon(\beta,N_\perp|d=3,\mathbf{b}) = N_\perp^{-1}\left(\frac{b_\perp}{b_\parallel}\right)\frac{2}{\pi^2}\Bigg\{\frac{1}{4}x_t(\tilde{y}-y_p) - \frac{1}{12\pi}(\tilde{y}^{3/2}-y_p^{3/2}) - \frac{1}{2\pi}\Big[\sqrt{\tilde{y}}\,\mathrm{Li}_2(-e^{-\sqrt{\tilde{y}}}) - \sqrt{y_p}\,\mathrm{Li}_2(e^{-\sqrt{y_p}}) + \mathrm{Li}_3(-e^{-\sqrt{\tilde{y}}}) - \mathrm{Li}_3(e^{-\sqrt{y_p}})\Big]\Bigg\}, \tag{4.8}$$

and

$$x_t = \frac{1}{2\pi}\sqrt{y_p} + \frac{1}{\pi}\ln[1-e^{-\sqrt{y_p}}], \tag{4.9}$$

respectively. The solution of Eq. (4.9) for periodic boundary conditions is

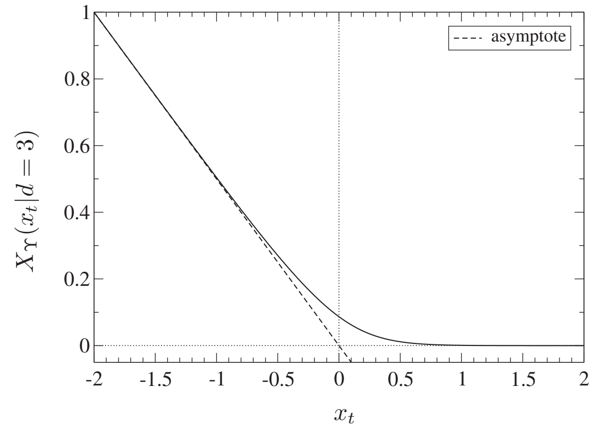

FIG. 2. The scaling function $X_\Upsilon(x_t)$ of the helicity modulus $\Upsilon(T,L)$ for $d=3$. One observes that it is a monotonically decreasing function of x_t. The asymptote of $X_\Upsilon(x_t)$ for $x_t \ll -1$ is given in Eq. (4.13).

$$\sqrt{y_p} = 2\,\mathrm{arcsinh}\left[\frac{1}{2}e^{\pi x_t}\right], \tag{4.10}$$

which has to be compared with the corresponding solution for the antiperiodic boundary conditions, see Eq. (3.45).

Let us determine the critical value of the finite-size helicity modulus $\Upsilon(\beta_c,N_\perp|d=3,\mathbf{b})$. Knowing the Casimir amplitude for antiperiodic boundary conditions $\Delta_{\mathrm{Casimir}}$ [see Eq. (3.50)] and that one under periodic boundary conditions [7] (see also [21])

$$\Delta_{\mathrm{Casimir}}^{\mathrm{per}} = -\frac{2}{5\pi}\zeta(3) \simeq -0.153\,051, \tag{4.11}$$

from Eq. (4.1) one obtains

$$\begin{aligned}\beta_c\Upsilon(\beta_c,N_\perp|d=3,\mathbf{b}) &= \frac{2}{\pi^2 N_\perp}\left(\frac{J_\perp}{J_\parallel}\right)[\Delta_{\mathrm{Casimir}}-\Delta_{\mathrm{Casimir}}^{\mathrm{per}}]\\ &= \frac{2}{\pi^2 N_\perp}\left(\frac{J_\perp}{J_\parallel}\right)\left[\frac{1}{3}\mathrm{Cl}_2\left(\frac{\pi}{3}\right)+\frac{7}{30\pi}\zeta(3)\right]\\ &\simeq 0.086\,649N_\perp^{-1}\left(\frac{J_\perp}{J_\parallel}\right).\end{aligned} \tag{4.12}$$

The dependence of the scaling function $X_\Upsilon(x_t)$ is plotted in Fig. 2. It is easy to show that $X_\Upsilon(x_t)$ decays exponentially fast for $x_t \gg 1$, while for $x_t \ll -1$ one derives that

$$X_\Upsilon(x_t) \underset{x_t\to-\infty}{\approx} -x_t/2. \tag{4.13}$$

The asymptote of X_Υ for $T<T_c$ leads to Eq. (4.7) for the behavior of the helicity modulus within the anisotropic $O(n)$ models when $n\to\infty$ in the limit $\lim_{N_\perp\to\infty}\beta\Upsilon(\beta,N_\perp|d=3,\mathbf{b})$.

