Critical Casimir force and its fluctuations in lattice spin models: Exact and Monte Carlo results

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We present general arguments and construct a stress tensor operator for finite lattice spin models. The average value of this operator gives the Casimir force of the system close to the bulk critical temperature T_c. We verify our arguments via exact results for the force in the two-dimensional Ising model, d-dimensional Gaussian, and mean spherical model with $2<d<4$. On the basis of these exact results and by Monte Carlo simulations for three-dimensional Ising, XY, and Heisenberg models we demonstrate that the standard deviation of the Casimir force F_C in a slab geometry confining a critical substance in-between is $k_bTD(T)(A/a^{d-1})^{1/2}$, where A is the surface area of the plates, a is the lattice spacing, and $D(T)$ is a slowly varying nonuniversal function of the temperature T. The numerical calculations demonstrate that at the critical temperature T_c the force possesses a Gaussian distribution centered at the mean value of the force $\langle F_C\rangle = k_bT_c(d-1)\Delta/(L/a)^d$, where L is the distance between the plates and Δ is the (universal) Casimir amplitude.

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I. INTRODUCTION

If material bodies are immersed in a fluctuating medium the surfaces of these bodies impose boundary conditions that select a certain mode spectrum for the fluctuations. This leads to a contribution into the ground state energy of a quantum mechanical system, or to the free energy of a critical statistical-mechanical system, which depends on the geometrical parameters characterizing the mutual position of the bodies and their shape. This is known as the Casimir effect [1–3].

According to our present understanding, the Casimir effect is a phenomenon common to all systems characterized by fluctuating quantities on which external boundary conditions are imposed. Casimir forces arise from an interaction between distant portions of the system mediated by fluctuations.

In quantum mechanics one usually considers fluctuations of the electromagnetic field. In this case correlations of the fluctuations are mediated by photons—massless excitations of the electromagnetic field [1,2,4,5]. In statistical mechanics the massless excitations can be generated by critical fluctuations of the order parameter around the critical temperature T_c of the system [3,6,7]. Goldstone modes (or spin wave excitations) in $O(n)$ models at temperatures below T_c also provide massless excitations [8–10]. Fluctuations of this type are scale invariant and therefore the Casimir force is long ranged in the above cases.

In this paper we discuss the behavior of the thermodynamic Casimir force in systems with short-ranged interactions undergoing a second-order phase transition.

To be more specific, let us consider a statistical-mechanical system, a magnet or a fluid, with the slab geometry $L_\parallel^{d-1}\times L_\perp$, where d is the dimensionality of the system and periodic boundary conditions are applied. In the limit $L_\parallel\to\infty$ ($L_\perp$ fixed) the Casimir force per unit area is defined as

$$\beta F_{\mathrm{Casimir}}(T,L_\perp) = -\frac{\partial f_{\mathrm{ex}}(T,L_\perp)}{\partial L_\perp}, \qquad (1.1)$$

where $f_{\mathrm{ex}}(T,L_\perp)$ is the excess free energy

$$f_{\mathrm{ex}}(T,L_\perp) = f(T,L_\perp) - L_\perp f_{\mathrm{bulk}}(T) \qquad (1.2)$$

of the system. Here $f(T,L_\perp)$ is the full free energy per unit area measured in units of k_BT and $f_{\mathrm{bulk}}(T)$ is the corresponding bulk free energy density.

According to the definition given by Eq. (1.1) the thermodynamic Casimir force is a generalized force conjugate to the distance $L_\perp$ between the boundaries of the system with the property $F_{\mathrm{Casimir}}(T,L_\perp)\to 0$ for $L_\perp\to\infty$. We are interested in the behavior of F_{Casimir} when $L_\perp \gg a$, where a is a typical microscopic length scale. In this limit finite-size scaling theory is applicable. Then one has [11]

$$\beta F_{\mathrm{Casimir}}(T,L_\perp) = L_\perp^{-d} X_{\mathrm{Casimir}}(L/\xi_\infty), \qquad (1.3)$$

where ξ_∞ is the true bulk correlation length, while X_{Casimir} is a universal scaling function.

At the critical point T_c of the bulk system one has $\xi_\infty=\infty$, and [3]

$$\beta_c F_{\mathrm{Casimir}}(T_c,L_\perp) = (d-1)\frac{\Delta}{L_\perp^d}, \qquad (1.4)$$

where Δ is the so-called Casimir amplitude. This amplitude is universal, i.e., Δ depends only on the universality class of the corresponding bulk system and the type of boundary conditions used across $L_\perp$. Obviously, one has $\Delta = X_{\mathrm{Casimir}}(0)/(d-1)$.

The Casimir force may also be viewed from the point of view of conformal invariance of, e.g., critical systems [12]. The Casimir force in its simple form for the film geometry ($L_\parallel\to\infty$, $L_\perp$ finite) is due to the $L_\perp$ dependence of the free energy $f(T,L_\perp)$ per unit area. The free energy therefore responds to any coordinate transformation which changes the value of $L_\perp$. On the other hand, any coordinate transformation which transforms a slab of thickness $L_\perp$ into a slab of a different thickness is nonconformal. Therefore, the Casimir force is the response of the free energy $f(T,L_\perp)$ of the original slab to a nonconformal coordinate transformation. The change of the free energy due to a nonconformal coordinate transformation is determined by the thermal average of the stress tensor $t_{\alpha\beta}$ associated with the Hamiltonian of the system [12]. If the coordinate perpendicular to the surfaces of the slab is denoted by z, it is easy to prove that the Casimir force in the slab is given by the thermal average of the stress tensor component t_{zz} [12] (see below).

Normally, one is interested in $\langle t_{zz}\rangle$, which determines the (average) value of the Casimir force. In addition, one can consider any realization t_{zz} of the stress tensor to be proportional to any realization, e.g., instantaneous value of the Casimir force F_C, where $\langle F_C\rangle \equiv F_{\rm Casimir}$. That is the approach undertaken recently by Bartolo, Ajdari, Fournier, and Golestenian [13]. They consider a statistical-mechanical model of a d-dimensional medium described by a scalar field Φ with an elastic energy density proportional to $(\vec{\nabla}\Phi)^2$, i.e., one considers an elastic Hamiltonian of the form

$$\mathcal{H}[\Phi] = \frac{K}{2}\int d^d\mathbf{R}[\{\vec{\nabla}\Phi(\mathbf{R})\}^2], \tag{1.5}$$

where $\mathbf{R}=(\mathbf{r},z)$. They assume that the plates impose Dirichlet boundary conditions, i.e., $\Phi(\mathbf{r},0)=\Phi(\mathbf{r},L_\perp)=0$.

For the total Casimir force $F_C^t \equiv L_\parallel^{d-1}F_C$ it has been found that

$$\langle F_C^t\rangle \equiv F_{\rm Casimir}^t = c(d)\frac{L_\parallel^{d-1}}{\beta L_\perp^d} = c(d)\frac{A}{\beta L_\perp^d}, \tag{1.6}$$

where $c(d)=(d-1)\Gamma(d/2)\zeta(d)/(4\pi)^{d/2}$ depends only on the spatial dimension d, while the variance of the force $(\Delta F_C^t)^2$ that can be considered as being produced of $N_a=(L_\parallel/a)^{d-1}$ independent strings is

$$(\Delta F_C^t)^2 \propto \frac{1}{\beta^2}\left(\frac{L_\parallel}{a}\right)^{d-1} = \frac{1}{\beta^2}\frac{A}{a^{d-1}}. \tag{1.7}$$

In the above expressions $A\equiv L_\parallel^{d-1}$ is the cross section of the system. From Eqs. (1.6) and (1.7) one obtains that the "noise-over-signal ratio" ρ is

$$\rho \equiv \frac{\Delta F_C^t}{\langle F_C^t\rangle} \propto \left(\frac{L_\perp}{L_\parallel}\right)^{(d-1)/2}\left(\frac{L_\perp}{a}\right)^{(d+1)/2}. \tag{1.8}$$

The probability distribution of the force has been found to be Gaussian, i.e.,

$$\mathcal{P}(F_C^t = x) = \frac{1}{\sqrt{2\pi}\Delta F_C^t}\exp\left[-\frac{(x-\langle F_C^t\rangle)^2}{2(\Delta F_C^t)^2}\right]. \tag{1.9}$$

The structure of the current paper is as follows: First, in Sec. II we present some general arguments and construct a stress tensor operator for finite *lattice* spin models. Then, in Sec. III, we verify our arguments by presenting exact results for the two-dimensional Ising model (see Sec. III A), d-dimensional Gaussian model (see Sec. III C), and for the mean spherical model with $2<d<4$ (see Sec. III B). Monte Carlo results, based on our definition, are given in Sec. IV for the behavior of the force and its variance. There the three-dimensional Ising (Sec. IV A), *XY* (Sec. IV B), and Heisenberg (Sec. IV C) models have been considered. The paper closes with a discussion given in Sec. V. The set of technical details needed in the main text is organized in a series of Appendixes.

II. THE STRESS TENSOR FOR LATTICE SPIN MODELS

We will now reconsider the Casimir force for a d-dimensional anisotropic lattice $O(N)$ spin system with the Hamiltonian (see also Ref. [13])

$$\mathcal{H}(\lambda) = -\sum_{\mathbf{R}}\sum_{k=1}^{d} J_k(\lambda)S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_k}, \tag{2.1}$$

where a d-dimensional simple hypercubic lattice with $L_\parallel^{d-1}\times L_\perp$ lattice sites and $L_\parallel \gg L_\perp$ is assumed. The vector $\mathbf{R}$ indicates a lattice site and the vectors $\mathbf{e}_k$, $k=1,2,\ldots,d$ connect nearest-neighbor lattice sites on the simple hypercubic lattice. The spins $S_{\mathbf{R}}$ are considered to be of $O(N)$ type. Following Ref. [14] and the general idea of conformal field theory [12], we define the coupling constants in Eq. (2.1) by

$$J_k(\lambda) \equiv J_\parallel(\lambda) = J(e^{\lambda}), \quad k=1,\ldots,d-1,$$

$$J_d(\lambda) \equiv J_\perp(\lambda) = J(e^{-(d-1)\lambda}), \tag{2.2}$$

which means that $\lambda=0$ marks the isotropic point of Eq. (2.1) due to $J_\parallel(0)=J_\perp(0)=J(1)$. The function $J(x)$ in Eq. (2.2) is supposed to be smooth and monotonic in the vicinity of $x=1$ but is otherwise arbitrary. The critical point of the bulk spin model defined by Eq. (2.1) is given by an implicit equation of the type

$$\mathcal{K}(\beta_c J_1(\lambda),\ldots,\beta_c J_{d-1}(\lambda),\beta_c J_d(\lambda)) = \mathcal{K}(\beta_c J_\parallel(\lambda),\ldots,\beta_c J_\parallel(\lambda),\beta_c J_\perp(\lambda)) = 1, \tag{2.3}$$

where $\beta_c = 1/(k_B T_c)$. The function $\mathcal{K}(u_1,\ldots,u_{d-1},u_d)$ is a smooth function of d variables $u_1,\ldots,u_d$. Furthermore, at $\mathcal{K}(u_1,\ldots,u_d)=1$ the function $\mathcal{K}$ is invariant with respect to any permutation of its arguments, because the location of the critical point is independent of the labeling of the lattice axes. This also implies that the derivatives $\partial\mathcal{K}/\partial u_k$, $k=1,\ldots,d$ for $\mathcal{K}=1$ all have the same value $\mathcal{K}'\neq 0$ at the isotropic point $u_1=u_2=\cdots=u_d$. For the two-dimensional Ising model the function $\mathcal{K}$ is rigorously known [15]:

$$\mathcal{K}(u_1,u_2) = \sinh(2u_1)\sinh(2u_2), \tag{2.4}$$

but for $d\geq 3$ exact results for $\mathcal{K}$ are extremely rare. From Eq. (2.3) one immediately concludes that in general the critical temperature T_c will depend on the anisotropy parameter λ. However, for the particular parametrization given by Eq. (2.2) one finds at the critical point (see also Ref. [14])

$$0 = \left.\frac{d\mathcal{K}}{d\lambda}\right|_{\lambda=0} = \beta_c'(0)\mathcal{K}'[(d-1)J_\parallel(0) + J_\perp(0)] + \beta_c(0)\mathcal{K}'[(d-1)J_\parallel'(0) + J_\perp'(0)] = \beta_c'(0)\mathcal{K}' dJ(1), \tag{2.5}$$

which immediately yields $\beta_c'(0)=0$, i.e., for an infinitesimal anisotropy ($\lambda \ll 1$) the value of the critical temperature remains unchanged and is given by its value for the isotropic model.

The correlation length of the anisotropic bulk spin system defined by Eqs. (2.1) and (2.2) will also be anisotropic. In the vicinity of the (isotropic) bulk critical temperature T_c one finds

$$\xi_\parallel(\lambda,t) = \xi_{\parallel,0}(\lambda)|t|^{-\nu} \quad \text{and} \quad \xi_\perp(\lambda,t) = \xi_{\perp,0}(\lambda)|t|^{-\nu}, \tag{2.6}$$

where $t=(T-T_c)/T_c$ is the reduced temperature and ν is the correlation length exponent which is universal, i.e., independent of the anisotropy parameter λ. At the isotropic point $\lambda=0$ one has $\xi_{\parallel,0}(0)=\xi_{\perp,0}(0)\equiv\xi_0$. To simplify the notation we ignore the fact that the correlation length amplitudes in general also depend on the sign of the reduced temperature t. We therefore assume that $t>0$ in the following.

