Critical Casimir forces for \( \mathcal{O}(n) \) systems with long-range interaction in the spherical limit

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We present exact results on the behavior of the thermodynamic Casimir force and the excess free energy in the framework of the \( d \)-dimensional spherical model with a power law long-range interaction decaying at large distances \( r \) as \( r^{-d-\sigma} \), where \( \sigma < d < 2\sigma \) and \( 0 < \sigma \leq 2 \). For a film geometry and under periodic boundary conditions we consider the behavior of these quantities near the bulk critical temperature \( T_c \), as well as for \( T > T_c \) and \( T < T_c \). The universal finite-size scaling function governing the behavior of the force in the critical region is derived and its asymptotics are investigated. While in the critical and under critical region the force is of the order of \( L^{-d} \), for \( T > T_c \) it decays as \( L^{-d-\sigma} \), where \( L \) is the thickness of the film. We consider both the case of a finite system that has no phase transition of its own, and the case with \( d-1 > \sigma \), when one observes a dimensional crossover from \( d \) to a \( d-1 \) dimensional critical behavior. The behavior of the force along the phase coexistence line for a magnetic field \( H = 0 \) and \( T < T_c \) is also derived. We have proven analytically that the excess free energy is always negative and monotonically increasing function of \( T \) and \( H \). For the Casimir force we have demonstrated that for any \( \sigma \geq 1 \) it is everywhere negative, i.e. an attraction between the surfaces bounding the system is to be observed. At \( T = T_c \) the force is an increasing function of \( T \) for \( \sigma > 1 \) and a decreasing one for \( \sigma < 1 \). For any \( d \) and \( \sigma \) the minimum of the force at \( T = T_c \) is always achieved at some \( H \neq 0 \).

I. INTRODUCTION

When a fluid is confined in a film geometry with a thickness \( L \), the boundary conditions which the order parameter has to fulfill at the surfaces bounding the system lead to a \( L \) dependence of the excess free energy. On its turn, the last lead to a force, conjugated to \( L \), which is called the Casimir (solvation) force and the corresponding effect - the thermodynamic Casimir effect. In this form it has been discussed for the first time by M. E. Fisher and de Gennes in 1978 \(^3\). The effect is dubbed alternating so after the Dutch physicist Hendrik Casimir who first, in 1948 \(^4\), predicted it considering the influence of the zero-point quantum mechanical vacuum fluctuations of the electromagnetic field on the resulting force between two infinite perfectly conducting planes placed against each other. In that form the effect is known as the quantum mechanical Casimir effect. For a long time the effect was considered as a theoretical curiosity but the interest in it has blossomed in the last decade. Numerous calculations and experiments have been performed both on the thermodynamic and the quantum Casimir effect. For a review on the thermodynamic effect the interested reader might consult \(^5\), \(^6\), \(^7\), and for the quantum one \(^8\), \(^9\).

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The Casimir force in statistical-mechanical systems at a temperature \( T \) and in the presence of an external magnetic field \( H \) is characterized by the excess free energy due to the finite-size contributions to the total free energy of the system. In the case of a film geometry \( L \times \infty^2 \) and under given boundary conditions \( \tau \) imposed across the direction \( L \), the Casimir force is defined as

\[
F_{\text{Casimir}}(T, H, L) = \frac{\partial f_{\text{ex}}(T, H, L)}{\partial L},
\]

where \( f_{\text{ex}}(T, H, L) \) is the excess free energy

\[
f_{\text{ex}}(T, H, L) = f(T, H, L) - f_{\text{bulk}}(T, H).
\]

Here \( f(T, H, L) \) is the full free energy per unit area and \( f_{\text{bulk}}(T, H) \) is the corresponding bulk free energy density. According to the standard finite-size scaling theory \(^8\), \(^10\), under periodic boundary conditions \( \tau = \beta \) near the critical point \( T = T_c, H = 0 \) (of the bulk system) one expects

\[
f_{\text{ex}}(T, H, L) = L^{-(d-1)} X^{(p)}(atL^{1/\nu}, bhL^{\Delta/\nu}),
\]

wherefrom one has

\[
F_{\text{Casimir}}^{(p)}(T, H, L) = L^{-d} X^{(p)}_{\text{Casimir}}(atL^{1/\nu}, bhL^{\Delta/\nu}).
\]

Here the universal scaling functions of the free energy \( X^{(p)}(x_1, x_2) \) and the Casimir force \( X^{(p)}_{\text{Casimir}}(x_1, x_2) \) are
related via the relation

\[ X^{(p)}_{\text{Casimir}}(x_1, x_2) = (d - 1)X^{(p)}(x_1, x_2) - \frac{1}{\nu} \frac{\partial}{\partial x_1} X^{(p)}(x_1, x_2) - \frac{\Delta}{\nu} \frac{\partial}{\partial x_2} X^{(p)}(x_1, x_2), \]

(1.5)

\[ \Delta \text{ and } \nu \text{ are the standard critical exponents, } a \text{ and } b \text{ are nonuniversal metric factors, } t = (T - T_c)/T_c \text{ is the reduced temperature and } h = \beta H \quad (\beta = (k_B T)^{-1}). \]

We recall that, according to the general theory of the thermodynamic Casimir effect \[3, 4, 5\], \( X^{(p)}_{\text{Casimir}}(x_1, x_2) \) is supposed to be negative under periodic boundary conditions (which corresponds to a mutual attraction of the ‘surfaces’ bounding the system). The boundaries influence the system to a depth given by the bulk correlation length \( \xi(T) \sim |T - T_c|^{-\nu} \), where \( \nu \) is its critical exponent. When \( \xi(T) \ll L \) the Casimir force, as a fluctuation induced force between the plates, is negligible. The force becomes long-ranged when \( \xi(T) \sim L \) the Casimir force as a fluctuation induced force between the plates, is negligible. The force becomes long-ranged when \( \xi(T) \ll L \) the Casimir force as a fluctuation induced force between the plates, is negligible.