V. DISCUSSION AND CONCLUDING REMARKS

In the current article we studied as a function of the temperature the behavior of the Casimir force and the helicity modulus in anisotropic $O(n)$ systems with continuous (n

≥ 2)-component order parameter. We envisaged systems with a film geometry when the boundary conditions imposed enforce the presence of a diffuse interface in them. The interaction along the film is characterized by a coupling constant $J_\parallel$ while in the direction perpendicular to the film it is $J_\perp$. We argued that in such anisotropic systems the Casimir force, the free energy and the helicity modulus differ from those of the corresponding isotropic systems, even at the bulk critical temperature, despite that these systems both belong to the same universality class. We suggested a relation between the scaling functions pertinent to the both systems; say, for the scaling functions of the excess free energies (normalized per $k_B T$) one has

$$X_f^{(a)}(x_t|J_\perp,J_\parallel) = \left[\frac{\xi_{\perp,0}}{\xi_{\parallel,0}}\right]^{d-1} X_f^{(a)}(x_t), \tag{5.1}$$

see Eq. (1.14), where $\xi_{\parallel,0}$ and $\xi_{\perp,0}$ are the correlation length amplitudes in the anisotropic system, while $X_f^{(a)}(x_t)$ is the universal scaling function of the isotropic one. Equation (5.1) implies the following relation between the corresponding scaling functions of the Casimir force

$$X_{\text{Casimir}}(x_t|d,J_\perp,J_\parallel) = \left[\frac{\xi_{\perp,0}}{\xi_{\parallel,0}}\right]^{d-1} X_{\text{Casimir}}(x_t|d), \tag{5.2}$$

and, thus, between the corresponding Casimir amplitudes

$$\Delta_{\text{Casimir}}(d|J_\perp,J_\parallel) = \left[\frac{\xi_{\perp,0}}{\xi_{\parallel,0}}\right]^{d-1} \Delta_{\text{Casimir}}(d). \tag{5.3}$$

In addition we argued that the presence of a diffuse interface leads to a strong repulsive Casimir force for $T \ll T_c$. For such systems one also expects that the force will remain repulsive even at T_c, i.e., that $\Delta_{\text{Casimir}} > 0$.

In order to further support and substantiate the above general statements, which are expected to be valid for any $O(n)$, $n \geq 2$ model system, in the current article we derived explicit exact analytical results for the scaling functions, as a function of the temperature T, of the free energy density, Casimir force, and the helicity modulus for the $n \to \infty$ limit of $O(n)$ models with antiperiodic boundary conditions applied along the finite dimension L of the film. Such boundary conditions enforce the existence of a diffuse interface within the investigated system. In full agreement with the presented above hypothesis, we have found that all scaling functions, including the Casimir amplitude, depend on the ratio $J_\perp/J_\parallel$ and are, thus, nonuniversal. More precisely, we have found that the Casimir force in a d-dimensional anisotropic system, with $2<d<4$, can be written in the form, see Eq. (3.38),

$$F_{\text{Casimir}}^{(a)}(T,N_\perp|d,J_\perp,J_\parallel) = (k_B T_c) N_\perp^{-d} X_{\text{Casimir}}(x_t|d,J_\perp,J_\parallel), \tag{5.4}$$

near the corresponding bulk critical temperature T_c of the anisotropic system, where x_t is a properly defined temperature-dependent scaling variable and the *nonuniversal* scaling function

$$X_{\text{Casimir}}(x_t|d,J_\perp,J_\parallel) = \left(\frac{J_\perp}{J_\parallel}\right)^{(d-1)/2} X_{\text{Casimir}}(x_t|d) \tag{5.5}$$

can be related to $X_{\text{Casimir}}(x_t|d)$, which is the *universal* scaling function characterizing the corresponding isotropic system. The explicit form of $X_{\text{Casimir}}(x_t|d)$, for $2<d<4$, is given in Eq. (3.32) and, equivalently, in Eq. (3.34). Similar relations can be written also for the helicity modulus, see Eq. (4.5),