In order to be able to apply finite-size scaling in the critical regime with respect to a *single* correlation length, say, $\xi_\parallel$, we employ the following anisotropic rescaling of the spatial coordinates:

$$x_k' = x_k, \quad k=1,\ldots,d-1, \quad \text{and} \quad x_d' = \frac{\xi_{\parallel,0}(\lambda)}{\xi_{\perp,0}(\lambda)} x_d. \tag{2.7}$$

This transformation has the desired property, namely, $\xi_\parallel' = \xi_\parallel$ and $\xi_\perp' = \xi_\parallel$ as can be easily verified from Eqs. (2.6) and (2.7). For the lattice sizes $L_\parallel$ and $L_\perp$ we find accordingly

$$L_\parallel' = L_\parallel \quad \text{and} \quad L_\perp' = \frac{\xi_{\parallel,0}(\lambda)}{\xi_{\perp,0}(\lambda)} L_\perp \equiv R(\lambda) L_\perp. \tag{2.8}$$

The link between the explicit λ dependence of the free energy of our spin system according to Eqs. (2.1) and (2.2) and the Casimir force defined by Eq. (1.1) is provided by Eq. (2.8). In the limit $L_\parallel \to \infty$ we find **(**see also Eqs. (24) and (33) of Ref. [14]**)**

$$\left.\frac{df_{\mathrm{ex}}}{d\lambda}\right|_{\lambda=0} = -\lim_{L_\parallel\to\infty} \frac{\beta J'(1)}{L_\parallel^{d-1}} \times \left\langle \sum_{\mathbf{R}} \left[\sum_{k=1}^{d-1} S_{\mathbf{R}} S_{\mathbf{R}+\mathbf{e}_k} - (d-1) S_{\mathbf{R}} S_{\mathbf{R}+\mathbf{e}_d} \right] \right\rangle, \tag{2.9}$$

where $\langle \cdots \rangle$ denotes the thermal average with respect to the Hamiltonian given by Eq. (2.1) at the isotropic point $\lambda=0$. From Eqs. (1.1) and (2.9) and the finite-size scaling form

$$f_{\mathrm{ex}}(t,L_\perp) = L_\perp^{-(d-1)} g_{\mathrm{ex}}[t(L_\perp/\xi_{\perp,0})^{1/\nu}] \tag{2.10}$$

of the excess free energy $f_{ex}(t,L_\perp)$ in the limit $L_\parallel \to \infty$, we obtain an expression of the Casimir force which is derived in detail in Appendixes A and B. From Eq. (B8) derived in Appendix B the operator form of the stress tensor component $t_{\perp\perp}(\mathbf{R})$ can be read off as

$$t_{\perp\perp}(\mathbf{R}) = \beta J'(1)[R'(0)]^{-1} \left[\sum_{k=1}^{d-1} S_{\mathbf{R}} S_{\mathbf{R}+\mathbf{e}_k} - (d-1) S_{\mathbf{R}} S_{\mathbf{R}+\mathbf{e}_d} \right] + \frac{1}{d\nu}(\hat{\mathcal{H}} - \hat{\mathcal{H}}_b)[\beta_c(0) - \beta], \tag{2.11}$$

where Eq. (B9) was used and the operators $\hat{\mathcal{H}}$ and $\hat{\mathcal{H}}_b$ are properly normalized Hamiltonians $\mathcal{H}(0)$ [see Eq. (2.1) and Appendix B].

Equation (2.11) provides the connection between the stress tensor component $t_{\perp\perp}$ parallel to the surfaces of the slab and the spin lattice model given by Eq. (2.1). It is valid also for temperatures $T>T_c$ and thus generalizes Eq. (36) of Ref. [14]. For $T<T_c$ Eq. (2.11) holds also for $O(N)$ symmetric spin models, because the correlation length ratio $\xi_\parallel/\xi_\perp$ remains finite at $T=T_c$ and it can be continued analytically into the Goldstone regime, where it can be used for the anisotropic rescaling of the coordinates according to Eq. (2.7). Finally, we note that Eq. (2.11) only holds for periodic boundary conditions.

For the purposes of this investigation Eq. (2.11) serves as a prescription to obtain the universal scaling function of the Casimir force in critical slabs with periodic boundary conditions by Monte Carlo simulations. However, Eq. (2.11) contains the ratio $\xi_{\parallel,0}(\lambda)/\xi_{\perp,0}(\lambda)$ of the correlation length amplitudes for Eq. (2.1) as a prefactor. For the two-dimensional (2D) Ising model this function is given by [15]

$$\frac{\xi_{\parallel,0}(\lambda)}{\xi_{\perp,0}(\lambda)} = \frac{J_\perp(\lambda) + J_\parallel(\lambda)\sinh[2\beta_c(\lambda)J_\perp(\lambda)]}{J_\parallel(\lambda) + J_\perp(\lambda)\sinh[2\beta_c(\lambda)J_\parallel(\lambda)]}, \tag{2.12}$$

and by virtue of Eq. (2.2), Eq. (2.11) can be made explicit. But in $d\geq 3$ no such information is available. However, in the critical regime, where Eq. (2.11) will be applied, the scaling argument $L_\perp/\xi$ will typically not exceed values of the order of 10. This means that we will be dealing with reduced temperatures in the range $|t|<10(L_\perp/\xi_0)^{-1/\nu}$, i.e., the relevant temperature range diminishes as the system size $L_\perp$ increases. As can be seen explicitly in Eq. (2.12) the correlation length amplitude ratio only depends on the temperature T and does *not* display any scaling behavior. Therefore, the generally unknown prefactor in Eq. (2.11) can be treated as a constant for sufficiently large system sizes which can be determined by a normalization of $\langle t_{\perp\perp}\rangle$ to known results at $T=T_c$ [6].

We end this section with some observations that turn out to be very helpful for analytical calculations of the variance of the force. Since they are model independent we give them before passing to explicit calculations presented in the following section. Let us consider an anisotropic Hamiltonian of the type given by Eq. (2.1), where $J_1(\lambda)=\cdots=J_{d-1}(\lambda)=J_\parallel(\lambda)=(1+\lambda)J$ and $J_d(\lambda)=J_\perp(\lambda)=[1-(d-1)\lambda]J$. Then, it is easy to see that

$$\mathcal{H}(\lambda)=\mathcal{H}(0)-\lambda J\sum_{\mathbf{R}}\left[\sum_{k=1}^{d-1}S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_k}-(d-1)S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_d}\right], \tag{2.13}$$

or, equivalently,

$$\beta\mathcal{H}(\lambda)=\beta\mathcal{H}(0)-\lambda\sum_{\mathbf{R}}\tilde{t}_{\perp,\perp}(\mathbf{R}), \tag{2.14}$$

where

$$\tilde{t}_{\perp,\perp}(\mathbf{R})=\beta J\left[\sum_{k=1}^{d-1}S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_k}-(d-1)S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_d}\right] \tag{2.15}$$

differs only by a multiplying factor from the stress tensor $t_{\perp,\perp}(\mathbf{R})$ defined in Eq. (2.11).

Let $\tilde{f}(T,\lambda)$ be the total free energy per unit spin of a system with the Hamiltonian (2.14). Then, taking into account the translational invariance symmetry, it is easy to see that

$$\langle\tilde{t}_{\perp,\perp}(\mathbf{R})\rangle=-\frac{\partial}{\partial\lambda}[\beta\tilde{f}(T,\lambda)]_{\lambda=0}=\beta J(d-1)[\langle S_{\mathbf{0}}S_{\mathbf{e}_1}\rangle-\langle S_{\mathbf{0}}S_{\mathbf{e}_d}\rangle]. \tag{2.16}$$

Therefore, in order to calculate the average value of $\tilde{t}_{\perp,\perp}(\mathbf{R})$ one needs either to know the finite-size free energy density of an anisotropic system, or, what is much simpler, the nearest-neighbor two-point correlations along the axes of the isotropic finite system.

III. ANALYTICAL RESULTS

In this section we summarize our analytical results for the two-dimensional Ising, for the spherical model with $2<d<4$, and for the Gaussian model. Their derivation for the Ising model is given in Appendix C, while ones for the spherical model is given in Appendix D.

A. Two-dimensional Ising model

For the two-dimensional Ising model on a square lattice with geometry $L\times M$ the lattice representation of the stress tensor is well known for a long time [14,16]. In our notations, using Eqs. (2.11) and (2.12), we obtain

$$\beta J'(1)\left[\frac{d}{d\lambda}\left(\frac{\xi_{\parallel,0}(\lambda)}{\xi_{\perp,0}(\lambda)}\right)\Bigg|_{\lambda=0}\right]^{-1}=\frac{\beta J[1+\sinh(2\beta J)]}{2[\sinh(2\beta J)-2\beta J\cosh(2\beta J)-1]}. \tag{3.1}$$

At the critical point β_c of the isotropic system one has [15]

$$1=\sinh(2\beta_c J), \tag{3.2}$$

and the right-hand side of the above equation simplifies essentially becoming simply $-1/(2\sqrt{2})$. Therefore, at $T=T_c$, the stress tensor reads

$$t_{x,x}(i,j)=\frac{1}{2\sqrt{2}}(S_{i,j}S_{i,j+1}-S_{i,j}S_{i+1,j}), \tag{3.3}$$

which is exactly the form considered in Ref. [14]. In the limit $M\to\infty$ at the critical point T_c of the bulk system one has [14]

$$\langle t_{x,x}\rangle=-\frac{\pi}{6}cL^{-2}, \tag{3.4}$$

where $c=1/2$ is the so-called central charge of the Ising model [12]. The Casimir amplitude is [12]

$$\Delta=-\frac{\pi}{6}c,\quad c=\frac{1}{2}. \tag{3.5}$$

It is easy to see that close to T_c the right-hand side of Eq. (3.1) becomes

$$-\frac{1}{2\sqrt{2}}\left(1+\frac{\beta-\beta_c}{\beta_c}\right)+O((\beta-\beta_c)^2). \tag{3.6}$$

Since $\nu=1$ for 2D Ising model, it is clear from Eq. (3.4) that the contributions to the Casimir force due to the term proportional to $\beta-\beta_c$ in the above expression will be of the order of L^{-3}. Such contributions will be neglected. Therefore, in the critical region of the finite system we conclude that the stress tensor is given by

$$t_{x,x}(i,j)=\frac{1}{2\sqrt{2}}(S_{i,j}S_{i,j+1}-S_{i,j}S_{i+1,j})+\frac{1}{2}(\beta_c-\beta)(\hat{\mathcal{H}}-\hat{\mathcal{H}}_b). \tag{3.7}$$

One can interpret the variance of the stress tensor $\Delta t_{x,x}(i,j)$ as a variance of a local measurement of the Casimir force made near the point (i,j). For the leading behavior of the variance at T_c one then has [see Eq. (C6)]

$$\Delta t_{x,x}(i,j)\simeq 1-2/\pi. \tag{3.8}$$

Definitely, in addition from the above nonuniversal part the variance contains also universal parts that are negligible in comparison with the nonuniversal one.

As we said above, we will interpret $\langle t_{x,x}(i,j)\rangle$ as a local measurement of the Casimir force made near the point (i,j). Let us imagine that we are collecting measurements from all the points belonging to the "surface" $(1,j)$, $j\in[1,\ldots,M]$ **(**in the very same way one can consider the opposite "surface" (L,j), $j\in[1,\ldots,M]$**)**. The surfaces are important because they are the only place where in an experiment the Casimir force is experimentally accessible. To characterize the force measured on the whole surface, instead of $t_{x,x}(i,j)$, one has to consider $\sum_j t_{x,x}(1,j)$. Taking, in a first approximation, any local measurement to be independent from the other ones, one obtains that

$$\Delta\sum_j t_{x,x}(1,j) \sim M\Delta t_{x,x}(1,1) \simeq 0.363M, \tag{3.9}$$

which implies that, indeed, in agreement with [13],

$$(\Delta\beta F_C^t)^2 \propto N_\parallel^{d-1} = (L_\parallel/a)^{d-1}, \tag{3.10}$$

where $d=2$.

An estimation can be also derived for $\Delta\Sigma_{i,j}\, t_{x,x}(i,j)$. With a variance of such a type one deals when, say, Monte Carlo simulations of the force are performed. One obtains [see Eq. (C10)]

$$\Delta\sum_{i,j} t_{x,x}(i,j) = \frac{1}{2}\left[-\frac{1}{2}+\frac{2}{\pi}\right]ML \simeq 0.068ML. \tag{3.11}$$

We again observe that the variance of the sum of $t_{x,x}(i,j)$ is proportional to the total number of summands in this sum. The coefficient of proportionality for 2D Ising model, when the sum is over all spins in the finite system, turns out to be 0.068.

Unfortunately, as far as we are aware, the finite-size properties of the free energy of the two-dimensional anisotropic Ising model under periodic boundary conditions are not available for $T\neq T_c$. This makes the comparison of the direct derivation of the force as a derivative of the finite-size scaling excess free energy and as average of the operator (2.11) a challenging task. Moreover the behavior of the finite-size free energy of the isotropic system is only known for moderate values of the scaling arguments [17]. Nevertheless, from Ref. [17] one can extract the following results for the scaling functions of the excess free energy and the Casimir force.

(a) Excess free energy: The scaling function of the excess free energy is [7]

$$X_{\rm ex} = -\frac{\pi}{12} - \pi\sum_{i=2}^{\infty}\binom{1/2}{i}\left(\frac{x}{2\pi}\right)^{2i}(1-2^{-2i+1})\zeta(2i-1), \tag{3.12}$$

where $-\pi<x<2\pi$, and the scaling variable is $x=8K_c tL$.

(b) Casimir force: The scaling function of the Casimir force $X_{\rm Casimir}$ is related to that one of the excess free energy via

$$X_{\rm Casimir} = X_{\rm ex}(x) - x\frac{\partial}{\partial x}X_{\rm ex}(x). \tag{3.13}$$

Then, from Eq. (3.12), one immediately obtains

$$X_{\rm Casimir} = -\frac{\pi}{12} - \pi\sum_{i=2}^{\infty}\binom{1/2}{i} \times\left(\frac{x}{2\pi}\right)^{2i}(1-2i)(1-2^{-2i+1})\zeta(2i-1). \tag{3.14}$$

B. The spherical model

We consider a spherical model on a d-dimensional hypercubic lattice $\Lambda\in Z^d$, where $\Lambda=L_1\times L_2\times\cdots\times L_d$. Let $L_i=N_i a_i$, $i=1,\ldots,d$, where N_i is the number of spins and a_i is the lattice constant along the axis $\mathbf{e}_i$ with $\mathbf{e}_i$ being a unit vector along that axis. With each lattice site $\mathbf{r}$ one associates a real-valued spin variable $S_{\mathbf{r}}$ which obey the constraint

$$\sum_{\mathbf{r}\in\Lambda}\langle S_{\mathbf{r}}^2\rangle = N, \tag{3.15}$$

where $N=N_1N_2\ldots N_d$ is the total number of spins in the system. The average in Eq. (3.15) is with respect to the Hamiltonian of the model which is

$$\beta\mathcal{H} = -\frac{1}{2}\beta\sum_{\mathbf{r},\mathbf{r}'} S_{\mathbf{r}}J(\mathbf{r},\mathbf{r}')S_{\mathbf{r}'} + s\sum_{\mathbf{r}} S_{\mathbf{r}}^2. \tag{3.16}$$

In the current paper we will consider only the case of nearest-neighbor interactions, i.e., we take $J(\mathbf{r},\mathbf{r}')=J(|\mathbf{r}-\mathbf{r}'|)=J_j$, if $\mathbf{r}-\mathbf{r}'=\pm\mathbf{e}_j$, $i=1,\ldots,d$, and $J(\mathbf{r},\mathbf{r}')=0$ otherwise.