The investigation of the Casimir effect in a classical system with long-range interaction possesses some peculiarities in comparison with the short-range system. Due to the long-range character of the interaction there exists a natural attraction between the surfaces bounding the system. One easily can estimate that in systems with

The temperature dependence of the Casimir force for two-dimensional systems has been investigated exactly only on the example of Ising strips \[14\]. In \( O(n) \) models for \( T > T_c \) the temperature dependence of the force has been considered in \[11\]. The only example where it is investigated exactly as a function of both the temperature and of the magnetic field scaling variables is that of the three-dimensional spherical model with short range interaction under periodic boundary conditions \[11, 12, 13\]. There results for the Casimir force in a mean-spherical model with \( L \times \infty^{d-1} \) geometry, \( 2 < d < 4 \), have been derived. The force is consistent with an attraction of the plates confining the system. In \[11\] some of the results of \[12, 13\] have been extended to a quantum version of the model. There the interaction has been taken to be long-ranged, with \( 0 < \sigma \leq 2 \), \( \sigma/2 < d < 3\sigma/2 \), and the corresponding quantum phase transition has been considered around \( T = 0 \). Very recently in \[15\], based on a derived there stress-tensor-like operator for critical lattice systems, the scaling functions of the force for the 3d Ising, XY and Heisenberg models have been obtained by Monte Carlo methods. The results suggest that, under periodic boundary conditions, the scaling function \( X^{(p)}_{\text{Casimir}}(x)/n \) of all the \( O(n) \) models practically coincide for large \( x \), say, for \( x = L/\xi \gtrsim 2 \), where \( \xi \) is the true bulk correlation length. The last increases the helpfulness of the spherical model results (i.e. of the results in the limit \( n \to \infty \)), which are available in an explicit analytic form.

Most of the results for the Casimir force are available only at \( T = T_c \), i.e. for the Casimir amplitudes. They are obtained for \( d = 2 \) by using conformal-invariance methods for a large class of models \[3\]. For \( d \neq 2 \) results for the amplitudes are available via field-theoretical renormalization group theory in \( 4 - \epsilon \) dimensions \[3, 11, 17\], Migdal-Kadanoff real-space renormalization group methods \[18\], and, by Monte Carlo methods \[15, 19\]. In addition to the flat geometries some results about the Casimir amplitudes between spherical particles in a critical fluid have been derived too \[15, 20\]. For the purposes of experimental verification that type of geometry seems especially suitable. For \( d = 3 \) the only exactly known amplitude is that one for the spherical model \[13\]. In the case \( d = \sigma \) the amplitude is also known \[14\] for the quantum version of the model with long-ranged power-law interaction (in that case the amplitude in question characterizes the leading temperature correction to the ground state of the quantum system).

It should be noted that in contrast to the quantum mechanical Casimir effect, that has been tested experimentally with high accuracy \[21, 22, 23, 24\] (for a recent review on the existing experiments see, e.g. \[25\]), the statistical-mechanical Casimir effect lacks so far a quantitatively satisfactory experimental verification. Nevertheless, one has to stress that all the existing experiments \[26, 27, 28, 29\] are in a qualitative agreement with the theoretical predictions.

In this paper a theory of the scaling properties of the Casimir force of a spherical model with a power-law leading long-ranged interactions (decreasing at long distances \( r \) as \( 1/r^{d+\sigma} \), with \( 0 < \sigma \leq 2 \), and \( \sigma < d < 2\sigma \)) is presented. The results represent an extension to leading long-ranged interactions of the corresponding ones for system with short-ranged interaction \[12, 13\]. The latter results, as we will see, can be reobtained by formally taking the limit \( \sigma \to 2^- \) in the expressions pertinent to the case of long-ranged interactions.

All the interactions enter the exact expressions for the free energy only through their Fourier transform which leading asymptotic behavior is \( U(q) \sim a_\sigma q^{\sigma'} \), where \( \sigma' = \min(2, \sigma) \). As it was shown for bulk systems by renormalization group arguments \( \sigma \geq 2 \) corresponds to the case of subleading long-ranged interactions, i.e. the universality class then does not depend on \( \sigma \) \[31\] and coincides with that one of systems with short-ranged interactions. Values satisfying \( 0 < \sigma < 2 \) correspond to leading long-ranged interactions and the critical behavior depends then on \( \sigma \) (see Ref. \[32, 33\] and references therein). In the current work we will restrict ourselves to the consideration of this case only. The other case of subleading long-ranged interaction, i.e. when \( \sigma > 2 \) is also of interest (involving, e.g., a serious modification of the standard finite-size scaling theory, see e.g. \[34, 35, 36, 37\]), but will be considered elsewhere \[38\].
real boundaries (i.e. with no translational invariance) in
the ordered state the $L$-dependent part of the excess free
energy that is raised by the direct inter-particle (spin) in-
teraction is of the order of $L^{−a+1}$. In the critical region
one still has some effects stemming from that interaction
on the background of which develops the fluctuating
induced new attraction between the surfaces that is in
fact the critical Casimir force. In the definition used here, that is the common one when one considers
short-range systems, these effects are superposed simulta-
neously. In the current article we will investigate their
interplay. An interesting case when forces of similar ori-
gin are acting simultaneously is that of the wetting when
the wetting layer is nearly critical and intrudes be-
tween two noncritical phases if one takes into account
the effect of long-range correlations and that one of the
long-range Van der Waals forces \cite{39,40,41}.