$$\Upsilon(T,N_\perp|d,J_\perp,J_\parallel) = (k_B T_c) N_\perp^{-(d-2)} X_\Upsilon(x_t|d,J_\perp,J_\parallel), \tag{5.6}$$

where, again, the *nonuniversal* scaling function, $X_\Upsilon(x_t|d,J_\perp,J_\parallel)$,

$$X_\Upsilon(x_t|d,J_\perp,J_\parallel) = \left(\frac{J_\perp}{J_\parallel}\right)^{(d-1)/2} X_\Upsilon(x_t|d) \tag{5.7}$$

can be related to an universal scaling function $X_\Upsilon(x_t|d)$ characterizing the corresponding isotropic system. The explicit form of $X_\Upsilon(x_t|d)$, for $2<d<4$, is given in Eq. (4.6).

From Eq. (5.5) one obtains, see Eq. (3.39),

$$\Delta_{\text{Casimir}}(d|J_\perp,J_\parallel) = \left(\frac{J_\perp}{J_\parallel}\right)^{(d-1)/2} \Delta_{\text{Casimir}}(d). \tag{5.8}$$

Since, within the spherical model, see Eq. (3.40),

$$\frac{\xi_\perp}{\xi_\parallel} = \sqrt{\frac{J_\perp}{J_\parallel}} \tag{5.9}$$

all the relations (5.5), (5.7), and (5.8) are in full conformity with our general predictions given by Eqs. (5.1) and (5.3).

In addition to the more general results valid for $2<d<4$, we have also derived some explicit closed-form results for the case $d=3$. The scaling function of the Casimir force then is given in Eq. (3.41) and, equivalently, in Eq. (3.42). The behavior of this function is visualized in Fig. 1. The scaling function for the helicity modulus is presented in Eq. (4.8) and is depicted in Fig. 2. For the value of the Casimir amplitude at $d=3$ one has, see Eq. (3.50) [63],

$$\Delta_{\text{Casimir}} = \left[\frac{1}{3}\text{Cl}_2\left(\frac{\pi}{3}\right) - \frac{\zeta(3)}{6\pi}\right]\left(\frac{J_\perp}{J_\parallel}\right), \tag{5.10}$$

while the value of the helicity modulus at T_c is [see Eq. (4.12)]

$$\beta_c \Upsilon(T_c,L) = \frac{2}{\pi^2}\left[\frac{1}{3}\text{Cl}_2\left(\frac{\pi}{3}\right) + \frac{7\zeta(3)}{30\pi}\right]\left(\frac{J_\perp}{J_\parallel}\right)L^{-1}. \tag{5.11}$$

Let us recall that the Casimir amplitude of the spherical model for periodic boundary conditions [7]

$$\Delta_{\text{Casimir}}^{\text{per}} = -\frac{2}{5\pi}\zeta(3) \simeq -0.153\,051 \tag{5.12}$$

numerically coincides (within the corresponding error bars) with the best known estimate of the Casimir amplitude $\Delta_{\text{Casimir}}^{\text{per,Ising}} \simeq -0.153$ for the three-dimensional Ising model [9] obtained via Monte Carlo methods. This fact still lacks adequate theoretical explanation. It will be very interesting to check if a similar relation also holds for the Casimir amplitudes of the spherical and Ising models under antiperiodic

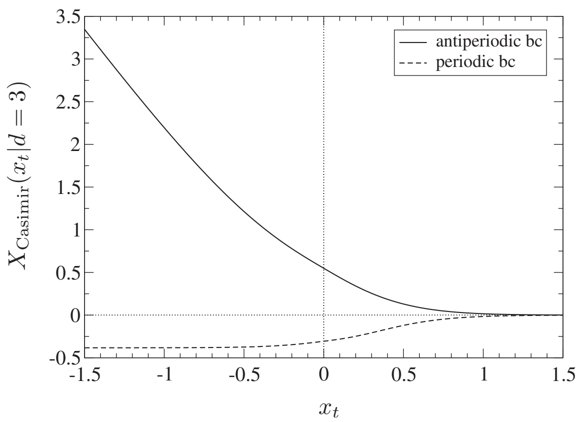

FIG. 3. The scaling functions $X_{\rm Casimir}(x_t)$ of the Casimir forces $F^{(a)}_{\rm Casimir}(\beta,N_\perp|d=3,\mathbf{b})$ and $F^{(p)}_{\rm Casimir}(\beta,N_\perp|d=3,\mathbf{b})$ for $d=3$. The difference is due to the contributions stemming from the helicity modulus. We see that this contribution is rather strong and dominates the behavior of the force under antiperiodic boundary conditions converting it from attractive (under periodic boundary condition) into a repulsive one (under antiperiodic boundary conditions).