For such a model it can be shown [7] that under periodic boundary conditions, the free energy of the model (per unit spin) is given by

$$\beta f(K,\mathbf{N}) = \frac{1}{2}\left[\ln\frac{K}{2\pi}-K\right] + \sup_{w>0}\left\{-\frac{1}{2}Kw+\frac{1}{2N}\sum_{\mathbf{k}\in\mathcal{B}_\Lambda}\ln\left[w+1-\frac{\hat{J}(\mathbf{k})}{\hat{J}(\mathbf{0})}\right]\right\}, \tag{3.17}$$

while the two-point correlation function is

$$G(\mathbf{r},K,\mathbf{N}) = \frac{1}{KN}\sum_{\mathbf{k}\in\mathcal{B}_\Lambda}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{w+1-\hat{J}(\mathbf{k})/\hat{J}(0)}. \tag{3.18}$$

Here $s=K(w+1)/2$, $K=\beta\hat{J}(\mathbf{0})$, where $\hat{J}(\mathbf{k})$ is given by the Fourier transform of the interaction

$$\hat{J}(\mathbf{k}) = \sum_{\mathbf{r}} J(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{3.19}$$

and the wave vector $\mathbf{k}=\{k_1,k_2,\ldots,k_d\}\in\mathcal{B}_\Lambda$ is with components $k_i=2\pi n_i/L_i$, where $n_i=1,\ldots,N_i$, $i=1,\ldots,d$. The equation for the spherical field w reads

$$\frac{1}{N}\sum_{\mathbf{k}\in\mathcal{B}_\Lambda}\frac{1}{w+1-\hat{J}(\mathbf{k})/\hat{J}(\mathbf{0})} = K, \tag{3.20}$$

which leads immediately to $G(\mathbf{0},t,\mathbf{N})=1$.

For nearest-neighbor anisotropic interactions it can be shown that [see Eq. (D16)]

$$\frac{\xi_j}{\xi_i} = \sqrt{\frac{b_j}{b_i}} = \sqrt{\frac{J_j}{J_i}}, \tag{3.21}$$

where ξ_j is the correlation length in direction j, and $b_j=J_j/\Sigma_{j=1}^d J_j$, which leads to the following explicit form of the stress tensor within the spherical model [see Eq. (D18)]:

$$t_{\perp\perp}(\mathbf{R}) = \frac{\beta J}{d/2}\left[\sum_{k=1}^{d-1} S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_k} - (d-1)S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_d}\right] + \frac{1}{d\nu}(\beta_c - \beta)(\hat{\mathcal{H}} - \hat{\mathcal{H}}_b). \tag{3.22}$$

Here $\hat{\mathcal{H}}$ is the Hamiltonian (normalized per unit particle) of the finite system and $\hat{\mathcal{H}}_b$ is that one of the infinite system.

1. Evaluation of the finite-size excess free energy of the anisotropic system

First, one can demonstrate that the critical coupling of the anisotropic bulk system is [see Eq. (D30)]

$$K_c \equiv 2\beta_c \sum_{j=1}^{d} J_j = W_d(0|\mathbf{b}) = \int_0^\infty dx \prod_{j=1}^{d} e^{-xb_j} I_0(xb_j). \tag{3.23}$$

Then, close to $K=K_c$, when $2<d<4$, for the scaling form of the *excess* free energy $\beta(f-f_b)$ (per spin) in the limit of a film geometry $N_1, N_2, \ldots, N_{d-1} \to \infty$ one obtains [see Eq. (D35)]

$$\beta[f(K,N_\perp|\mathbf{b}) - f_b(K|\mathbf{b})] = \left\{ \frac{1}{4}x_1(y-y_\infty) - \frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2}(y^{d/2} - y_\infty^{d/2}) - \frac{2}{(2\pi)^{d/2}}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2} y^{d/4}\sum_{q=1}^{\infty}\frac{K_{d/2}(q\sqrt{y})}{q^{d/2}} \right\} N_\perp^{-d}. \tag{3.24}$$

In the above equation

$$x_1 = b_\perp (K_c - K) N_\perp^{1/\nu}, \quad \nu = \frac{1}{d-2} \tag{3.25}$$

is the temperature scaling variable, $y_\infty = 2w_b N_\perp^2 / b_\perp$ is the solution of the bulk spherical field equation [see Eq. (D37)]

$$-\frac{1}{2}x_1 = \frac{\Gamma(1-d/2)}{(4\pi)^{d/2}}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2} y_\infty^{d/2-1}, \tag{3.26}$$

while $y=2wN_\perp^2/b_\perp$ is the solution of the finite-size spherical field equation [see Eq. (D38)]

$$-\frac{1}{2}x_1 = \frac{\Gamma(1-d/2)}{(4\pi)^{d/2}}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2} y^{d/2-1} + \frac{2}{(2\pi)^{d/2}}\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2} y^{d/4-1/2}\sum_{q=1}^{\infty}\frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}}. \tag{3.27}$$

For the Casimir force one derives [see Eq. (D40)]

$$\beta F_{\mathrm{Casimir}} = N_\perp^{-d}\left\{ \frac{1}{4}x_1(y-y_\infty) - (d-1)\left(\frac{b_\perp}{b_\|}\right)^{(d-1)/2} \times \left[\frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}(y^{d/2} - y_\infty^{d/2}) + \frac{2}{(2\pi)^{d/2}} y^{d/4}\sum_{q=1}^{\infty}\frac{K_{d/2}(q\sqrt{y})}{q^{d/2}} \right] \right\}, \tag{3.28}$$

whereas for the Casimir amplitudes Δ we derive [see Eq. (D44)]

$$\Delta = -\frac{2}{d(2\pi)^{d/2}} y_c^{d/4+1/2}\sum_{q=1}^{\infty}\frac{K_{d/2+1}(q\sqrt{y_c})}{q^{d/2-1}}, \tag{3.29}$$

with $\beta_c F_{\mathrm{Casimir}}(K_c, L_\perp) = (d-1)\Delta L_\perp^{-d}$. The exact value of y_c and Δ in an explicit form is only known for $d=3$. Then

$$y_c = 4\ln^2[(1+\sqrt{5})/2] \tag{3.30}$$

(this value is well known and seems that has been derived for the first time in Ref. [18]), and, then, one obtains [19]

$$\Delta = -\frac{2\zeta(3)}{5\pi}. \tag{3.31}$$

This is the only exactly known Casimir amplitude for a three-dimensional system.

2. Evaluation of the average value of the stress tensor

For the scaling form of the average value of the stress tensor one derives [see Eq. (D54)]

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = -\left\{ \frac{2(d-1)}{(2\pi)^{d/2}}\left[y^{d/4}\sum_{q=1}^{\infty}\frac{K_{d/2}(q\sqrt{y})}{q^{d/2}} + \frac{1}{d}y^{(d+2)/4}\sum_{q=1}^{\infty}\frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}} \right] + \frac{(d-2)}{4d}x_1(y-y_\infty) \right\} N_\perp^{-d}. \tag{3.32}$$

It is also possible to demonstrate (see Appendix D) that the above expression is equivalent to $\beta F_{\mathrm{Casimir}}$ given by Eq. (3.28) for the isotropic system (when $b_\| = b_\perp$), i.e., indeed,

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = \beta F_{\mathrm{Casimir}} \tag{3.33}$$

for the spherical model.

3. Evaluation of the variance of the stress tensor

For the variance of the Casimir force in the spherical model at $T=T_c$ one obtains [see Eq. (3.34)]

$$\Delta t_{\perp,\perp} \equiv \Delta \sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) \simeq 0.107 N_\perp N_\|^2. \tag{3.34}$$

This will be also the leading result everywhere in the critical region, since it is coming from the nonsingular part of the free energy around $T=T_c$ an analytical expansion should be possible. It is also clear that if the summation over **R** in Eq. (3.34) is not over the total number of particles in Λ, which is $N_\perp N_\parallel^{d-1}$, but over, say, all the spins from one of the boundaries, then the corresponding variance will be proportional to the total number of spins there, i.e.,

$$(\Delta\beta F_C^t)^2 \propto N_\parallel^{d-1} = (L_\parallel/a)^{d-1}, \tag{3.35}$$

exactly as it has been found in Ref. [13], see Eq. (1.7).

C. The Gaussian model

In order to simplify the notations we define the Gaussian model in the same way that we have defined the spherical model. Actually the spherical model is a Gaussian-type model with one additional constraint, given by Eq. (3.15) fixing the average length of all the spins in the system. To be more precise, we suppose that the Hamiltonian $\mathcal{H}$ of the model is again given by Eq. (3.16), where, as before, $s = K(1+w)/2$ and $K=\beta\tilde{J}(\mathbf{0})$. The only difference is that now Eq. (3.15) is missing and w is not a quantity whose behavior has to be derived from it, but a parameter which describes the deviation from the critical point, i.e., $w=(\beta_c-\beta)/\beta$. As a result, the free energy density of the model becomes

$$\beta f(K,\mathbf{N}) = \frac{1}{2}\left[\ln\frac{K}{2\pi} - K\right] + U(w,\mathbf{N}) - \frac{1}{2}Kw, \tag{3.36}$$

where $U(w,\mathbf{N})$ is given by Eq. (D3), while the two-point correlation function is still determined by Eq. (3.18). Then, for a system with anisotropic short-range interaction, proceeding in the same way as in Sec. III B, we derive that Eqs. (D13)–(D17) are still valid, wherefrom we conclude that in the Gaussian model the stress tensor again is

$$t_{\perp\perp}(\mathbf{R}) = \frac{\beta J}{d/2}\left[\sum_{k=1}^{d-1} S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_k} - (d-1)S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_d}\right] + \frac{1}{d\nu}(\beta_c-\beta)(\hat{\mathcal{H}}-\hat{\mathcal{H}}_b), \tag{3.37}$$

where $\hat{\mathcal{H}}$ is the Hamiltonian (normalized per unit particle) of the finite and $\hat{\mathcal{H}}_b$ of the infinite model.

1. Evaluation of the finite-size excess free energy of the anisotropic system

The analysis of the excess free energy can be performed along the same lines as in the case of a spherical model. For example, for $U(w,\mathbf{N})$ Eqs. (D19)–(D23) and (D28) are still valid. On the basis of these equations we immediately obtain that in the case of a Gaussian model the excess free energy in a film geometry is

$$\beta[f(K,N_\perp|\mathbf{b}) - f_b(K|\mathbf{b})] = -\frac{2}{(2\pi)^{d/2}}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} y^{d/4}\sum_{q=1}^{\infty}\frac{K_{d/2}(q\sqrt{y})}{q^{d/2}}N_\perp^{-d}. \tag{3.38}$$

In the above equation the temperature scaling variable is

$$y = 2wN_\perp^{1/\nu}/b_\perp, \tag{3.39}$$

where $\nu=1/2$ and $w=\beta_c/\beta-1$.

From Eq. (3.38), using the property of the $K_\nu(x)$ functions [20] that

$$\frac{\partial}{\partial y}[y^\nu K_\nu(ay)] = -ay^\nu K_{\nu-1}(ay), \tag{3.40}$$

we immediately derive that the Casimir force in such an anisotropic Gaussian model is given by

$$\beta F_{\text{Casimir}} = -\frac{2}{(2\pi)^{d/2}}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} N_\perp^{-d} \times\left\{(d-1)y^{d/4}\sum_{q=1}^{\infty}\frac{K_{d/2}(q\sqrt{y})}{q^{d/2}} + y^{d/4+1/2}\sum_{q=1}^{\infty}\frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}}\right\}. \tag{3.41}$$

Note that despite the similarities with the spherical model both the excess free energy and the Casimir force differs essentially for the two models. Let us demonstrate that even more explicitly on the example of the Casimir amplitudes Δ. We are reminded that in the spherical model they are given, for $2<d<4$, by Eq. (3.29) where y_c is the solution of the spherical field equation at $\beta=\beta_c$. In explicit form we have been able to solve this equation and to calculate Δ only for $d=3$. The situation with the Gaussian model is much simpler. At the critical point $\beta=\beta_c$ one has $y=0$, and, therefore, from Eq. (3.41), or Eq. (3.38), we obtain (in the isotropic system)

$$\Delta = -\frac{\Gamma(d/2)\zeta(d)}{\pi^{d/2}}. \tag{3.42}$$

So, for $d=3$ one has $\Delta=-\zeta(3)/2\pi$ and, therefore,

$$\Delta_{\text{spherical model}} = \tfrac{4}{5}\Delta_{\text{Gaussian model}}, \quad d=3. \tag{3.43}$$

2. Evaluation of the average value of the stress tensor

Having in mind that $u=(\partial/\partial\beta)(\beta f)$ and using Eq. (3.40), for the difference of the finite-size and bulk internal energy densities one can easily derive from Eqs. (3.36) and (3.38),

$$u - u_b = -\frac{\beta_c/\beta}{(2\pi)^{d/2}}\frac{y^{d/4+1/2}}{(\beta_c-\beta)}\sum_{q=1}^{\infty}\frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}}N_\perp^{-d}, \tag{3.44}$$

where $y=2dwN_\perp^2$ and $w=\beta_c/\beta-1$. Next, from Eq. (3.18), or Eq. (3.36), for the stress tensor (3.37) of the Gaussian model we derive that

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = \frac{d-1}{d}\frac{1}{N}\sum_{\mathbf{k}\in\mathcal{B}_\Lambda}\frac{\cos(k_1a_1)-\cos(k_da_d)}{d(1+w)-\sum_{j=1}^{d}\cos(k_ja_j)} - \frac{\beta_c/\beta}{d}\frac{2}{(2\pi)^{d/2}}y^{d/4+1/2}\sum_{q=1}^{\infty}\frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}}N_\perp^{-d}, \tag{3.45}$$

where we have taken into account that $\nu=1/2$. Applying to the first row in the above equation the same way of acting as in the case of the spherical model, and replacing β_c/β by 1 (since we are close to the critical point), we derive

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = -\frac{2}{d(2\pi)^{d/2}}\left\{y^{d/4+1/2}\sum_{q=1}^{\infty}\frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}} + (d-1)y^{(d+2)/4}\sum_{q=1}^{\infty}\frac{K_{1+d/2}(q\sqrt{y})}{q^{d/2-1}}\right\}N_\perp^{-d}. \tag{3.46}$$

Now it only remains to show that the right-hand side of the above equation is indeed equal to the right-hand side of Eq. (3.41) (for $b_\perp = b_\parallel$), which gives the Casimir force calculated in a direct manner as a derivative of the finite-size free energy with respect to the size of the system. In order to demonstrate this, let us note that, according to the identity (D43),

$$K_{d/2+1}(x) = K_{d/2-1}(x) + \frac{d}{x}K_{d/2}(x). \tag{3.47}$$

Inserting Eq. (3.47) in Eq. (3.46) and comparing the result with Eq. (3.41), we conclude that, indeed,

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = \beta F_{\text{Casimir}} \tag{3.48}$$

for the Gaussian model.

3. Evaluation of the variance of the stress tensor

For the variance of the stress tensor all the equations from the corresponding part of Appendix D for the spherical model are still valid. That is because the leading contribution of the variance is stemming from the regular part of the bulk free energy $U_b(0|\mathbf{b})$ [see Eq. (D25)] evaluated at $T=T_c$ [see Eq. (D65)]. This observation leads to the conclusion that, as in the spherical model case,

$$\Delta t_{\perp,\perp} \equiv \Delta\sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) \simeq 0.107 N_\perp N_\parallel^2, \tag{3.49}$$

where the summation is over all the spins of the system.