The structure of the article is as follows. In Section II we briefly describe the spherical model (which,
in systems with a translational invariance, is equivalent
to the $n \to \infty$ limit of the $O(n)$ models) and give all ba-
sic expressions needed to investigate the behavior of the
Casimir force. In Section III we derive the scaling func-
tion of the excess free energy and the Casimir force, and
investigate the leading asymptotic behavior of the force
both above and below the critical point. In Section IV we
consider in some details the behavior of the force along
the phase coexistence line $T < T_c$, $H = 0$. In Section V
we investigate the monotonicity properties of the excess
free energy, and the Casimir force, and prove analytically
that both the excess free energy and the force are nega-
tive for any $T$ and $H$ (for $\sigma > 1$). The last implies that
the force between the boundary surfaces of the system is
always attractive. The article closes with a discussion
given in Section VI. The technical details needed in the
main text are organized in a series of Appendices.

II. THE MODEL

We consider the ferromagnetic mean spherical model
with long-range interaction confined to a fully finite $d$-
dimensional hypercubic lattice $L_d$ of $N = |L_d|$ sites.
The model is defined by

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} S_i S_j - H \sum_i S_i,$$  \hspace{1cm} (2.1)

where $S_i$ is the spin variable at site $i$, $J_{ij}$ is the inter-
action matrix between spins at sites $i$ and $j$, and $H$ is an
ordering external magnetic field. The long-wavelength
asymptotic form of the Fourier transform $\mathcal{F}(\mathbf{q})$ of
the interaction potential $J_{ij}$ is

$$\mathcal{F}(\mathbf{q}) \approx \mathcal{F}(0) [1 - \rho_\sigma \omega_\sigma(\mathbf{q})], \quad |\mathbf{q}| \to 0, \quad \rho_\sigma > 0.$$  

We suppose that the interaction in the system is long-
ranged with $0 < \sigma < 2$, i.e. $\omega_\sigma(\mathbf{q}) \sim |\mathbf{q}|^\sigma$. This corre-
sponds to the inverse power-law behavior $\mathcal{F}(r) \sim r^{-d-\sigma}$,
for large spin separations $r = |r|$. The spins in the model
under consideration obey the spherical constraint

$$\sum_i \langle S_i^2 \rangle = N,$$  \hspace{1cm} (2.2)

where $\langle \cdots \rangle$ denotes standard thermodynamic averages
taken with the Hamiltonian $\mathcal{H}$ and $N$ is the total number of
spins located at sites $i$ of finite hypercubic lattice $L_d$
of size $L_1 \times L_2 \times \cdots \times L_d = N$ (here $L_i$ are the linear sizes
of the system measured in units of the lattice constants).

Under periodic boundary conditions imposed along the
finite directions of the system, the free energy density of
the model is given by

$$\beta \mathcal{F}_{d,\sigma}(\beta, H, L|\mathbf{A}) = \frac{1}{2} \sup_{\phi > 0} \{ U_{d,\sigma}(\phi, L|\mathbf{A})$$
$$+ \ln \left[ \frac{\beta \mathcal{F}(0) \rho_\sigma}{2\pi} \right] - \frac{\beta H^2}{\mathcal{F}(0) \rho_\sigma \phi}$$
$$- \beta \mathcal{F}(0) \rho_\sigma \left( \phi + \frac{1}{\rho_\sigma} \right) \}, \hspace{1cm} (2.3a)$$

where

$$U_{d,\sigma}(\phi, L|\mathbf{A}) = \frac{1}{N} \sum_{\mathbf{q}} \ln[\phi + \omega_\sigma(\mathbf{q})]. \hspace{1cm} (2.3b)$$

Here the vector $\mathbf{q}$ has the components \{ $q_1, q_2, \ldots, q_d$\}
where $q_j = 2\pi n_j / L_j$ and $n_j \in \{-M_j, \ldots, M_j - 1\}$ with
$M_j = L_j \Lambda_j / (2\pi) \gg 1$ being integer numbers, and $\Lambda_j$
the cutoff at the boundaries of the first Brillouin zone along
the $j$ direction. The spherical field $\phi$ is introduced to
ensure the fulfillment of the constraint (2.2). It is the solu-
tion of the equation

$$\beta \mathcal{F}(0) \rho_\sigma \left( 1 - \frac{H^2}{\phi^2 \mathcal{F}(0) \rho_\sigma^2} \right) = \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{\phi + \omega_\sigma(\mathbf{q})}. \hspace{1cm} (2.3c)$$

Equations (2.3a) and (2.3b) contain all the necessary
information for the investigation of the critical behavior
of the model under consideration.