boundary conditions. For such boundary conditions we are also not aware about any Monte Carlo data for the critical value of the helicity modulus in the three-dimensional *XY* and Heisenberg models. Let us note that, under antiperiodic boundary conditions, both the Casimir amplitude, as well as the Casimir force, are positive, i.e., they correspond to a repulsion between the plates of the system. Let us stress that this effect is solely due to the existence of a diffuse interface in the system. We recall that under periodic boundary conditions for $d=3$ and in the notations of the current article the Casimir force under periodic boundary conditions is given by the expression [19]

$$\beta F^{(p)}_{\rm Casimir}(\beta,N_\perp|d=3,\mathbf{b}) = N_\perp^{-3}\left(\frac{b_\perp}{b_\parallel}\right)\Bigg\{\frac{1}{4}x_t(y_p-y_b) - \frac{1}{6\pi}(y_p^{3/2}-y_b^{3/2}) - \frac{\sqrt{y_p}}{\pi}\mathrm{Li}_2(e^{-\sqrt{y_p}}) - \frac{1}{\pi}\mathrm{Li}_3(e^{-\sqrt{y_p}})\Bigg\}, \qquad (5.13)$$

where y_p and y_b are given by Eqs. (4.10) and (3.47), respectively. The comparison between the force under antiperiodic and periodic boundary conditions is shown in Fig. 3. We observe that the contribution of the helicity energy is so strong that the Casimir force converts from being everywhere attractive (under periodic boundary conditions) into everywhere repulsive (under antiperiodic boundary conditions).

The idea of creating a diffuse interface in a nanosystem can eventually be used for practical purposes when applying some ordering external field might cause border spins, electric or magnetic dipoles, etc., to order in a parallel or in an antiparallel way to each other. More concretely, in order to avoid sticking of the working metal surfaces of a nanomachine, e.g., it is possible to immerse it in a dipolar, or a magnetic fluid, and to create a diffuse interface between its working surfaces by imposing opposite (or tilted, at a given angle) electric, or magnetic fields on them. Of course, by changing the degree of helicity the force will pass from being attractive through being zero into being repulsive. Obviously, it will be interesting to consider such a scenario in more details by say, studying a system under twisted at a given angle boundary conditions. We hope to return to this problem in a future work.

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APPENDIX A: EVALUATION OF $U(w,N_\perp|d,\mathbf{b})$

In the current appendix we prove the validity of Eq. (3.25) for the behavior of $U(w,N_\perp|d,\mathbf{b})$ when $N_\perp \gg 1$ and $0 \leq w \ll 1$. Because of the representation (3.6) of $U(w,N_\perp|d,\mathbf{b})$ and the asymptotes (3.10) of $S_N^{(a)}(x)$ one divides the region of integration in two subregions, from 0 to $aN_\perp^2$ and from $aN_\perp^2$ to infinity, where a is a fixed real number such that $0<a<1$. Let us denote the integral over the first region (over "moderate" values of x) by U_m and let U_l is the integral over the "large" values of x, i.e., let

$$U_m \equiv \frac{1}{2}\int_0^{aN_\perp^2}\frac{dx}{x}\Bigg\{\exp(-x) - \exp\Bigg\{-x\Bigg[w - b_\perp\left(1-\cos\frac{\pi}{N_\perp}\right)\Bigg]\Bigg\}\Bigg[e^{-xb_\perp}I_0(xb_\perp) + \sqrt{\frac{2}{\pi x b_\perp}}R^{(-)}\left(\frac{2N_\perp^2}{xb_\perp}\right)\Bigg]\times[e^{-xb_\parallel}I_0(xb_\parallel)]^{d-1}\Bigg\} \qquad (A1)$$

and

$$U_l \equiv \frac{1}{2}\int_{aN_\perp^2}^{\infty}\frac{dx}{x}\Bigg\{e^{-x} - e^{-xw}[e^{-xb_\parallel}I_0(xb_\parallel)]^{d-1}\times\Bigg[\frac{2}{N_\perp} + \frac{2}{N_\perp}R^{(+)}\left(\frac{\pi^2 b_\perp}{2N_\perp^2}x\right)\Bigg]\Bigg\}. \qquad (A2)$$