IV. MONTE CARLO RESULTS

The foundation of our Monte Carlo investigations of the critical Casimir force is laid by Eqs. (2.11) and (B8), respectively. Apart from the *a priori* unknown coefficient $J'(1)/R'(0)$ and the bulk energy density u_b the numerical evaluation of Eq. (2.11) is absolutely straightforward and apart from usual algorithmic precautions in the critical regime no special techniques are required. However, as has become obvious in, e.g., Eq. (3.11), the statistical error of the estimate will increase with the system size if the number of Monte Carlo sweeps is kept constant. In order to approach the asymptotic regime larger system sizes, say, $N_\parallel=120$ and $N_\perp=20$ lattice sites in $d=3$ are required which means that a reliable estimation of the Casimir force remains computationally demanding as far as the required CPU time is concerned.

We employ a hybrid algorithm [21] which consists of Metropolis [22] and single cluster updates [23] for the Ising model, for XY, and Heisenberg simulations over-relaxation updates [24] are employed as a third update method. Cluster updates are only used in the immediate vicinity of the critical point, e.g., for $-0.02\leqslant t\leqslant 0.02$ for the system size indicated above. Typically, we have performed between 4.8×10^6 and 9.6×10^6 Monte Carlo steps per spin. In order to cope with the high demand of CPU time for larger systems we have performed part of our simulation in parallel on two-processor Intel Xeon system and on a four-processor DEC Alpha system using the OpenMP Standard for SMP programming. A few runs have also been performed on a two-processor AMD Opteron system.

We first investigated the energy dependent contribution $[\beta_c(0)-\beta](u-u_b)$ to Eqs. (2.11) and (B8) by a series of simulations on a cubic geometry for $N_\parallel=N_\perp=20,\ldots,80$ in order to obtain reliable estimates for the bulk energy density u_b. It turns out that within the range $-0.2\leqslant t\leqslant 0.2$ of reduced temperatures, various aspect ratios $N_\parallel/N_\perp=3,4,6,8$, and several system sizes $N_\parallel=60,\ldots,120$ the energy dependent contribution $[\beta_c(0)-\beta](u-u_b)/d\nu$ is always negligible. As a typical result we obtained that for forces of the order of 10^{-1} with a statistical error in the range 10^{-2}–10^{-3}, the energy contribution $[\beta_c(0)-\beta](u-u_b)/d\nu$ remains in the range 10^{-4}–10^{-5} for all models. The prefactor $J'(1)/R'(0)$ roughly evaluates to $J'(1)/R'(0)\simeq 0.3$ in all cases. We therefore conclude that we can safely ignore the energy contribution to the Casimir force for our Monte Carlo investigations of the Ising, the XY, and the Heisenberg model in three dimensions.

A. Three-dimensional Ising model

As expounded above, we have neglected the energy dependent contribution to Eq. (B8) for our Monte Carlo evaluations of the scaling function $\theta_{per}(x)$, $x=t(L_\perp/a)^{1/\nu}$ of the Casimir force. From extended simulations for various aspect ratios $N_\parallel/N_\perp=3$, 4, 6, and 8 we have arrived at the conclusion that corrections to $\theta_{per}(x)$ due to finite aspect ratio are by far negligible within the statistical error for $N_\parallel/N_\perp=6$. In fact, our results for $N_\parallel/N_\perp=4$ can hardly be distinguished from corresponding results for larger aspect ratios. We have therefore fixed the aspect ratio to the value 6 and performed simulations for $N_\perp=16$, 20, 24, and 30. The resulting scaling plot for $\theta_{per}(x)$ is shown in Fig. 1.

For $T\geqslant T_c$ finite-size scaling works very well, whereas for $T<T_c$ data collapse for $N_\perp=30$ is not as good. However, the data collapse improves upon increasing the statistics and so we have performed 9.6×10^6 Monte Carlo steps per lattice site for the largest lattice $N_\perp=30$ for $T<T_c$. With the esti-

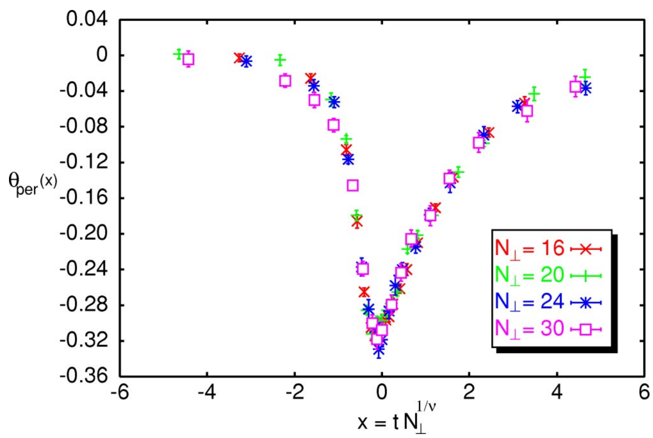

FIG. 1. Scaling function $\theta_{per}(x)$ of the Casimir force for the $d=3$ Ising model in a slab geometry for periodic boundary conditions as a function of the scaling variable $x=tN_\perp^{1/\nu}$, where $N_\perp=L_\perp/a$ is the number of lattice layers. The aspect ratio is chosen as $N_\parallel/N_\perp=6$ (see main text). Finite-size scaling according to our expectation is confirmed within two standard deviations, where $\nu=0.63$ has been chosen. The vertical scale has been adjusted according to the estimate $\theta_{per}(0)\equiv 2\Delta_{per,n=1}=-0.306$ (see Ref. [25]). The error bars displayed here correspond to one standard deviation.

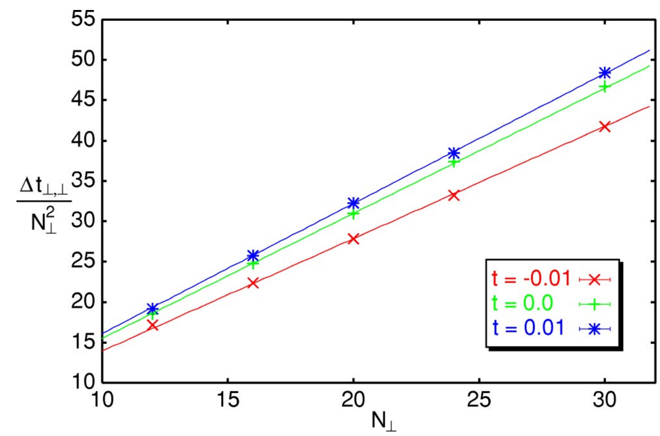

FIG. 2. Variance $\Delta t_{\perp,\perp}$ of the stress tensor for the Ising model in $d=3$ [see Eqs. (3.34) and (3.49)], normalized to $N_\perp^2$ at fixed aspect ratio $N_\parallel/N_\perp=6$ as a function of $N_\perp$ for different reduced temperatures t in the critical regime. The behavior is linear as indicated by the straight lines connecting the data points. Their slopes have been evaluated as 1.39 for $t=-0.01$, 1.55 for $t=0$, and 1.61 for $t=0.01$. The statistical error of the data (one standard deviation) is smaller than the symbol size.

mate $\nu=0.63$ for the correlation length exponent we finally obtain scaling within two standard deviations. The scaling function $\theta_{per}(x)$ decays exponentially for $x\to\pm\infty$ and has its minimum *below* T_c. However, due to the magnitude of the statistical error its location cannot be determined accurately enough to exclude $x=0$ with reasonable certainty. The Monte Carlo data for the Casimir force are not normalized due to the *a priori* unknown prefactor $J'(1)/R'(0)$ in Eq. (B8). The data displayed in Fig. 1 have therefore been scaled in such a way that $\theta_{per}(0)\equiv 2\Delta_{per,n=1}$ is given by the best known estimate $\Delta_{per,n=1}\simeq -0.153$ for the Casimir amplitude $\Delta_{per,n=1}$ for the three-dimensional Ising model [25].

The scaling function displayed in Fig. 1 has been obtained from Eq. (B8), where a spatial average over all lattice sites is performed. As expounded in Sec. III (see also Ref. [14]) this leads to a certain size dependence of the *variance* of the stress tensor as, e.g., given by Eq. (3.34) for the spherical model and by Eq. (3.49) for the Gaussian model. In order to investigate the variance also for the Ising model in $d=3$ we have recorded the distribution function of the stress tensor during our Monte Carlo simulations. It turns out that the shape of the distribution function is captured by a Gaussian distribution to a very high degree of accuracy also for the Ising model (see Ref. [13]). We are therefore able to extract the variance of the stress tensor average from a least square fit of the measured distribution function to a Gaussian, where the variance is one of the fit parameters. Guided by Eqs. (3.34) and (3.49) we have normalized the variance to $N_\perp^2$ in order to obtain a linear law at fixed aspect ratio. Our results for $N_\parallel/N_\perp=6$ are displayed in Fig. 2.

The functional dependence is indeed linear and the slope at $t=0$ $(T=T_c)$ is 1.55 as compared to $0.107(N_\parallel/N_\perp)^2\simeq 3.85$ for $N_\parallel/N_\perp=6$ according to Eqs. (3.34) and (3.49) for the spherical and the Gaussian model. The strict linearity also prevails for other temperatures in the scaling regime as shown in Fig. 2. The quadratic dependence of $\Delta t_{\perp,\perp}/N_\perp^2$ on the aspect ratio has also been confirmed for the Ising model in $d=3$ at $T=T_c$ from simulations at different aspect ratios (not shown).

B. Three-dimensional *XY* model

In accordance with our findings for the Ising model we find that the value 6 for the aspect ratio of the simulation lattice is also a good choice for the *XY* model. We have performed simulations for $N_\perp=16$, 20, 24, and 30, where 4.8×10^6 Monte Carlo steps per lattice site have been performed for all lattice sizes. It turns out that the energy dependent contribution to Eq. (B8) can again be disregarded within the statistical error obtained from the simulations.

As in the Ising case we determine the normalization factor $J'(1)/R'(0)$ in Eq. (B8) from the requirement $\theta_{per}(0)=2\Delta_{per,n=2}$. Unfortunately, all estimates for $\Delta_{per,n=2}$, which are currently available, are based on the ε expansions quoted, e.g., in Ref. [6]. Independent Monte Carlo estimates for the Casimir amplitudes of the *XY* model do not exist and rigorous results for the two-dimensional *XY* model are limited to temperatures below the Kosterlitz-Thouless temperature, where the model renormalizes towards the two-dimensional Gaussian fixed point. The Gaussian model in $d=2$ is characterized by the central charge $c=1$ and therefore the Casimir amplitude for the two-dimensional *XY* model in the low temperature limit is given by $\Delta_{per,n=2,d=2}=-\pi c/6=-\pi/6\simeq -0.5236$ [26].

Apparently, the ε expansion underestimates the magnitude of the Casimir amplitude $\Delta_{per,n=1}$ of the critical Ising model in $d=3$, i.e., $\varepsilon=1$. From the structure of the critical Ginzburg-Landau ϕ^4 theory and the nature of the two-loop approximation to the Casimir amplitude we expect that the ε expansion will also underestimate the magnitude of $\Delta_{per,n}$ for any n. This leads us to the conclusion that the ε expansion of

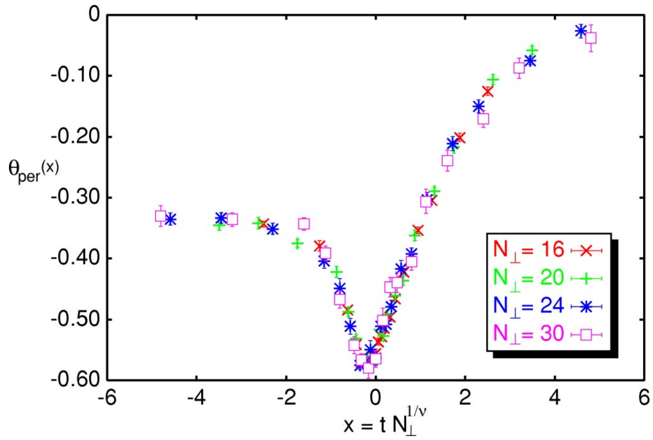

FIG. 3. Scaling function $\theta_{per}(x)$ of the Casimir force for the $d=3XY$ model in a slab geometry for periodic boundary conditions as a function of the scaling variable $x=tN_\perp^{1/\nu}$, where $N_\perp=L_\perp/a$ is the number of lattice layers. The aspect ratio is chosen as $N_\parallel/N_\perp=6$ (see main text). Finite-size scaling according to our expectation is confirmed within two standard deviations, where $\nu=0.67$ has been chosen. The vertical scale has been adjusted according to the estimate $\theta_{per}(0)\equiv 2\Delta_{per,n=2}=-0.56$ (see main text). The error bars displayed here correspond to one standard deviation.

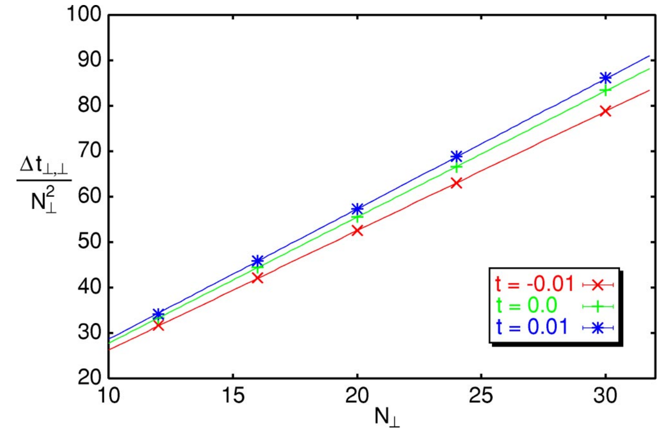

FIG. 4. Variance $\Delta t_{\perp,\perp}$ of the stress tensor for the XY model in $d=3$ [see Eqs. (3.34) and (3.49)], normalized to $N_\perp^2$ at fixed aspect ratio $N_\parallel/N_\perp=6$ as a function of $N_\perp$ for different reduced temperatures t in the critical regime. The behavior is linear as indicated by the straight lines connecting the data points. Their slopes have been evaluated as 2.63 for $t=-0.01$, 2.78 for $t=0$, and 2.86 for $t=0.01$. The statistical error of the data (one standard deviation) is smaller than the symbol size.

the *ratio*

$$\frac{\Delta_{per,n}}{\Delta_{per,n=1}} = n\left[1-\frac{5}{4}\varepsilon\left(\frac{n+2}{n+8}-\frac{1}{3}\right)+O(\varepsilon^2)\right] \tag{4.1}$$

is more accurate in $d=3$ than the ε expansion for numerator and denominator individually (see Ref. [6]). We therefore adopt the approximation

$$\Delta_{per,n} \simeq -0.153n\left[1-\frac{5}{4}\left(\frac{n+2}{n+8}-\frac{1}{3}\right)\right] \tag{4.2}$$

as our estimate for $\Delta_{per,n}$ in $d=3$ in the following, where $\Delta_{per,n=1}=-0.153$ (see above) has been used. From Eq. (4.2) we then have

$$\Delta_{per,2} \simeq -0.28 \tag{4.3}$$

for the three-dimensional XY model. The resulting scaling plot for $\theta_{per}(x)$ is shown in Fig. 3.