In the bulk limit, when all the sizes of the system are
infinite, the $d$-dimensional sums over the momentum vec-
tor $\mathbf{q}$ in Eqs. (2.3b) and (2.3c) transform into integrals
over the first Brillouin zone. For example one has

$$U_{d,\sigma}(\phi|\Lambda) = \frac{1}{(2\pi)^d} \int_{-\Lambda}^{\Lambda} dq_1 \cdots \int_{-\Lambda}^{\Lambda} dq_d$$
$$\ln[\phi + \omega_\sigma(q_1, q_2, \ldots, q_d)]. \hspace{1cm} (2.4)$$

By analyzing the equation for the spherical field \( \phi \) in
the bulk limit it is easy to show that the system ex-
hibits a phase transition for $d > \sigma$ at the critical point,
$\beta_c$, given by

$$\beta_c \mathcal{F}(0) \rho_\sigma = \frac{1}{(2\pi)^d} \int_{-\Lambda}^{\Lambda} dq_1 \cdots \int_{-\Lambda}^{\Lambda} dq_d \frac{1}{\omega_\sigma(q_1, q_2, \ldots, q_d)}. \hspace{1cm} (2.5)$$
III. SCALING FORM OF THE EXCESS FREE ENERGY AND THE CRITICAL CASIMIR FORCE

In the remainder we consider a system with a film geometry \( L \times \infty^{d-1} \), which results after taking the limits \( L_2 \to \infty, \cdots, L_d \to \infty \) and setting \( L_1 = L \). For the simplicity of notations we will only consider the case when all cut-off variables are taken to be equal to each other, i.e. \( \Lambda_i = \Lambda, i = 1, \cdots, d \). Then \( U_{d,\sigma}(\phi, L|\Lambda) \) becomes

\[
U_{d,\sigma}(\phi, L|\Lambda) = \frac{1}{L} \sum_{q_i} \left( \frac{1}{(2\pi)^{d-1}} \int_{-\Lambda}^{\Lambda} dq_2 \cdots \int_{-\Lambda}^{\Lambda} dq_d \ln[\phi + \omega_\sigma(q_1, q_2, \cdots, q_d)] \right).
\]

(3.1)

The above sum can be evaluated using the Poisson summation formula and the identity

\[
\ln(1 + z^\alpha) = a \int_0^\infty \frac{dx}{x} \left( 1 - e^{-xz} \right) E_\alpha(-x^\alpha),
\]

where \( E_\alpha(x) \equiv E_{\alpha,1}(x) \), and

\[
E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{(\alpha k + \beta)}
\]

(3.3)

are the Mittag-Leffler functions. For a review on the properties of \( E_{\alpha,\beta}(z) \) and other related to them functions, as well as for their application in statistical and continuum mechanics see Ref. 12 (see also Ref. 12). The properties used in the current article are summarized in Appendix A.

After some algebra for the full free energy density we receive:

\[
\beta F_{d,\sigma}(\beta, H, L) = \beta F_{d,\sigma}(\beta, H) - \frac{1}{2} L^{-\sigma} K_{d,\sigma}(L^\sigma \phi),
\]

(3.4)

where

\[
F_{d,\sigma}(\beta, H) \equiv \lim_{L \to \infty} F_{d,\sigma}(\beta, H, L),
\]

and

\[
K_{d,\sigma}(y_L) = \frac{\sigma}{(4\pi)^{d/2}} \sum_{l=1}^{\infty} \int_0^\infty dx e^{-d-1} \exp \left( -\frac{l^2}{4x} \right)
\times E_{\sigma/2,1} \left( -x^{\sigma/2} \right),
\]

(3.5)

The main advantage of the above expression for the free energy, despite its complicated form in comparison to equation (2.3a), is the simplified dependence on the size \( L \) which now enters only via the arguments of some functions. This gives the possibility, as it is explained below, to obtain the scaling functions of the excess free energy and the Casimir force. It is worthwhile noting that under a sharp cutoff \( \Lambda \) a special care has to be taken when performing finite-size scaling calculations in order to avoid receiving artificial, i.e. not existing in real systems, finite-size \( \Lambda \)-dependent contributions. This question is considered in details in 37. In obtaining (3.3) the suggested there receipt has been applied (see Eq. (27) in 37 and the discussion devoted to it). According to these findings, for the finite-size contributions in the following we are going to send the cutoff to infinity.

In equation (3.4), \( \phi \) is the solution of the corresponding spherical field equation that follows by requiring the partial derivative of the right hand side of equation (3.1) with respect to \( \phi \) to be zero. Let us denote the solution of the corresponding bulk spherical equation by \( \phi_\infty \). Then, for the excess free energy (per unit area) it is possible to obtain from equations (3.1) and (3.3) the finite size scaling form, valid for \( \sigma < d < 2\sigma \)

\[
f_{ex}(\beta, H, L|d) = \beta L^{-(d-1)} X_f(x_1, x_2),
\]

with scaling variables

\[
x_1 = (\beta - \beta_c) \mathcal{J}(0) \rho L^{1/\nu},
\]

(3.6a)

and

\[
x_2 = H L^{\Delta/\nu} \sqrt{\beta/\mathcal{J}(0)} \rho \sigma.
\]

(3.6b)

Here \( \nu = 1/(d - \sigma) \) and \( \Delta = (d + \sigma)/(2(d - \sigma)) \) are the critical exponents of the spherical model (for \( \sigma < d < 2\sigma \), and \( 0 < \sigma \leq 2 \)). In equation (3.6b) the universal scaling function \( X_{ex}(x_1, x_2) \) of the excess free energy has the form

\[
X_f(x_1, x_2) = \frac{1}{2} x_2 \left( \frac{1}{y_L} - \frac{1}{y_\infty} \right) - \frac{1}{2} x_1 (y_L - y_\infty),
\]