Obviously $U=U_l+U_m$. The evaluation of U_l is straightforward. Since $x \gg 1$ in calculating U_l one can use the large value asymptote of the Bessel function [60]

$$I_\nu(x) = \frac{\exp(x-\nu^2/2x)}{\sqrt{2\pi x}}\left[1 + \frac{1}{8x} + \frac{9-32\nu^2}{2!(8x)^2} + \cdots\right] \qquad (A3)$$

with the help of which one directly obtains that

$$U_l = -N_\perp^{-d}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2}\frac{1}{(4\pi)^{(d-1)/2}} \times \int_{ab_\perp/2}^{\infty}\frac{dx}{x}x^{-(d-1)/2}e^{-yx}[1+R^{(+)}(\pi^2 x)], \quad (A4)$$

where y is defined in Eq. (3.18). Let us deal now with the term U_m. We divide this term into "bulklike" contributions $U_{m,b}$ and "finite-size" contributions $U_{m,fs}$ where $U_m = U_{m,b} + U_{m,fs}$ with

$$U_{m,b} \equiv \frac{1}{2}\int_0^{aN_\perp^2}\frac{dx}{x}\{e^{-x} - e^{-x\tilde{w}}[e^{-xb_\perp}I_0(xb_\perp)] \times [e^{-xb_\|}I_0(xb_\|)]^{d-1}\} \quad (A5)$$

and

$$U_{m,fs} \equiv -\int_0^{aN_\perp^2}\frac{dx}{x}e^{-x\tilde{w}}\frac{1}{\sqrt{2\pi x b_\perp}}R^{(-)}\left(\frac{2N_\perp^2}{xb_\perp}\right) \times [e^{-xb_\|}I_0(xb_\|)]^{d-1}, \quad (A6)$$

where

$$\tilde{w} = w - b_\perp\left(1-\cos\frac{\pi}{N_\perp}\right). \quad (A7)$$

It is straightforward to evaluate $U_{m,fs}$. Due to the representation (3.15), for all $x \ll N_\perp^2$ the corresponding contribution into the integral on the right-hand side of Eq. (A6) will be exponentially small. Thus, one again can use in Eq. (A6) the large-value asymptote (A3) of the Bessel function $I_0(x)$ which leads to

$$U_{m,fs} = -N_\perp^{-d}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2}\frac{1}{(4\pi)^{d/2}} \times \int_0^{ab_\perp/2}\frac{dx}{x}x^{-d/2}e^{-\tilde{y}x}R^{(-)}\left(\frac{1}{x}\right). \quad (A8)$$

It now remains only to deal with the term $U_{m,b}$. By subtracting and adding, up to the linear in x term, the asymptote of $\exp[xb_\perp(1-\cos\frac{\pi}{N_\perp})]$ for small values of x one rewrites Eq. (A5) into the form

$$U_{m,b} = \frac{1}{2}\int_0^{aN_\perp^2}\frac{dx}{x}\left\{e^{-x} - \left(1+\frac{1}{2}b_\perp\frac{\pi^2}{N_\perp^2}x\right)e^{-xw}[e^{-xb_\perp}I_0(xb_\perp)] \times [e^{-xb_\|}I_0(xb_\|)]^{d-1}\right\} + \frac{1}{2}\int_0^{aN_\perp^2}\frac{dx}{x}\left[\left(1 + \frac{1}{2}b_\perp\frac{\pi^2}{N_\perp^2}x\right)e^{-xw} - e^{-x\tilde{w}}\right][e^{-xb_\perp}I_0(xb_\perp)] \times [e^{-xb_\|}I_0(xb_\|)]^{d-1}. \quad (A9)$$

It is easy to understand that the integration over small values of x in the second line of the above equation will provide contributions of the order of $O(N_\perp^{-4})$ which we will neglect, since we are only interested in contributions that are not smaller than $O(N_\perp^{-d})$, with $2<d<4$. Thus, in this integral one again can use the large value asymptote (A3) of the Bessel function $I_0(x)$, which leads to

$$U_{m,b} = \frac{1}{2}\int_0^{aN_\perp^2}\frac{dx}{x}\{e^{-x} - e^{-xw}[e^{-xb_\perp}I_0(xb_\perp)][e^{-xb_\|}I_0(xb_\|)]^{d-1}\} - \frac{1}{4}b_\perp\frac{\pi^2}{N_\perp^2}\int_0^{aN_\perp^2}dx e^{-xw}[e^{-xb_\perp}I_0(xb_\perp)] \times [e^{-xb_\|}I_0(xb_\|)]^{d-1} + N_\perp^{-d}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2}\frac{1}{2}\frac{1}{(4\pi)^{d/2}}\int_0^{ab_\perp/2}\frac{dx}{x}[e^{-xy}(1+\pi^2 x) - e^{-x\tilde{y}}]x^{-d/2}. \quad (A10)$$