For $T\geqslant T_c$ finite-size scaling works very well, whereas for $T<T_c$ data collapse for $N_\perp=30$ is again not as good. However, the data collapse is still acceptable within two standard deviations, so we refrain from performing additional runs here. The scaling function $\theta_{per}(x)$ decays exponentially above T_c for $x\to\infty$ and displays a minimum below T_c. Unlike the Ising model the XY model exhibits long-ranged correlations also below T_c (Goldstone modes) which are a prominent feature in Fig. 3. The scaling function $\theta_{per}(x\to-\infty)$ saturates at about half its minimum value and does no longer decay to zero.

We have also evaluated the size dependence of the variance of the stress tensor for the XY model along the lines of the previous analysis for the Ising model. The distribution function of the stress tensor is again given by a Gaussian to a very high accuracy. The corresponding result for $\Delta t_{\perp,\perp}/N_\perp^2$ is shown in Fig. 4.

The functional dependence is again linear and the slope at $t=0$ $(T=T_c)$ is 2.78 as compared to $0.107(N_\parallel/N_\perp)^2\simeq 3.85$ [see preceding section and Eqs. (3.34) and (3.49)] for the spherical and the Gaussian model. The strict linearity also prevails for other temperatures in the scaling regime as shown in Fig. 4. In summary the XY model behaves just as the Ising model with respect to the variance of the stress tensor.

C. Three-dimensional Heisenberg model

We have repeated the simulations finally for the Heisenberg model in $d=3$ with the same geometric and statistical data as for the XY model for the same reasons discussed above. We note again that the energy dependent contribution to Eq. (B8) can be disregarded within the statistical error obtained from the simulations.

The normalization factor $J'(1)/R'(0)$ in Eq. (B8) is determined from the requirement $\theta_{per}(0)=2\Delta_{per,n=3}$, where the estimate

$$\Delta_{per,3} \simeq -0.39 \tag{4.4}$$

used here has been obtained from Eq. (4.2) for $n=3$. The resulting scaling plot for $\theta_{per}(x)$ is shown in Fig. 5. For $T\geqslant T_c$ finite-size scaling works very well, whereas for $T<T_c$ the scatter of the date is larger than for the XY model. However, the data collapse is still acceptable within two standard deviations. The qualitative shape of the scaling function $\theta_{per}(x)$ is the same as for the XY model. The Heisenberg model also exhibits long-ranged correlations below T_c (Goldstone modes) which is a prominent feature in Fig. 5. The scaling function $\theta_{per}(x\to-\infty)$ saturates at about three quarters of its minimum value.

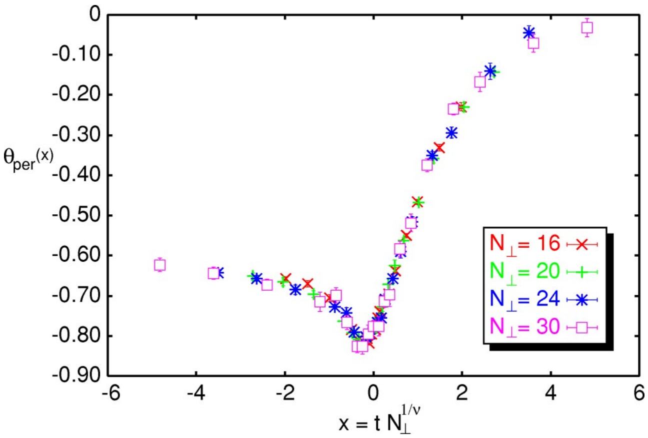

FIG. 5. Scaling function $\theta_{per}(x)$ of the Casimir force for the $d=3$ Heisenberg model in a slab geometry for periodic boundary conditions as a function of the scaling variable $x=tN_\perp^{1/\nu}$, where $N_\perp = L_\perp/a$ is the number of lattice layers. The aspect ratio is chosen as $N_\parallel/N_\perp = 6$. Finite-size scaling according to our expectation is confirmed within two standard deviations, where $\nu=0.71$ has been chosen. The vertical scale has been adjusted according to the estimate $\theta_{per}(0) \equiv 2\Delta_{per,n=3} = -0.78$ (see main text). The error bars displayed here correspond to one standard deviation.

Finally, we have evaluated the size dependence of the variance of the stress tensor for the Heisenberg model along the lines of the previous analyses for the Ising and the *XY* model. As before the distribution function of the stress tensor is given by a Gaussian to a very high accuracy. The corresponding result for $\Delta t_{\perp,\perp}/N_\perp^2$ is shown in Fig. 6.

The functional dependence is linear and the slope at $t=0$ ($T=T_c$) is 3.92 as compared to $0.107(N_\parallel/N_\perp)^2 \simeq 3.85$ [see previous sections and Eqs. (3.34) and (3.49)] for the spherical and the Gaussian model. The strict linearity also prevails for other temperatures in the scaling regime as shown in Fig. 4. In summary the Heisenberg model behaves just as the Ising and the *XY* model with respect to the variance of the stress tensor.

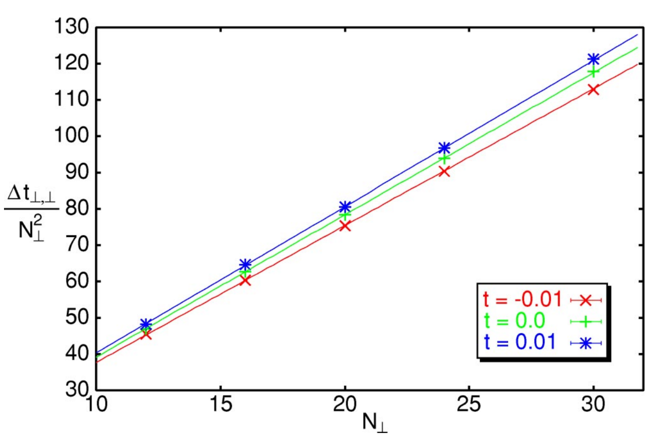

FIG. 6. Variance $\Delta t_{\perp,\perp}$ of the stress tensor for the Heisenberg model in $d=3$ [see Eqs. (3.34) and (3.49)], normalized to $N_\perp^2$ at fixed aspect ratio $N_\parallel/N_\perp = 6$ as a function of $N_\perp$ for different reduced temperatures t in the critical regime. The behavior is linear as indicated by the straight lines connecting the data points. Their slopes have been evaluated as 3.77 for $t=-0.01$, 3.92 for $t=0$, and 4.03 for $t=0.01$. The statistical error of the data (one standard deviation) is smaller than the symbol size.

Apart from different slopes there are no specific differences in the behavior of the variance of the stress tensor for all spin models investigated here in $d=3$. However, the scaling function of the Casimir force does display specific differences as one may expect from the presence and the increasing dominance of Goldstone modes below T_c.

V. SUMMARY AND CONCLUDING REMARKS

In the current paper an operator—the stress tensor operator—on a finite lattice system has been constructed so that its average value gives the universal behavior of the thermodynamic Casimir force near the critical point of a system with short-ranged interactions [see Eq. (2.11)]. The definition of the operator holds in systems in which the hyperscaling is valid [for $O(n)$ models that are systems with dimensionality $2<d<4$]. Its explicit form for the two-dimensional Ising model is [see Eq. (3.7)]

$$t_{x,x}(i,j) = \frac{1}{2\sqrt{2}}(S_{i,j}S_{i,j+1} - S_{i,j}S_{i+1,j}) + \frac{1}{2}(\beta_c - \beta)(\hat{\mathcal{H}} - \hat{\mathcal{H}}_b), \tag{5.1}$$

while that one for the d-dimensional ($2<d<4$) spherical and the d-dimensional Gaussian models is [see Eqs. (3.22) and (3.37), respectively]

$$t_{\perp\perp}(\mathbf{R}) = \frac{\beta J}{d/2}\left[\sum_{k=1}^{d-1} S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_k} - (d-1)S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_d}\right] + \frac{1}{d\nu}(\beta_c - \beta)(\hat{\mathcal{H}} - \hat{\mathcal{H}}_b). \tag{5.2}$$

Here $\hat{\mathcal{H}}$ is the Hamiltonian (normalized per unit particle) of the finite system and $\hat{\mathcal{H}}_b$ is that one of the infinite system. For the spherical model one has to take into account that $\nu = 1/(d-2)$, while $\nu=1/2$ for the Gaussian model. In the example of the two-dimensional Ising model, the spherical model with $2<d<4$, and the Gaussian model we have verified via exact calculations the correctness of the above presentation. They reproduce the correct values of the Casimir amplitudes at $T=T_c$ and, for the spherical and the Gaussian models the expressions for the force derived via the excess free energy and via averaging the stress tensor operator are giving the same results. The amplitudes and the force near the critical point of the bulk system turns out, as expected, to be universal and is in full accordance with the finite-size scaling theory. An evaluation of the variance of the so defined Casimir force has been also performed. If the summation is performed over all the particles within the system the corresponding result for the two-dimensional Ising model is [see Eq. (3.11)]

$$\Delta \sum_{i,j} t_{x,x}(i,j) = \frac{1}{2}\left[-\frac{1}{2} + \frac{2}{\pi}\right] N_\perp N_\parallel \simeq 0.068 N_\perp N_\parallel, \quad (5.3)$$

while that one for the three-dimensional spherical and the Gaussian models is [see Eqs. (3.34) and (3.49)]

$$\Delta t_{\perp,\perp} \equiv \Delta \sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) \simeq 0.107 N_\perp N_\parallel^2. \quad (5.4)$$

The average values of the above stress tensor operator are

$$\left\langle \sum_{i,j} t_{x,x}(i,j) \right\rangle = -\frac{\pi}{12 N_\perp^2}(N_\perp N_\parallel), \quad (5.5)$$

for the two-dimensional Ising model [see Eq. (3.4)],

$$\langle t_{\perp,\perp}\rangle \equiv \left\langle \sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) \right\rangle = -\frac{4\zeta(3)}{5\pi N_\perp^3}(N_\perp N_\parallel^2) \quad (5.6)$$

$$\simeq -\frac{0.306}{N_\perp^3}(N_\perp N_\parallel^2), \quad (5.7)$$

for the three-dimensional spherical model [see Eq. (3.31)], and

$$\langle t_{\perp,\perp}\rangle \equiv \left\langle \sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) \right\rangle = -\frac{\zeta(3)}{2\pi N_\perp^3}(N_\perp N_\parallel^2) \quad (5.8)$$

$$\simeq -\frac{0.382}{N_\perp^3}(N_\perp N_\parallel^2), \quad (5.9)$$

for the three-dimensional Gaussian model [see Eq. (3.42)]. For the "noise-over-signal" ratio

$$\rho_V = \frac{\sqrt{\Delta t_{\perp,\perp}}}{\langle t_{\perp,\perp}\rangle} \quad (5.10)$$

of the so-measured force from the above results one then derives

$$\rho_V \simeq 0.159\left(\frac{N_\perp}{N_\parallel}\right)^{1/2} N_\perp, \quad (5.11)$$

for the Ising model,

$$\rho_V \simeq 1.069\left(\frac{N_\perp}{N_\parallel}\right) N_\perp^{3/2}, \quad (5.12)$$

for the spherical model, and

$$\rho_V \simeq 0.856\left(\frac{N_\perp}{N_\parallel}\right) N_\perp^{3/2}, \quad (5.13)$$

for the Gaussian model. In the general case of a d-dimensional critical system the corresponding ratio at the bulk critical point is

$$\rho_V = \frac{D}{(d-1)\Delta}\left(\frac{N_\perp}{N_\parallel}\right)^{(d-1)/2} N_\perp^{d/2}, \quad (5.14)$$

where $D = D(T \to T_c)$ is a nonuniversal constant that describes the behavior of the variance of the tensor, i.e.,

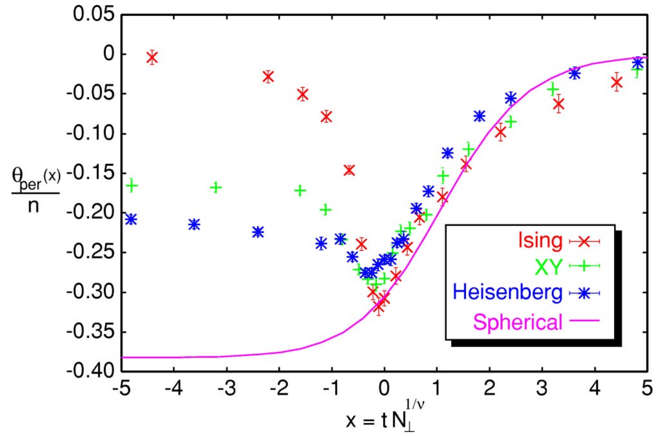

FIG. 7. Scaling function $\theta_{per}(x)/n$ of the Casimir force in $d=3$ in a slab geometry for periodic boundary conditions as a function of the scaling variable $x = tN_\perp^{1/\nu}$, where $N_\perp = L_\perp/a$ is the number of lattice layers. Monte Carlo data are shown for the Ising model $(+, n=1)$, the XY model $(\times, n=2)$, and the Heisenberg model $(*, n=3)$ with lattice size $N_\parallel = 180$ and $N_\perp = 30$. The solid line shows $\theta_{per}(x)/n$ in the spherical limit $(n \to \infty)$.

$$\Delta t_{\perp,\perp} \simeq \frac{D^2(T)}{\beta^2} N_\perp N_\parallel^{d-1}, \quad (5.15)$$

where $D(T)$ is a slowly varying nonuniversal function of T close to T_c and Δ is the usual Casimir amplitude.

Based on the proposed operator, Monte Carlo calculations have been performed and the Casimir force scaling functions have been determined for the three-dimensional Ising, XY, and Heisenberg models. The scaling functions decay exponentially to zero above the critical temperature. The same happens for the Ising model also below T_c, while for the XY and Heisenberg models they tend to a constant because of the existence of the Goldstone modes in this regime in these two models. Our results for $O(n)$ spin models, $n=1,2,3,\infty$, are summarized in Fig. 7. The data for $\theta_{per}(x)$ are normalized to n in order to obtain a direct comparison with the spherical limit, for which the exact result is shown.

Our results confirm that one has to take into account the ratio between the thickness of the film and its lateral dimensions, when planning the settlement of an experiment, in order to achieve the desired noise-over-signal ratio. The numerical results that are presented can be considered as a type of such measuring of the force by Monte Carlo methods. They demonstrate clearly that high accuracy in such type of measurement of the force is indeed possible to achieve.

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APPENDIX A: THE CORRELATION LENGTH AMPLITUDE RELATION

The coordinate transformation given by Eq. (2.7) removes the anisotropy from the spin model defined by Eq. (2.1) in the vicinity of the critical point. From the coordinate transformation and the principle of two scale factor universality a relation between the correlation length amplitudes $\xi_{\parallel,0}(\lambda)$ and $\xi_{\perp,0}(\lambda)$ [see Eq. (2.6)] can be established, which will be derived in the following under the assumption that hyperscaling is also valid, e.g., for $2<d<4$ and short-ranged interactions.