(3.7a)

\[
-\frac{\sigma}{2d} |D_{d,\sigma}| \left( y_L^{d/\sigma} - y_\infty^{d/\sigma} \right) - \frac{1}{2} K_{d,\sigma}(y_L),
\]

(3.7b)

where the \( y_L = \phi_L L^\sigma, y_\infty = \phi_\infty L^\sigma \), and

\[
D_{d,\sigma} = 2\pi \left( \frac{4\pi}{d} \right)^{d/2} \Gamma \left( \frac{d}{2} \right) \sigma \sin \left( \frac{\pi d}{\sigma} \right) \right)^{-1}.
\]

(3.8)

In Eq. (3.8), \( y_L \) is the solution of the spherical field equation for the finite system obtained by minimizing the free energy with respect to \( y_L \)

\[
x_1 = \frac{x_2^2}{y_L^2} - |D_{d,\sigma}| y_L^{d/\sigma - 1} - \frac{\partial}{\partial y_L} K_{d,\sigma}(y_L).
\]

(3.9)

For the infinite system the corresponding equation is

\[
x_1 = \frac{x_2^2}{y_\infty^2} - |D_{d,\sigma}| y_\infty^{d/\sigma - 1}.
\]

(3.10)

According to equation (3.11), the finite-size scaling function of the Casimir force for the system under consideration is

\[
X_{\text{Casimir}}(x_1, x_2) = \frac{\sigma}{2} \frac{x_2^2}{y_L^2} \left( \frac{1}{y_L} - \frac{1}{y_\infty} \right)
\]

\[
-\frac{\sigma - 1}{2} x_1 (y_L - y_\infty) - \frac{\sigma(d - 1)}{2d} |D_{d,\sigma}| \left( y_L^{d/\sigma} - y_\infty^{d/\sigma} \right)
\]

\[
- \frac{1}{2} (d - 1) K_{d,\sigma}(y_L).
\]

(3.12)
Note that in the limit $\sigma \to 2^-$ Eqs. (3.6)-(3.12) reproduce exactly the corresponding ones for the case of the short-range interaction \cite{12,13,14}. In such a case the above equations simplify greatly since then $E_{1,1}(z) = \exp(z)$, and the function $K_{d,\sigma}(y)$ defined in Eq. (3.5) becomes

$$K_{d,\sigma}(y) = \frac{4}{(2\pi)^{d/2}} y^{d/4} \sum_{l=1}^{\infty} l^{-d/2} K_{d/2}(l\sqrt{y}), \quad (3.13)$$

where $K_{\nu}$ is the modified Bessel function.

In the present article we will concentrate on the investigation of the behavior of the Casimir force and the excess free energy in different regions of the phase diagram. We will also evaluate some critical amplitudes for selected values of the parameters $d$ and $\sigma$. The analysis will be done analytically for the cases where one can obtain simple expressions and is then extended numerically to cases which are not accessible by analytical means.

In FIG. 1 we present the numerical evaluation of the Casimir force at $T = T_c$. We recall that the finite-size correlation length $\xi_L$ is related to $y_L$ via $\xi_L = L^{1/\sigma} y_L$.

![FIG. 1: Behavior of the Casimir amplitude as a function of $d$.](image)

In order to obtain the amplitudes, one needs to know the value of $y_L(T)$ at the critical point $T = T_c$ that is the solution of the equation for the spherical field \cite{8,10}. These results have their own important physical meaning. We recall that $y_L$ is directly connected to the finite-size correlation length $\xi_L = L^{1/\sigma} y_L$ of the system \cite{8}. The results for $y_L(T_c)$ are shown in FIG. 2.

![FIG. 2: Behavior of the scaling variable $y_L$ as a function of $d$ at the critical point $T = T_c$.](image)

In FIG. 3 we present our results for the Casimir force evaluated at the bulk critical point of the model as a function of $d$ for some selected values of $\sigma$. We observe that the Casimir force behaves in a different way depending on whether $\sigma$ is smaller or larger than $\sigma = 1$. For $\sigma \leq 1$ it is decreasing monotonically as a function of $d$, while for $\sigma > 1$ it is not.

![FIG. 3: The behavior of the Casimir force at $T = T_c$ as a function of $d$.](image)

In the following we turn our attention to the investigation of the thermodynamic functions of interest as a function of the scaling variable $x_1$ for fixed $d$ and $\sigma$. Let us first consider the situations where it is possible to obtain some results analytically.

Let us first consider the asymptotic of the excess free energy and the Casimir force in the under critical region (i.e. $T < T_c$). Taking into account that then (i.e. when $x_1 \gg 1, x_2 = 0$), according to Eqs. (3.6) and (3.11) $y_L \to 0^+, y_\infty = 0$, as well as the asymptotic (3.13) of the function $K_{d,\sigma}(y_L)$ for small values of the argument (derived in Appendix B) it is easy to see that below the critical temperature

$$X_f(x_1 \to \infty, 0) \simeq -\frac{\sigma}{2\pi^{d/2}} \Gamma\left(\frac{d}{2}\right) \zeta(d), \quad (3.14)$$
The obtained analytical results are supported by numerical analysis of the expressions for the scaling functions of the excess free energy and the Casimir force at zero external field. The corresponding data is presented in FIG. 2 (for the excess free energy) and in FIG. 5 (for the Casimir force). While the scaling function of the excess free energy is monotonic regardless of the used values of \(d\) and \(\sigma\), the behavior of Casimir force depends strongly on the range of the interaction \(\sigma\). For \(\sigma > 1\) it is monotonically increasing as it can be seen from the case \(\sigma = 2\), corresponding to short range interaction, and the long-range case with \(\sigma = 1.5\). For \(\sigma = 1\) the monotonicity changes and \(X_{\text{Casimir}}(x_1, 0)\) becomes decreasing for values of \(\sigma < 1\). As example we show its behavior for \(\sigma = 0.75\).