One can complete the integral in the first and second line of the above equation so that the integration is from 0 to ∞ and to subtract the parts of integration from $aN_\perp^2$ to ∞. In the subtracted parts one can again use the large value asymptote (A3) of the Bessel function $I_0(x)$. In this way one obtains

$$U_{m,b} = U_d(w|\mathbf{b}) - \frac{1}{4}b_\perp\frac{\pi^2}{N_\perp^2}W_d(w|\mathbf{b}) + N_\perp^{-d}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2}\frac{1}{2}\frac{1}{(4\pi)^{d/2}}\left[\int_{ab_\perp/2}^{\infty}\frac{dx}{x}e^{-xy}(1 + \pi^2 x)x^{-d/2} + \int_0^{ab_\perp/2}\frac{dx}{x}[e^{-xy}(1+\pi^2 x) - e^{-x\tilde{y}}]x^{-d/2}\right]. \quad (A11)$$

Expressing from Eq. (3.28) function $R^{(-)}(x)$ in terms of $R^{(+)}(x)$ and substituting the so-obtained representation in Eq. (A8) one obtains

$$U_{m,fs} = -N_\perp^{-d}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2}\frac{1}{(4\pi)^{(d-1)/2}}\int_0^{ab_\perp/2}\frac{dx}{x}x^{-(d-1)/2}e^{-yx}\left[1+R^{(+)}(\pi^2 x) - \frac{1}{2}\frac{1}{\sqrt{4\pi x}}e^{\pi^2 x}\right] = -N_\perp^{-d}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2}\frac{1}{(4\pi)^{(d-1)/2}}\left\{\int_0^{ab_\perp/2}\frac{dx}{x}x^{-(d-1)/2}e^{-yx}\left[1+R^{(+)}(\pi^2 x) - \frac{1}{2}\frac{1}{\sqrt{4\pi x}}(1+\pi^2 x)\right] + \frac{1}{2}\frac{1}{\sqrt{4\pi}}\int_0^{ab_\perp/2}\frac{dx}{x}x^{-d/2}e^{-yx}[(1+\pi^2 x) - e^{\pi^2 x}]\right\}. \quad (A12)$$

In a similar way, by adding and subtracting the asymptote of $1+R^{(+)}(\pi^2 x)$ for small values of the argument, one can rewrite U_l [see Eq. (A4)] into the form

$$U_l = - N_\perp^{-d}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\frac{1}{(4\pi)^{(d-1)/2}}\left\{\int_{ab_\perp/2}^{\infty}\frac{dx}{x}x^{-(d-1)/2}e^{-yx}\times\left[1+R^{(+)}(\pi^2 x)-\frac{1}{2}\frac{1}{\sqrt{4\pi x}}(1+\pi^2 x)\right]+\frac{1}{2}\frac{1}{\sqrt{4\pi}}\int_0^{ab_\perp/2}\frac{dx}{x}x^{-d/2}e^{-yx}(1+\pi^2 x)\right\}. \tag{A13}$$

By adding $U_{\mathrm{m,b}}$, $U_{\mathrm{m,fs}}$, and U_l as given by Eqs. (A11)–(A13), respectively, one obtains, after using the representation (3.20) for $U_d(w|\mathbf{b})$, as well as the fact that $W_d(w|\mathbf{b}) = \partial U_d(w|\mathbf{b})/\partial\omega$, the final result for $U(w,N_\perp|d,\mathbf{b})$ given in Eq. (3.25) in the main text.

APPENDIX B: DERIVATION OF THE SERIES REPRESENTATION OF $I(y,d)$

In this appendix we derive the power series representation (3.30) of the integral $I(y,d)$ defined in Eq. (3.27). The procedure described in the following employs dimensional regularization and is analogous to the one discussed in Appendix C of reference [27].