According to the coordinate transformation given by Eq. (2.7) we obtain $\xi'_{\parallel}=\xi_{\parallel}$ and $\xi'_{\perp}=R(\lambda)\xi_{\perp}=\xi_{\parallel}$ [see Eq. (2.8)], i.e., the parallel correlation length $\xi_{\parallel}$ of the (untransformed) anisotropic system remains as the only correlation length of the (transformed) isotropic system. According to the principles of two scale factor universality and hyperscaling the singular part of the (bulk) free energy density $f'_{b,\text{sing}}(t)$ of the transformed spin system can then be written in the form

$$f'_{b,\text{sing}}(\lambda,t)=\mathcal{A}[\xi_{\parallel}(\lambda,t)]^{-d}, \tag{A1}$$

where $t=\beta_c(\lambda)/\beta-1$ is the reduced temperature and $\mathcal{A}$ is a *universal* amplitude. Strictly speaking, one has to distinguish between *two* universal amplitudes $\mathcal{A}_+$ for $T>T_c$ and $\mathcal{A}_-$ for $T<T_c$. We disregard this distinction in Eq. (A1) in order to simplify the notation. Equation (A1) is valid for $T>T_c$ and $T<T_c$ *separately*, provided, the correlation length remains finite for $T<T_c$. According to Eq. (2.7) the unit volume v of the system transforms as

$$v'=R(\lambda)v \tag{A2}$$

and therefore we find

$$\begin{aligned} f_{b,\text{sing}}(\lambda,t)&=R(\lambda)f'_{b,\text{sing}}(\lambda,t)\\ &=\mathcal{A}R(\lambda)[\xi_{\parallel}(\lambda,t)]^{-d}\\ &=\mathcal{A}R(\lambda)[\xi'_{\perp}(\lambda,t)]^{-1}[\xi'_{\parallel}(\lambda,t)]^{-(d-1)}\\ &=\mathcal{A}[\xi_{\perp}(\lambda,t)]^{-1}[\xi_{\parallel}(\lambda,t)]^{-(d-1)} \end{aligned} \tag{A3}$$

for the singular part of the bulk free energy density of the anisotropic, i.e., the untransformed system.

According to Eq. (2.6) we have the alternative form

$$\begin{aligned} f_{b,\text{sing}}(\lambda,t)&=\mathcal{A}[\xi_{\perp,0}(\lambda)]^{-1}[\xi_{\parallel,0}(\lambda)]^{-(d-1)}|t|^{d\nu}\\ &\equiv A(\lambda)|\beta_c(\lambda)/\beta-1|^{d\nu} \end{aligned} \tag{A4}$$

for Eq. (A3). The nonuniversal amplitudes $A(\lambda)$ and $\beta_c(\lambda)$ must be independent of the labeling of the lattice axes, i.e., the direction which is chosen to be the "perpendicular" one. From this symmetry argument and the particular choice of the coupling constants $J_{\parallel}(\lambda)$ and $J_{\perp}(\lambda)$ in Eq. (2.2) we have already obtained $\beta'(\lambda=0)=0$ in Eq. (2.5). Likewise, we obtain $A'(\lambda=0)=0$ from this symmetry argument. We therefore conclude that

$$\left.\frac{d}{d\lambda}f_{b,\text{sing}}(\lambda,t)\right|_{\lambda=0}=0 \tag{A5}$$

and that due to

$$A(\lambda)=\mathcal{A}[\xi_{\perp,0}(\lambda)]^{-1}[\xi_{\parallel,0}(\lambda)]^{-(d-1)}, \tag{A6}$$

one also concludes from $A'(\lambda=0)=0$ that

$$\left.\frac{d}{d\lambda}\{[\xi_{\perp,0}(\lambda)]^{-1}[\xi_{\parallel,0}(\lambda)]^{-(d-1)}\}\right|_{\lambda=0}=0. \tag{A7}$$

From Eq. (A7) we finally obtain the important correlation length amplitude relation

$$(d-1)\left.\frac{d}{d\lambda}\xi_{\parallel,0}(\lambda)\right|_{\lambda=0}+\left.\frac{d}{d\lambda}\xi_{\perp,0}(\lambda)\right|_{\lambda=0}=0, \tag{A8}$$

which is needed in the derivation of the stress tensor representation of the Casimir force for lattice spin models presented in Appendix B.

APPENDIX B: THE STRESS TENSOR REPRESENTATION OF THE CASIMIR FORCE

The derivative of the excess free energy f_{ex} with respect to λ at the isotropic point $\lambda=0$ is given by Eq. (2.9) in the main text. The relation between Eq. (2.9) and the Casimir force defined by Eq. (1.1) yields a lattice expression of the stress tensor. This will be investigated here in the critical regime. Above the critical temperature all expressions will be exponentially small and can be neglected. Below the critical temperature Goldstone modes in $O(N\geqslant 2)$ systems also give rise to algebraically decaying finite-size effects, which will not be considered here.

In order to find the relation between Eqs. (1.1) and (2.9) we use the coordinate transformation given by Eq. (2.7) and note that unlike the unit volume v [see Eq. (A2)] the unit area remains *invariant* under Eq. (2.7). We recall that in the transformed (isotropic) system we have $\xi'_{\perp,0}(\lambda)=\xi'_{\parallel,0}(\lambda)=\xi_{\parallel,0}(\lambda)$ and we therefore find

$$\begin{aligned} \left.\frac{df_{\text{ex}}}{d\lambda}\right|_{\lambda=0}&=\left.\frac{df'_{\text{ex}}}{d\lambda}\right|_{\lambda=0}\\ &=\left.\frac{\partial f'_{\text{ex}}}{\partial L'_{\perp}}\right|_{\lambda=0}\left.\frac{dL'_{\perp}}{d\lambda}\right|_{\lambda=0}+\left.\frac{\partial f'_{\text{ex}}}{\partial \xi'_{\perp,0}}\right|_{\lambda=0}\left.\frac{d\xi'_{\perp,0}}{d\lambda}\right|_{\lambda=0}\\ &=-\beta F_{\text{Casimir}}R'(0)L_{\perp}+\left.\frac{\partial f'_{\text{ex}}}{\partial \xi'_{\perp,0}}\right|_{\lambda=0}\left.\frac{d\xi'_{\perp,0}}{d\lambda}\right|_{\lambda=0}, \end{aligned} \tag{B1}$$

where Eqs. (1.1) and (2.8) have been used. In order to evaluate the derivative $\partial f'_{\text{ex}}/\partial\xi'_{\perp,0}$ in the critical regime, we use the critical finite-size scaling form

$$f'_{\text{ex}}(t,L'_{\perp})=L'^{-(d-1)}_{\perp}g'_{\text{ex}}[t(L'_{\perp}/\xi'_{\perp,0})^{1/\nu}], \tag{B2}$$

and disregard the exponentially small contributions to Eq. (B1) from the regular part of the excess free energy. Note that for periodic boundary conditions the free energy of the finite system $f'(t,L'_{\perp})$ can be decomposed, as usual, in a regular $f'_{\text{reg}}(t,L'_{\perp})$ and a singular $f'_{\text{sing}}(t,L'_{\perp})$ parts, where the regular part $f'_{\text{reg}}(t,L'_{\perp})$ can be taken to be equal (up to, eventually, exponentially small corrections) to that one of the infinite system, i.e., $f'_{\text{reg}}(t,L'_{\perp})=f'_{\text{reg}}(t,\infty)$ [11]. That is why, for the periodic boundary conditions, the above equation (B2) is valid for the *total* excess free energy (and not only for its singular part). From Eq. (B2), we immediately obtain

$$\left.\frac{\partial f'_{\rm ex}}{\partial \xi'_{\perp,0}}\right|_{\lambda=0} = -\frac{t}{\nu\xi_0}\frac{\partial f'_{\rm ex}}{\partial t}, \tag{B3}$$

where all terms on the right-hand side of Eq. (B3) have already been evaluated at $\lambda=0$. To further evaluate Eq. (B3) we note that the excess internal energy $u_{\rm ex}$ is given by

$$u_{\rm ex} = \frac{\partial f_{\rm ex}}{\partial \beta} = -\frac{\beta_c(0)}{\beta^2}\frac{\partial f_{\rm ex}}{\partial t}. \tag{B4}$$

In the vicinity of $\beta=\beta_c(0)$, Eq. (B3) can be rewritten as

$$\left.\frac{\partial f'_{ex}}{\partial \xi'_{\perp,0}}\right|_{\lambda=0} = \frac{1}{\nu\xi_0}[\beta_c(0)-\beta]u_{\rm ex}. \tag{B5}$$

In order to evaluate the derivative $d\xi'_{\perp,0}/d\lambda|_{\lambda=0}$ in Eq. (B1) we note that according to Eq. (2.7) we have $\xi'_{\perp,0}(\lambda)=\xi_{\parallel,0}(\lambda)$. From the definition of $R(\lambda)$ given by Eq. (2.8) we find by taking the derivative $R'(\lambda)$ with respect to λ at $\lambda=0$,

$$R'(0) = \frac{1}{\xi_0}\left[\left.\frac{d\xi_{\parallel,0}}{d\lambda}\right|_{\lambda=0} - \left.\frac{d\xi_{\perp,0}}{d\lambda}\right|_{\lambda=0}\right]. \tag{B6}$$

We eliminate $d\xi_{\perp,0}/d\lambda|_{\lambda=0}$ from Eq. (B6) using Eq. (A8) of Appendix A and obtain

$$\left.\frac{d\xi_{\parallel,0}}{d\lambda}\right|_{\lambda=0} = \frac{\xi_0}{d}R'(0). \tag{B7}$$

We finally insert Eqs. (B5) and (B7) into Eq. (B1) and, by rearranging the terms, we obtain for the Casimir force

$$\begin{aligned}\beta F_{\rm Casimir} &= [R'(0)]^{-1}\lim_{L_\parallel\to\infty}\frac{\beta J'(1)}{L_\parallel^{d-1}L_\perp}\\ &\quad\times\left\langle\sum_{\mathbf{R}}\left[\sum_{k=1}^{d-1}S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_k}-(d-1)S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_d}\right]\right\rangle\\ &\quad+\frac{1}{d\nu}[\beta_c(0)-\beta]\frac{u_{\rm ex}}{L_\perp}\\ &\equiv\langle t_{\perp\perp}\rangle,\end{aligned} \tag{B8}$$

where Eq. (2.9) has also been used. Note that the first term in Eq. (B8) is generated by the anisotropy variation whereas the second term originates from a change in length scales enforced by the coordinate transformation given by Eq. (2.7).

In order to express Eq. (B8) as the thermal average $\langle t_{\perp\perp}\rangle$ of the normal component of the stress tensor we note that

$$u_{\rm ex}/L_\perp = u - u_b, \tag{B9}$$

where u is the volume energy density of the slab and u_b the volume energy density in the bulk. Naturally, u and u_b are thermal averages of properly normalized Hamiltonians $\hat{\mathcal{H}}$ and $\hat{\mathcal{H}}_b$. More specifically, $\hat{\mathcal{H}}$ is the Hamiltonian of the finite system normalized per unit volume, while $\hat{\mathcal{H}}_b$ is the corresponding Hamiltonian for the bulk system (i.e., one imagines an arbitrary finite connected region of spins whose mutual probability distribution is obtained by taking the thermodynamic limit while integrating out all spins *outside* that fixed region. This is done for any finite region of the lattice). From Eqs. (B8) and (B9) the operator form of the stress tensor given by Eq. (2.11) in the main text can then be read off.

APPENDIX C: THE TWO-DIMENSIONAL ISING MODEL

As it has been shown in the main text, see Eq. (3.7), in the critical region of the finite system the stress tensor is given by

$$t_{x,x}(i,j) = \frac{1}{2\sqrt{2}}(S_{i,j}S_{i,j+1}-S_{i,j}S_{i+1,j}) + \frac{1}{2}(\beta_c-\beta)(\hat{\mathcal{H}}-\hat{\mathcal{H}}_b). \tag{C1}$$

Let us now calculate the variance of the stress tensor $\Delta t_{x,x}(i,j)$, which we will interpret as a variance of a local measurement of the Casimir force made near the point (i,j). For the leading behavior of the variance near T_c one has

$$\begin{aligned}\Delta t_{x,x}(i,j) &= \tfrac{1}{2}\langle S_{i,j}^2(S_{i,j+1}-S_{i+1,j})^2\rangle - \langle t_{x,x}(i,j)\rangle^2\\ &= 1-\langle S_{i,j+1}S_{i+1,j}\rangle - \langle t_{x,x}(i,j)\rangle^2.\end{aligned} \tag{C2}$$

Obviously, it holds that $\langle S_{i,j+1}S_{i+1,j}\rangle=\langle S_{0,1}S_{1,0}\rangle=\langle S_{0,0}S_{1,1}\rangle$, because of the symmetry of the Ising model on a square lattice under periodic boundary conditions. The correlations $\langle S_{0,0}S_{1,1}\rangle$ are well known for the bulk system [15].

(i) For $T<T_c$,

$$\langle S_{0,0}S_{1,1}\rangle = \frac{2}{\pi}\mathbf{E}\left(\frac{1}{u}\right). \tag{C3}$$

(ii) For $T>T_c$,

$$\langle S_{0,0}S_{1,1}\rangle = \frac{2}{\pi u}[\mathbf{E}(u)+(u^2-1)\mathbf{K}(u)], \tag{C4}$$

where, according to Eq. (2.4),

$$u = \sinh(2\beta J_x)\sinh(2\beta J_y). \tag{C5}$$

(iii) For $T=T_c$, which is given by $u=1$, it follows that $\langle S_{0,0}S_{1,1}\rangle=2/\pi$.

In the above expressions **K** and **E** are the complete elliptic integrals of first and of second kind, respectively. From them and Eq. (C2) one easily obtains expressions for the behavior of the variance $\Delta t_{x,x}(i,j)$ of the stress tensor below, above, and at T_c. At $T=T_c$, for example, one has that

$$\Delta t_{x,x}(i,j) \simeq 1-2/\pi. \tag{C6}$$

Definitely, in addition from the above nonuniversal part the variance contains also universal parts that are negligible in comparison with the nonuniversal one.