![FIG. 4: The universal finite-size scaling function of the excess free energy \(X_f(x_1, 0)\) from Eq. (3.8) as a function of \(-x_1\); (T - Tc)L^\nu/\sigma, for some selected values of \(\sigma\) at zero external magnetic field. One observes that, in full accordance with the corresponding statement from Section XI, \(X_{\text{Casimir}}(x_1, 0)\) is a monotonically increasing function of the temperature \(T\) regardless of value of \(\sigma\).](image)

We close this section by presenting the outcome of the numerical analysis of the behavior of the scaling functions of the excess free energy, shown in FIG. 6 and that of the Casimir force, shown in FIG. 7, as a function of the scaling variable \(x_2\) at the bulk critical temperature. One observes that the excess free energy is a monotonically increasing function of the external magnetic field \(H\) independently of the range of the interaction. However the Casimir force is a nonmonotonic function of \(H\) and has a minimum at \(x_2 \neq 0\) which depth depends of the parameter \(\sigma\). The minimum is found to be at \(x_2 = 0.084, 0.145, 0.263\) and 0.416 for \(\sigma = 2, 1.5, 1\) and 0.75, respectively. So, as long as \(\sigma\) goes smaller the minimum becomes deeper. Indeed the ratio of the Casimir force evaluated at the minimum to its value at \(H = 0\) is a decreasing function of \(\sigma\). It is given by 1.017, 1.073, 1.215 and 1.513 for \(\sigma = 2, 1.5, 1\) and 0.75, respectively.

IV. CASIMIR (SOLVATION) FORCE ALONG THE PHASE COEXISTENCE LINE

Here we investigate the behavior of the Casimir force along the line \(H = 0\) when \(T < T_c\). This is a line of a first
order phase transition with respect to the magnetic field $H$. The finite-size rounding of the first-order transitions in $O(n)$ models has been already studied by Fisher and Privman in [48] for a fully finite and cylinder geometries. Later their predictions have been verified in details for the spherical model system with such a geometry in [48], while in [48] their arguments have been extended to a geometry of the type $L^{d-d'} \times \infty$, where $d'$ has been chosen so that no phase transition of its own exists in the finite system, i.e. $d' < \sigma$ has been supposed. Here we extend these investigations to cover also the cases $d' = \sigma$ and $d' > \sigma$ in systems with a film geometry, i.e. when $d' = d - 1$. We will be only interested in the behavior of the Casimir force.

For $T < T_c$ and small $H$ Eqs. (3.6)-(3.12) are still valid, but there the limit $y_L \ll 1$ has to be taken (i.e. we suppose that $x_1 \gg x_2^1$). As it is clear from Eq. (3.13), then there are three subcases to be considered.

i) The case $d - 1 < \sigma$.

Then in the finite system there is no phase transition on its own. For the excess free energy one obtains

$$f^\text{ex}(\beta, H) = -\frac{\sigma}{2\pi d/2} \Gamma(d/2) \zeta(d) L^{-(d-1)} + \beta m_0 H L \left\{ 1 - \frac{1}{2} \left( \frac{m_0}{m_L} + \frac{m_L}{m_0} \right) + \frac{\sigma}{2(d-1)} \left( \frac{m_0}{m_L} - \frac{m_L}{m_0} \right) \right\},$$

(4.1) where

$$\frac{m_L}{m_0} = \sqrt\left( \frac{D_{d-1,\sigma}}{2x_m} \right)^2 + 1 - \frac{D_{d-1,\sigma}}{2x_m}. \quad (4.2)$$

Here $m_L = H/|\rho_0 J(0)|\phi$ is the magnetization of the finite system, $m_0 = \sqrt{1 - T/T_c}$ is the spontaneous magnetization, and $x_m = \beta m_0(T) L\xi^{-1} L\xi^{-1} T$, which has the meaning of the ratio of the total magnetic energy in the correlated volume $V_{corr} = L_d^{d-1}$ to the thermal energy $k_b T$ per degree of freedom, is the scaling variable. (We recall that in the spherical model the true finite-size correlation length $\xi_L$ is equal to $\phi^{-1/\sigma}$.) Next, it is easy to see from Eq. (4.2) that $x_m = O(1)$ involves $H = O(L^{-\sigma/(1+\sigma-d')}$, that is the scale on which the jump in the bulk magnetization is rounded off. From
this observation and from Eq. (4.1) one obtains that the $H$ dependent correction to the Casimir force is then of the order of $L^{-\sigma/(1+\sigma-d)}$ (Note that $\sigma/(1+\sigma-d) > d$ for $d > \sigma$, and, so, the term proportional to $H$ in Eq. (4.1) will indeed contribute as a correction towards the Casimir force).

ii) The case $d-1 = \sigma$.