First, let us note that using the representation (3.11) for the function $R^{(+)}(x)$, the integral $I(y,d)$ can be decomposed as $I(y,d)=I^{[1]}(y,d)+I^{[2]}(y,d)$, where

$$I^{[1]}(y,d) = -\frac{1}{(4\pi)^{(d-1)/2}}\sum_{n=1}^{\infty}\int_0^{\infty}dx x^{-(d+1)/2}e^{-yx}e^{-4\pi^2 n(n+1)x} \tag{B1}$$

and

$$I^{[2]}(y,d) = -\frac{1}{(4\pi)^{(d-1)/2}}\int_0^{\infty}dx x^{-(d+1)/2}e^{-yx}\left[1-\frac{1+\pi^2 x}{2\sqrt{4\pi x}}\right]. \tag{B2}$$

Employing dimensional regularization, the latter integral can be done analytically and becomes

$$I^{[2]}(y,d) = \frac{y^{(d-2)/2}}{2(4\pi)^{d/2}}\{\pi^2\Gamma(1-d/2)-4\sqrt{\pi y}\Gamma[(1-d)/2]+y\Gamma(-d/2)\}. \tag{B3}$$

Introducing the variable $\tilde{y}\equiv y-\pi^2$, the integral $I^{[1]}(y,d)$ can be written as

$$I^{[1]}(y,d) = -\frac{1}{(4\pi)^{(d-1)/2}}\sum_{n=1}^{\infty}\int_0^{\infty}\frac{dx}{x^{(d+1)/2}}e^{-\tilde{y}x}e^{-[\pi^2+4\pi^2 n(n+1)]x} \tag{B4}$$

and upon replacing $\exp(-\tilde{y}x)$ by its Taylor series representation the integral $I^{[1]}(y,d)$ becomes

$$I^{[1]}(y,d) = -\frac{1}{(4\pi)^{(d-1)/2}}\sum_{n=1}^{\infty}\sum_{m=0}^{\infty}b_{n,m}^{(d)}\frac{(-\tilde{y})^m}{m!} \tag{B5}$$

with the coefficients

$$b_{n,m}^{(d)} = \int_0^{\infty}dx x^{m-(d+1)/2}e^{-[\pi^2+4\pi^2 n(n+1)]x}. \tag{B6}$$

Again in the sense of dimensional regularization the x integration in the latter equation can be performed to give

$$b_{n,m}^{(d)} = \frac{\left(n+\frac{1}{2}\right)^{d-2m-1}\Gamma\left(m+\frac{1-d}{2}\right)}{(2\pi)^{2m+1-d}}. \tag{B7}$$

Inserting this into Eq. (B5), the n summation can be done analytically leading to

$$I^{[1]}(y,d) = \pi^{(d-1)/2}\left[2^{1-d}\sum_{m=0}^{\infty}\frac{(-\tilde{y})^m\Gamma\left(m+\frac{1-d}{2}\right)}{\pi^{2m}m!}-\sum_{m=0}^{\infty}a_m^{(d)}(-\tilde{y})^m\right] \tag{B8}$$

with the coefficients $a_m^{(d)}$ defined in Eq. (3.31). The first m sum in square brackets can also be done analytically and we obtain

$$I^{[1]}(y,d) = (4\pi)^{(1-d)/2}\Gamma[(1-d)/2](\tilde{y}+\pi^2)^{(d-1)/2}-\pi^{(d-1)/2}\sum_{m=0}^{\infty}a_m^{(d)}(-\tilde{y})^m. \tag{B9}$$

If we now add up $I^{[1]}(y,d)$ and $I^{[2]}(y,d)$ we arrive at the power series representation (3.30) of $I(y,d)$ given in the main text. Note that no terms being nonanalytic with respect to $\tilde{y}$ are present, and furthermore that the radius of convergence of the expansion is $|\tilde{y}|=|y-\pi^2|<4\pi^2$.

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$$f_{\text{ex}}^{(a)}(T,L) = f_{\text{ex}}^{(p)}(T,L) + \frac{1}{2L}\alpha^2\Upsilon(T,L),$$

which, on its turn, can be considered as a definition of the helicity modulus in a system with boundary spins twisted with respect to each other at an angle α, which corresponds to a system under "twisted boundary conditions." In the case of antiperiodic boundary conditions $\alpha=\pi$ and both definitions are equivalent.
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