An estimation can be also derived for $\Delta\Sigma_{i,j}\, t_{x,x}(i,j)$. With a variance of such a type one deals when, say, Monte Carlo simulations of the force are performed. According to Eqs. (2.14) and (2.15), at $T=T_c$,

$$\Delta\sum_{i,j}\tilde{t}_{x,x}(i,j)=\frac{\partial^2}{\partial\lambda^2}\Big[\ln\sum e^{-\beta\mathcal{H}(\lambda)}\Big]=ML\frac{\partial^2}{\partial\lambda^2}[-\beta\tilde{f}(T_c,\lambda)], \tag{C7}$$

and, therefore, from Eq. (3.7) it follows that

$$\Delta\sum_{i,j}t_{x,x}(i,j)=\frac{1}{2\ln^2(1+\sqrt{2})}ML\frac{\partial^2}{\partial\lambda^2}[-\beta\tilde{f}(T_c,\lambda)]. \tag{C8}$$

It is clear that the leading-order behavior of the variance will stem from the bulk contribution to the free energy—the finite-size terms will produce only corrections to it. The bulk free energy of the anisotropic two-dimensional Ising model is well known (see, e.g., Ref. [15])

$$-\beta f=\ln 2+\frac{1}{2}\int_{-\pi}^{\pi}\frac{d\theta_1}{2\pi}\int_{-\pi}^{\pi}\frac{d\theta_2}{2\pi}\ln[\cosh(2\beta J_x)\cosh(2\beta J_y)-\sinh(2\beta J_x)\cos(\theta_1)-\sinh(2\beta J_y)\cos(\theta_2)]. \tag{C9}$$

Setting here $J_x=(1+\lambda)J$ and $J_x=(1-\lambda)J$, we immediately obtain $-\beta\tilde{f}(\beta J,\lambda)$, and from Eq. (C8) one then derives (at $T=T_c$) that

$$\Delta\sum_{i,j}t_{x,x}(i,j)=\frac{1}{2}\left[-\frac{1}{2}+\frac{1}{\pi^2}\int_{-\pi}^{\pi}d\theta_1\int_{-\pi}^{\pi}d\theta_2\times\frac{\sin^2\left(\frac{\theta_1}{2}\right)\sin^2\left(\frac{\theta_2}{2}\right)}{\left(1-\frac{\cos(\theta_1)+\cos(\theta_2)}{2}\right)^2}\right]=\frac{1}{2}\left[-\frac{1}{2}+\frac{2}{\pi}\right]ML\simeq 0.068ML. \tag{C10}$$

We again observe that the variance of the sum of $t_{x,x}(i,j)$ is proportional to the total number of summands in this sum. This is the result given in Eq. (3.11) in the main text.

APPENDIX D: THE SPHERICAL MODEL

Using the identity

$$\ln(1+z)=\int_0^\infty\frac{dx}{x}(1-e^{-zx})e^{-x}, \tag{D1}$$

the equation for the free energy (3.17) becomes

$$\beta f(K,\mathbf{N})=\frac{1}{2}\left[\ln\frac{K}{2\pi}-K\right]+\sup_{w>0}\left\{U(w,\mathbf{N})-\frac{1}{2}Kw\right\}, \tag{D2}$$

where

$$U(w,\mathbf{N})=\frac{1}{2N}\sum_{\mathbf{k}\in\mathcal{B}_\Lambda}\ln\left[w+1-\frac{\hat{J}(\mathbf{k})}{\hat{J}(\mathbf{0})}\right]=\frac{1}{2}\int_0^\infty\frac{dx}{x}\left(e^{-x}-e^{-xw}\frac{1}{N}\sum_{\mathbf{k}\in\mathcal{B}_\Lambda}e^{-x[1-\hat{J}(\mathbf{k})/\hat{J}(\mathbf{0})]}\right). \tag{D3}$$

The supremum is attained at the value of w that is a solution of the (spherical field) equation

$$\frac{1}{N}\sum_{\mathbf{k}\in\mathcal{B}_\Lambda}\int_0^\infty e^{-xw}e^{-x[1-\hat{J}(\mathbf{k})/\hat{J}(\mathbf{0})]}dx=K. \tag{D4}$$

For nearest-neighbor interactions the Fourier transform of the interaction reads

$$\hat{J}(\mathbf{k})=2\sum_{j=1}^{d}J_j\cos(k_ja_j). \tag{D5}$$

Then, for the spherical field equation and the sum $U(w,\mathbf{N})$, we obtain

$$\int_0^\infty e^{-xw}\left[\prod_{j=1}^{d}\frac{1}{N_j}\sum_{k_j}e^{-xb_j(1-\cos k_ja_j)}\right]=K, \tag{D6}$$

$$U(w,\mathbf{N})=\frac{1}{2}\int_0^\infty\frac{dx}{x}\left(e^{-x}-e^{-xw}\left[\prod_{j=1}^{d}\frac{1}{N_j}\sum_{k_j}e^{-xb_j(1-\cos k_ja_j)}\right]\right), \tag{D7}$$

where $b_j=J_j/\Sigma_{j=1}^d J_j$. Using the identity [27]

$$\sum_{n=0}^{N-1}\exp\left[x\cos\frac{2\pi n}{N}\right]=N\sum_{q=-\infty}^{\infty}I_{qN}(x), \tag{D8}$$

Equations (D6) and (D7) can be written in the form

$$\int_0^\infty e^{-xw}\prod_{j=1}^{d}\left[e^{-xb_j}\sum_{q_j=-\infty}^{\infty}I_{q_jN_j}(b_jx)\right]dx=K \tag{D9}$$

and

$$U(w,\mathbf{N})=\frac{1}{2}\int_0^\infty\frac{dx}{x}\left(e^{-x}-e^{-xw}\prod_{j=1}^{d}\left[e^{-xb_j}\sum_{q_j=-\infty}^{\infty}I_{q_jN_j}(b_jx)\right]\right). \tag{D10}$$

In analogical way one can consider the behavior of the bulk system. Then, in the limit $N_j\to\infty$, $j=1,\ldots,d$, one obtains the bulk equation for the spherical field

$$K=\int_0^\infty e^{-xw}\prod_{j=1}^{d}[e^{-xb_j}I_0(b_jx)]dx$$
$$=\frac{1}{(2\pi)^d}\int_0^{2\pi}dn_1\cdots\int_0^{2\pi}dn_d\frac{1}{w+\sum_{j=1}^{d}b_j(1-\cos n_j)},\tag{D11}$$

and the following contribution into the free energy:

$$U_b(w)=\frac{1}{2}\int_0^\infty\frac{dx}{x}\left(e^{-x}-e^{-xw}\prod_{j=1}^{d}[e^{-xb_j}I_0(b_jx)]\right)$$
$$=\frac{1}{2}\frac{1}{(2\pi)^d}\int_0^{2\pi}dn_1\cdots\int_0^{2\pi}dn_d$$
$$\times\ln\left[w+\sum_{j=1}^{d}b_j(1-\cos n_j)\right].\tag{D12}$$

In a similar way, starting from Eq. (3.18), one can show that the bulk two-point correlation function in such an anisotropic system is

$$G(\mathbf{r},t)=\frac{1}{w\beta\hat{J}(\mathbf{0})}\int_0^\infty d\rho\, e^{-\rho}\prod_{j=1}^{d}\exp\left(\rho\frac{b_j}{w}\right)$$
$$\times\frac{1}{2\pi}\int_0^{2\pi}\exp\left[in_jl_j+\rho\frac{b_j}{w}\cos n_j\right].\tag{D13}$$

Supposing that $l_j\gg1$, $j=1,\ldots,d$, from Eq. (D13) one obtain

$$G(\mathbf{r},t)\simeq\frac{1}{w\beta\hat{J}(\mathbf{0})}\int_0^\infty d\rho\, e^{-\rho}\prod_{j=1}^{d}\frac{\exp\left[-\frac{w}{2\rho b_j}l_j^2\right]}{\sqrt{\rho b_j/w}},\tag{D14}$$

wherefrom one concludes that the correlation length ξ_j in direction j is

$$\xi_j=\sqrt{2b_j/w}\tag{D15}$$

with the critical point of the system given by $w=0$ [note that in the spherical model, because of the so-called equation of the spherical field, Eq. (D11), w depends on the coupling K, dimensionality d, and on the anisotropy described by the constants b_j, $j=1,\ldots,d$]. Therefore, one has

$$\frac{\xi_j}{\xi_i}=\sqrt{\frac{b_j}{b_i}}=\sqrt{\frac{J_j}{J_i}}.\tag{D16}$$

Taking J_j, $j=1,\ldots,j$ in the form prescribed by Eq. (2.2) one obtains

$$\frac{d}{d\lambda}\left(\frac{\xi_{\parallel,0}}{\xi_{\perp,0}}\right)\Bigg|_{\lambda=0}=\frac{d}{2}\frac{J'(1)}{J(1)},\tag{D17}$$

and, thus, making use of Eq. (2.11), we derive the explicit form of the stress tensor within the spherical model

$$t_{\perp\perp}(\mathbf{R})=\frac{\beta J}{d/2}\left[\sum_{k=1}^{d-1}S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_k}-(d-1)S_{\mathbf{R}}S_{\mathbf{R}+\mathbf{e}_d}\right]$$
$$+\frac{1}{d\nu}(\beta_c-\beta)(\hat{\mathcal{H}}-\hat{\mathcal{H}}_b),\tag{D18}$$

where $\hat{\mathcal{H}}$ is the Hamiltonian (normalized per unit particle) of the finite system and $\hat{\mathcal{H}}_b$ of the infinite system.

1. Evaluation of the finite-size excess free energy of the anisotropic system

From Eqs. (D10) and (D12) one has

$$U(w,\mathbf{N})=U_b(w)+\Delta U(w,\mathbf{N}),\tag{D19}$$

where

$$\Delta U(w,\mathbf{N})=-\frac{1}{2}\sum_{\mathbf{q}\neq\mathbf{0}}\int_0^\infty\frac{dx}{x}e^{-xw}\prod_{j=1}^{d}e^{-xb_j}I_{q_jN_j}(xb_j).\tag{D20}$$

Next, with the help of the expansion [27]

$$I_\nu(x)=\frac{\exp(x-\nu^2/2x)}{\sqrt{2\pi x}}\left(1+\frac{1}{8x}+\frac{9-32\nu^2}{2!\,(8x)^2}+\cdots\right),\tag{D21}$$

$\Delta U(w,\mathbf{N})$ can be cast in the form

$$\Delta U(w,\mathbf{N})=-\frac{1}{2}\sum_{\mathbf{q}\neq\mathbf{0}}\int_0^\infty\frac{dx}{x}e^{-xw}\prod_{j=1}^{d}\frac{e^{-N_j^2q_j^2/2xb_j}}{\sqrt{2\pi xb_j}},\tag{D22}$$

wherefrom, in the limit of a film geometry $N_1,N_2,\ldots,N_{d-1}\to\infty$, with $N_d=N_\perp$, one obtains

$$\Delta U(w,N_\perp)=-\frac{2}{(2\pi)^{d/2}}\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}y^{d/4}\sum_{q=1}^{\infty}\frac{K_{d/2}(q\sqrt{y})}{q^{d/2}}N_\perp^{-d}.\tag{D23}$$

Here we have taken $J_1=J_2=\cdots J_{d-1}=J_\parallel$ and $J_d=J_\perp$, which corresponds to $b_1=b_2=\cdots b_{d-1}=b_\parallel$ and $b_d=b_\perp$, whereas $y=2wN_\perp^2/b_\perp$.

All what remains now is to deal with the behavior of the bulk term $U_b(w)$ when K is close to K_c, i.e., when $w\ll1$. This analysis is well known for the isotropic case, here we will, very briefly, extend it to cover the anisotropic case also. Starting from Eq. (D12), one obtains

$$U_b(w)=U_b(0)+\frac{1}{2}\int_0^w d\omega\, W_d(\omega|\mathbf{b}),\tag{D24}$$

where

$$U_b(0)=\frac{1}{2}\int_0^\infty\frac{dx}{x}\left[e^{-x}-\prod_{j=1}^{d}e^{-xb_j}I_0(xb_j)\right]\tag{D25}$$

is a temperature independent constant and

$$W_d(\omega|\mathbf{b}) = \int_0^\infty dx e^{-x\omega} \prod_{j=1}^{d} e^{-xb_j} I_0(xb_j) \tag{D26}$$

is the generalized Watson-type integral (the standard one is with $b_j=b$ for all $j=1,\ldots,d$). Using the standard technique for evaluation of such type of integrals (see, e.g., Ref. [7]) one derives that, for $2<d<4$,

$$W_d(\omega|\mathbf{b}) \simeq W_d(0|\mathbf{b}), \tag{D27}$$

wherefrom it follows that, again for $2<d<4$,

$$U_b(w) \simeq U_b(0) + \frac{1}{2} w W_d(0|\mathbf{b}) - \frac{1}{2} \frac{\Gamma(-d/2)}{(2\pi)^{d/2} \prod_{j=1}^{d} \sqrt{b_j}} \omega^{d/2}. \tag{D28}$$

Taking into account that in terms of the "anisotropic" Watson integral the equation of the spherical field simply is

$$K = W_d(w|\mathbf{b}), \tag{D29}$$

and that, according to Eq. (D15), the critical point is fixed by $w=0$, we conclude that the critical coupling of the anisotropic system is

$$K_c \equiv 2\beta_c \sum_{j=1}^{d} J_j = W_d(0|\mathbf{b}) = \int_0^\infty dx \prod_{j=1}^{d} e^{-xb_j} I_0(xb_j). \tag{D30}$$

Then, close to $K=K_c$, for the free energy density of bulk system from Eqs. (D2), (D28), and (3.23) one obtains

$$\beta f_b(K|\mathbf{b}) = \frac{1}{2}\left[\ln\frac{K}{2\pi} - K\right] + \frac{1}{2} w_b (K_c - K) + U_b(0) - \frac{1}{2} \frac{\Gamma(-d/2)}{(2\pi)^{d/2} \prod_{j=1}^{d} \sqrt{b_j}} \omega^{d/2}, \tag{D31}$$

where, for $K \leqslant K_c$, the parameter w_b is the solution of the equation

$$K = K_c + \frac{\Gamma(1-d/2)}{(2\pi)^{d/2} \prod_{j=1}^{d} \sqrt{b_j}} \omega_b^{d/2-1}, \tag{D32}$$

whereas for $K>K_c$ the supremum of the free energy is attained at $w_b=0$. Similarly, for the free energy density of the *finite* system from Eqs. (D2), (D22), (D28), and (3.23) we obtain

$$\beta f(K,\mathbf{N}|\mathbf{b}) = \frac{1}{2}\left[\ln\frac{K}{2\pi} - K\right] + \frac{1}{2} w (K_c - K) + U_b(0) - \frac{1}{2} \frac{\Gamma(-d/2)}{(2\pi)^{d/2} \prod_{j=1}^{d} \sqrt{b_j}} \omega^{d/2} - \frac{1}{2} \sum_{\mathbf{q}\neq\mathbf{0}} \int_0^\infty \frac{dx}{x} e^{-xw} \prod_{j=1}^{d} \frac{e^{-N_j^2 q_j^2/2xb_j}}{\sqrt{2\pi x b_j}}, \tag{D33}$$

where w is the solution of the finite-size equation for the spherical field

$$K = K_c + \frac{\Gamma(1-d/2)}{(2\pi)^{d/2} \prod_{j=1}^{d} \sqrt{b_j}} \omega^{d/2-1} + \sum_{\mathbf{q}\neq\mathbf{0}} \int_0^\infty dx\, e^{-xw} \prod_{j=1}^{d} \frac{e^{-N_j^2 q_j^2/2xb_j}}{\sqrt{2\pi x b_j}}. \tag{D34}$$