This is the borderline case between that one when in the finite system there is no phase transition of its own (for $d-1 < \sigma$) and that one in which in the finite system there is such a phase transition (for $d-1 > \sigma$). In this case an essential singular point exists in the finite-size system at $T = H = 0$. For the excess free energy one now obtains

$$f^{\text{ex}}(\beta, H) = -\frac{\sigma}{2\pi d/2} \Gamma(d/2) \zeta(d) L^{-(d-1)} + \beta m_0 H L \left(1 - \frac{m_0}{m_L}\right),$$

where

$$\frac{m_L}{m_0} = \sqrt{\left(\frac{L}{4\pi}\right)^{\sigma/2} \Gamma(\sigma/2) \frac{1}{x_m}} + 1 + \frac{1}{\left(4\pi\right)^{\sigma/2} \Gamma(\sigma/2) \frac{1}{x_m}} \right),$$

and $x_m = \beta m_0(T) H L \xi_L^{-d-1}/\ln(L/\xi_L)$. The above equations are to be compared with the previous case. One observes, that the main difference is the existence of logarithmic-in-$L$ dependence that is introduced via the scaling field variable $x_m$. As a result the rounding of the jump in the magnetization takes place on a scale given by $H = L^{-\sigma} \exp(-\text{const} \cdot L)$, i.e. the scale in this case is exponentially small in $L$.

ii) The case $d-1 > \sigma$.

In this case there is a true phase transition of its own in the finite system at some $T_{c,L} = T_c - \xi_L^{-1/\nu}$, i.e. no rounding of the jump of the magnetization is possible. One only observes $L$-dependent corrections of the finite-size magnetization $m_L$ with respect to the spontaneous magnetization $m_0$. One finds that the crossover from $d$ to $d-1$ critical behavior happens at $T_{c,L}$, with

$$\xi = \frac{\pi^{(d-1)/2}}{(2\pi)^{\sigma}} \frac{C_{d,\sigma}}{\Gamma(d/2) \beta_c \zeta(0)} \frac{1}{\rho_\sigma},$$

and, when $|H| L^{\sigma} \ll 1$,

$$f^{\text{ex}}(\beta, H) = -\frac{\sigma}{2\pi d/2} \Gamma(d/2) \zeta(d) L^{-(d-1)} + \beta m_0 H L \left(1 - \frac{m_0}{m_L}\right),$$

with

$$\alpha = \frac{\pi^{(d-1)/2}}{(2\pi)^{\sigma}} \frac{C_{d,\sigma}}{\Gamma(d/2) \beta m_0^2(T) \zeta(0)} \frac{1}{\rho_\sigma},$$

and $m_L \approx m_0(1-\alpha/2)$.

Finally, we would like to note that in $O(n)$ systems one observes for $T < T_c$ in addition to the rounding of the jump of the order parameter also rounding of the spin wave singularities. According to the general theory, their rounding occurs on the scale for which $x_s = [H]|L^{\sigma} = O(1)$. As it is clear from Eq. (4.19) and taking into account that if $T < T_c$ one can rewrite $x_1$ as $x_1 = \beta m_0(T)^2 \rho \zeta(0)$, with $x_1 \gg 1$ the scale on which the rounding of the spin wave singularities sets in involves that $x_1 \sim x_2^2$ there. Then, in this regime, the solution of the spherical field equations for the finite and the infinite system $\xi_{L,\sigma}^c$ and $\xi_{\infty,\sigma}^c$ will be again $y_L = O(1)$ and $y_\infty = O(1)$. Since $x_1$ and $x_2$ can be expressed from Eqs. (3.10) and (3.11) in terms of $y_L$ and $y_\infty$, we conclude that, according to (5.1.4), in the regime in which the spin waves are of importance, the Casimir force will be $F_{\text{Casimir}} = O(L^{-d})$, possessing a nontrivial $H$ dependence. If one would like to reveal more on this dependence the numerical treatment is unavoidable. Note that when the field is strong enough to suppress the spin-wave excitations, i.e. when $x_s \gg 1$ and $T < T_c$, one will have an Ising-like system. In this regime $y_L \gg 1$, $y_\infty \gg 1$, and the Casimir force will be of the order of $L^{-(d+\sigma)}$ (see Eq. (5.1.5)) under periodic boundary conditions. (If the system was possessing real bounding surfaces like, say, under Dirichlet-Dirichlet boundary conditions, one would expect that the corresponding contribution in the force is of the order of $L^{-\sigma}$.)

V. MONOTONICITY PROPERTIES OF THE EXCESS FREE ENERGY AND THE CASIMIR FORCE

Let us denote by $g_L(x_2,y)$ and $g_\infty(x_2,y)$ the right-hand side of Eqs. (3.10) and (3.11), respectively. Now we prove that

i) $g_L(x_2,y) > g_\infty(x_2,y)$ and

ii) that $g_L(x_2,y)$ and $g_\infty(x_2,y)$ are monotonically decreasing functions of $y$.

i) First, let us note that $E_{\alpha,\sigma}(-x)$ is a completely monotonic function of $x \geq 0$ for $0 < \alpha \leq 1$ and $\beta \geq \alpha$. (In [49] and [50] this property was shown to hold for $E_{\alpha,1}(-x) \equiv E_{\alpha,\sigma}(-x)$ and was later extended to $E_{\alpha,\beta}(-x)$ in [51] and [52]; see also [52].) This means that for all $n = 0, 1, 2, \ldots$ one has

$$(1-x)^n \frac{d^n}{dx^n} E_{\alpha,\beta}(-x) \geq 0, x \geq 0, 0 < \alpha \leq 1, \beta \geq \alpha. \quad (5.1)$$

Then, from $n = 0$ it immediately follows that $E_{\alpha,\sigma}(-x) > 0$ when $x \geq 0$. Now, from Eqs. (5.1) and (3.11), it immediately follows that $g_L(x_2,y) > g_\infty(x_2,y)$.

ii) The required property follows from the monotonicity of the function $E_{\alpha,\sigma}(-x)$ for $x \geq 0$ and the explicit form of the right hand sides of Eqs. (3.10) and (3.11).