Recalling that, for $2<d<4$, the spherical model has a critical exponent $\nu=1/(d-2)$ one can, in the limit of a film geometry $N_1,N_2,\ldots,N_{d-1}\to\infty$, from Eqs. (D23), (D31), and (D33), obtain an expression for the *excess* free energy $\beta(f - f_b)$ (per spin),

$$\beta\left[f(K,N_\perp|\mathbf{b}) - f_b(K|\mathbf{b})\right] = \left\{ \frac{1}{4} x_1 (y - y_\infty) - \frac{1}{2} \frac{\Gamma(-d/2)}{(4\pi)^{d/2}} \left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} (y^{d/2} - y_\infty^{d/2}) - \frac{2}{(2\pi)^{d/2}} \left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} y^{d/4} \sum_{q=1}^{\infty} \frac{K_{d/2}(q\sqrt{y})}{q^{d/2}} \right\} N_\perp^{-d} \tag{D35}$$

in a scaling form. In the above equation

$$x_1 = b_\perp (K_c - K) N_\perp^{1/\nu}, \quad \nu = \frac{1}{d-2} \tag{D36}$$

is the temperature scaling variable, $y_\infty = 2w_b N_\perp^2/b_\perp$ is the solution of the bulk spherical field equation

$$-\frac{1}{2} x_1 = \frac{\Gamma(1-d/2)}{(4\pi)^{d/2}} \left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} y_\infty^{d/2-1}, \tag{D37}$$

while $y=2wN_\perp^2/b_\perp$ is the solution of the finite-size spherical field equation

$$-\frac{1}{2} x_1 = \frac{\Gamma(1-d/2)}{(4\pi)^{d/2}} \left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} y^{d/2-1} + \frac{2}{(2\pi)^{d/2}} \left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2} y^{d/4-1/2} \sum_{q=1}^{\infty} \frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}}. \tag{D38}$$

For the Casimir force [see also Eq. (1.1)]

$$\beta F_{\text{Casimir}} = -\frac{\partial}{\partial N_\perp}[N_\perp \beta(f-f_b)] \tag{D39}$$

from Eqs. (3.24), (3.26), and (3.27) one obtains

$$\beta F_{\text{Casimir}} = N_\perp^{-d}\Bigg\{\frac{1}{4}x_1(y-y_\infty)-(d-1)\times\left(\frac{b_\perp}{b_\parallel}\right)^{(d-1)/2}\Bigg[\frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}(y^{d/2}-y_\infty^{d/2})+\frac{2}{(2\pi)^{d/2}}y^{d/4}\sum_{q=1}^{\infty}\frac{K_{d/2}(q\sqrt{y})}{q^{d/2}}\Bigg]\Bigg\}. \tag{D40}$$

We are ready now to determine the Casimir amplitudes Δ in the spherical model. Having in mind Eq. (1.4), at $K=K_c$ (then $y_\infty=0$), for the isotropic system (then $b_\perp=b_\parallel=1/d$) one obtains from Eq. (3.28),

$$\Delta = -\left[\frac{1}{2}\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}y_c^{d/2}+\frac{2}{(2\pi)^{d/2}}y_c^{d/4}\sum_{q=1}^{\infty}\frac{K_{d/2}(q\sqrt{y_c})}{q^{d/2}}\right], \tag{D41}$$

where

$$\frac{\Gamma(-d/2)}{(4\pi)^{d/2}}y_c^{d/2} = \frac{4}{d(2\pi)^{d/2}}y_c^{d/4+1/2}\sum_{q=1}^{\infty}\frac{K_{d/2-1}(q\sqrt{y_c})}{q^{d/2-1}}. \tag{D42}$$

Using now that (see, e.g., Ref. [19])

$$K_{\nu+1}(z) = K_{\nu-1}(z)+\frac{2\nu}{z}K_\nu(z), \tag{D43}$$

from Eqs. (D41) and (D42) we derive

$$\Delta = -\frac{2}{d(2\pi)^{d/2}}y_c^{d/4+1/2}\sum_{q=1}^{\infty}\frac{K_{d/2+1}(q\sqrt{y_c})}{q^{d/2-1}}, \tag{D44}$$

with $\beta_c F_{\text{Casimir}}(K_c,L_\perp)=(d-1)\Delta L_\perp^{-d}$. The exact value of y_c and Δ in an explicit form is only known for $d=3$. Then

$$y = 4\ln^2[(1+\sqrt{5})/2] \tag{D45}$$

(this value is well known and seems that has been derived for the first time in Ref. [18] and [19]

$$\Delta = -\frac{2\zeta(3)}{5\pi}. \tag{D46}$$

This is the only exactly known Casimir amplitude for a three-dimensional system. In Ref. [21] it has been shown [see there Eq. (27)] that this value can also be written in the form

$$\Delta = -\frac{1}{2\pi}\left[\mathrm{Li}_3(e^{-\sqrt{y_c}})+\sqrt{y_c}\,\mathrm{Li}_2(e^{-\sqrt{y_c}})+\frac{1}{6}y_c^{3/2}\right], \tag{D47}$$

where $\mathrm{Li}_p(z)=\sum_{k=1}^{\infty}z^k/k^p$ is the polylogarithm function of order p. Taking into account that $K(5/2,x)=\sqrt{\pi/2x}(1+2/x+3/x^2)\exp(-x)$ [20] and Eq. (3.30), one can easily check that the right-hand side of Eq. (3.29) can indeed be written in the form given in Eq. (D47).

2. Evaluation of the average value of the stress tensor

Taking into account Eq. (2.16), for the difference of the finite size and bulk internal energy densities $u=\langle\hat{\mathcal{H}}\rangle$ and $u_b=\langle\hat{\mathcal{H}}_b\rangle$, one can easily derive from Eq. (D2),

$$u-u_b = -\frac{1}{2}J(w-w_b) = -\frac{1}{4d}J(y-y_\infty)N_\perp^{-2}, \tag{D48}$$

where $y=2dwN_\perp^2$, and then from Eq. (3.18) or Eq. (D2), to obtain for the stress tensor (3.22) that

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = \frac{d-1}{d}\frac{1}{N}\sum_{\mathbf{k}\in\mathcal{B}_\Lambda}\frac{\cos(k_1a_1)-\cos(k_da_d)}{d(1+w)-\sum_{j=1}^{d}\cos(k_ja_j)} - \frac{d-2}{4d}x_1(y-y_\infty)N_\perp^{-d}, \tag{D49}$$

where, we recall, $x_1=d^{-1}(K_c-K)N_\perp^{d-2}$ [see Eq. (3.25)]. Using the identity [see Eq. (D8)]

$$\sum_{n=0}^{N-1}\cos\left(\frac{2\pi n}{N}\right)\exp\left[x\cos\left(\frac{2\pi n}{N}\right)\right] = N\sum_{q=-\infty}^{\infty}I'_{qN}(x), \tag{D50}$$

where $I'_\nu(x)=(d/dx)I_\nu(x)$, in the limit of a film geometry, i.e., when $N_1,N_2,\ldots,N_{d-1}\to\infty$, the above expression can be rewritten in the form

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = \frac{2(d-1)}{d}\sum_{q=1}^{\infty}\int_0^\infty dx\, e^{-dw\,x}[e^{-x}I_0(x)]^{d-2}\times e^{-2x}[I'_0(x)I_{qN}(x)-I_0(x)I'_{qN}(x)] - N_\perp^{-d}\frac{(d-2)}{4d}x_1(y-y_\infty). \tag{D51}$$

It is worth mentioning that till now no approximation in the calculation of the average of the stress tensor operator has been made. In order to obtain the scaling form of the above expression such a step will be performed only now. Indeed, with the help of the expansion (D21),

$$I_\nu(x) = \frac{\exp(x-\nu^2/2x)}{\sqrt{2\pi x}}\left(1+\frac{1}{8x}+\frac{9-32\nu^2}{2!\,(8x)^2}+\cdots\right), \tag{D52}$$

one can set the above expression in scaling form

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = -\frac{2(d-1)}{d(2\pi)^{d/2}} y^{(d+2)/4} \sum_{q=1}^{\infty} \frac{K_{1+d/2}(q\sqrt{y})}{q^{d/2-1}} N_{\perp}^{-d} - N_{\perp}^{-d} \frac{(d-2)}{4d} x_1 (y - y_\infty). \tag{D53}$$

Now it only remains to show that the right-hand side of the above equation is indeed equal to the right-hand side of Eq. (3.28) (for $b_\perp = b_\|$), which gives the Casimir force calculated in a direct manner as a derivative of the finite-size free energy with respect to the size of the system. In order to demonstrate that, let us first, with the help of identity (D43), rewrite the above expression for the stress tensor in the form

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = -\left\{ \frac{2(d-1)}{(2\pi)^{d/2}} \left[y^{d/4} \sum_{q=1}^{\infty} \frac{K_{d/2}(q\sqrt{y})}{q^{d/2}} + \frac{1}{d} y^{(d+2)/4} \sum_{q=1}^{\infty} \frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}} \right] + \frac{(d-2)}{4d} x_1 (y - y_\infty) \right\} N_\perp^{-d}. \tag{D54}$$

Next, from the bulk (3.26) and finite-size equations (3.27) of the spherical field one directly derives

$$-\frac{1}{4} x_1 y_\infty = \frac{\Gamma(1-d/2)}{2(4\pi)^{d/2}} y_\infty^{d/2} \tag{D55}$$

and

$$-\frac{1}{4} x_1 y = \frac{\Gamma(1-d/2)}{2(4\pi)^{d/2}} y^{d/2} + \frac{1}{(2\pi)^{d/2}} y^{(d+2)/4} \sum_{q=1}^{\infty} \frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}}, \tag{D56}$$

wherefrom

$$\frac{1}{(2\pi)^{d/2}} y^{(d+2)/4} \sum_{q=1}^{\infty} \frac{K_{d/2-1}(q\sqrt{y})}{q^{d/2-1}} = -\frac{1}{4} x_1 (y - y_\infty) - \frac{\Gamma(1-d/2)}{2(4\pi)^{d/2}} (y^{d/2} - y_\infty^{d/2}). \tag{D57}$$

Inserting now Eq. (D57) in Eq. (3.32) we conclude that, indeed,

$$\langle t_{\perp\perp}(\mathbf{R})\rangle = \beta F_{\text{Casimir}} \tag{D58}$$

for the spherical model.

c. Evaluation of the variance of the stress tensor

If $\Delta\zeta$ is the variance of the random variable ζ, i.e., $\Delta\zeta = \langle(\zeta - \langle\zeta\rangle)^2\rangle = \langle\zeta^2\rangle - \langle\zeta\rangle^2$, then at $T = T_c$,

$$\Delta \sum_{\mathbf{R}\in\Lambda} \tilde{t}_{\perp,\perp}(\mathbf{R}) = \frac{\partial^2}{\partial\lambda^2}\Big[\ln \sum e^{-\beta\mathcal{H}(\lambda)}\Big] = N_\perp N_\|^{d-1} \frac{\partial^2}{\partial\lambda^2}[-\beta\tilde{f}(T_c,\lambda)] \tag{D59}$$

[for the definition of $\mathcal{H}(\lambda)$] and $\tilde{f}(T,\lambda)$ see Eqs. (2.13)–(2.15). Comparing now Eqs. (2.15) and (3.22), we conclude that, at $T = T_c$, in the case of a spherical model

$$\Delta \sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) = \frac{4}{d^2} N_\perp N_\|^{d-1} \frac{\partial^2}{\partial\lambda^2}[-\beta\tilde{f}(T_c,\lambda)]. \tag{D60}$$

The finite-size free energy density of the anisotropic system is given in Eq. (D33), where the anisotropy is characterized by the constants

$$b_1 = b_2 = \cdots = b_{d-1} = b_\| = \frac{J_\|}{(d-1)J_\| + J_\perp} = \frac{1+\lambda}{d} \tag{D61}$$

and

$$b_d = b_\perp = \frac{J_\perp}{(d-1)J_\| + J_\perp} = \frac{1}{d} - \frac{d-1}{d}\lambda. \tag{D62}$$

Let us now first note that

$$K = \beta\hat{J}(\mathbf{0}) = 2\beta[(d-1)J_\| + J\perp] = 2\beta J d \tag{D63}$$

does not depend on λ and that

$$\frac{\partial b_\|}{\partial\lambda} = \frac{1}{d}, \quad \frac{\partial b_\perp}{\partial\lambda} = -\frac{d-1}{d}. \tag{D64}$$

It is clear from Eqs. (D33) and (3.24) that the contributions to the variance of the stress tensor stemming from the "finite-size" and the singular "bulk" parts will be of the order of $(N_\perp N_\|^{d-1})/N_\perp^d$, while that one from the bulk regular part will be of the order of $N_\perp N_\|^{d-1}$. Because of that the leading contributions will be nonuniversal. In addition to them one will have also universal corrections, but we will neglect them in the current treatment and will deal only with the leading-order behavior of the variance of the Casimir force. Then, from Eq. (D33), one has

$$\Delta \sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) \sim \frac{4}{d^2} N_\perp N_\|^{d-1} \frac{\partial^2}{\partial\lambda^2}[-U_b(0|\mathbf{b})], \tag{D65}$$

where $U_b(0|\mathbf{b}) \equiv U_b(0)$ is defined in Eq. (D25). Having in mind Eq. (D64), it is easy to show that

$$\frac{\partial}{\partial\lambda} U_b(0|\mathbf{b}) = \frac{d-1}{d}\left(\frac{\partial}{\partial b_\|} U_b(0|\mathbf{b}) - \frac{\partial}{\partial b_\perp} U_b(0|\mathbf{b})\right), \tag{D66}$$

wherefrom one immediately derives

$$\frac{\partial^2}{\partial \lambda^2} U_b(0|\mathbf{b}) = \frac{d-1}{d}\left(\frac{\partial^2}{\partial b_\parallel^2} U_b(0|\mathbf{b}) - \frac{\partial^2}{\partial b_\perp \partial b_\parallel} U_b(0|\mathbf{b})\right). \tag{D67}$$

Performing now the calculations, from Eqs. (D25) and (D67), we obtain

$$\frac{\partial^2}{\partial \lambda^2} U_b(0|\mathbf{b}) = \frac{1}{2} d(d-1) \int_0^\infty dx\, x e^{-dx} I_0^{d-2}(x) \times \left\{ I_1^2(x) - \frac{1}{2} I_0(x)[I_0(x) + I_2(x)] \right\}, \tag{D68}$$

which leads to the following result:

$$\Delta \sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) \simeq -\frac{2(d-1)}{d} N_\perp N_\parallel^{d-1} \int_0^\infty dx\, x I_0^{d-2}(x) \times \left\{ I_1^2(x) - \frac{1}{2} I_0(x)[I_0(x) + I_2(x)] \right\} e^{-dx}, \tag{D69}$$

for the variance of the Casimir force in the spherical model at $T = T_c$. This will be also the leading result everywhere in the critical region. A numerical evaluation of Eq. (D69) gives

$$\Delta t_{\perp,\perp} \equiv \Delta \sum_{\mathbf{R}\in\Lambda} t_{\perp,\perp}(\mathbf{R}) \simeq 0.107 N_\perp N_\parallel^2. \tag{D70}$$

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