Having proved i) and ii), it is easy to understand now that for any given values $x_1$ and $x_2$ of the scaling variables the solution of the spherical field equation for the finite system will be larger than that for the infinite system, i.e. $y_L(x_1,x_2) > y_\infty(x_1,x_2)$. (Since the correlation lengths in the finite and the infinite system are $\xi_L = y_L^{-1/\sigma}$ and $\xi_\infty = y_\infty^{-1/\sigma}$, respectively, the difference in the solutions will be largest for the smallest correlation length $\xi_\infty$.)
\( \xi_\infty = y_\infty^{-1/\sigma} \), correspondingly, the physical meaning of the above result is that the correlation length of the finite system is always smaller than that of the infinite one. We are then ready to prove that

A) For \( x_1 \geq 0 \) and \( x_2 = 0 \) the excess free energy scaling function is negative, i.e. \( X_f(x_1 \geq 0, x_2 = 0) < 0 \).

B) The excess free energy scaling function \( X_f(x_1, x_2) \) is a monotonically increasing function of the temperature \( T \) and the magnetic field \( |H| \).

Let us start with statement A).

A) From the explicit form of the Eq. \( 3.8 \) it is clear that the statement A) will be true if \( E_\alpha,1(-x) \geq 0 \) when \( x \geq 0 \). The last follows from \( 5.1 \) for \( n = 0 \), and, thus, \( X_f(x_1, x_2) < 0 \).

Let us now prove the statement B.

B) From Eq. \( 3.8 \) one obtains

\[
\frac{\partial X_f}{\partial x_1} = \frac{1}{2} \left( y_\infty - y_L \right) < 0, \tag{5.2}
\]

and

\[
\frac{\partial X_f}{\partial x_2} = x_2 \left( \frac{1}{y_\infty} - \frac{1}{y_L} \right) > 0. \tag{5.3}
\]

Eq. \( 5.2 \) implies that \( X_f(x_1, x_2) \) is a monotonically increasing function of \( T \), whereas Eq. \( 5.3 \) states that it is a monotonically increasing function of \( |H| \) too.

Using B) one can now prove that:

C) The excess free energy scaling function is negative for any \( T \) and \( H \), i.e. \( X_f(x_1, x_2) < 0 \) for any \( x_1 \) and \( x_2 \).

Indeed, from the monotonicity property B) and from A) it is clear that in order to prove C) it is enough to show that it holds for values of \( T \) above \( T_c \), i.e. when \( y_L \gg 1 \) and \( y_\infty \gg 1 \). Then, from Eqs. \( 3.10, 3.11 \) and the asymptotic \( 5.14 \) one obtains \( y_L = y_\infty (1 + \varepsilon) \), \( 0 < \varepsilon \ll 1 \), where

\[
\varepsilon = \frac{a_{d,\sigma}}{y_\infty} \left[ \frac{x_1^2}{y_\infty^2} + |D_{d,\sigma}| y_\infty^{-d/\sigma - 1} (d/\sigma - 1) + \frac{2 a_{d,\sigma}}{y_\infty} \right]. \tag{5.4}
\]

Next, from Eq. \( 3.8 \) it follows that

\[
X_f(x_1, x_2) \approx -\frac{1}{2} \frac{a_{d,\sigma}}{y_\infty} (1 - \varepsilon) < 0. \tag{5.5}
\]

Thus, the excess free energy is indeed always negative.

Finally, we prove that

D) For \( \sigma \geq 1 \) the Casimir force is always negative, i.e. it is a force of attraction between the surfaces bounding the system.

We start by multiplying Eq. \( 3.11 \) with \( y_\infty \) and Eq. \( 5.10 \) with \( y_L \), and then adding the results together. One
obtains
\[ x_1(y_L - y_\infty) = x_2^t\left(\frac{1}{y_L} - \frac{1}{y_\infty}\right) - |D_{d,\sigma}|(y_1^{d/\sigma} - y_2^{d/\sigma}) - y_L \frac{d}{dy_L}K_{d,\sigma}(y_L). \] (5.6)

Inserting the above expression in Eq. 5.12, one obtains
\[ X_{\text{Casimir}}(x_1, x_2) = x_2^t\left(\frac{1}{y_L} - \frac{1}{y_\infty}\right) - \frac{1}{2}\left(1 - \frac{\sigma}{d}\right)|D_{d,\sigma}|(y_1^{d/\sigma} - y_2^{d/\sigma}) - \frac{1}{2}(d - 1)K_{d,\sigma}(y_L) + \frac{\sigma - 1}{2}y_L \frac{d}{dy_L}K_{d,\sigma}(y_L). \] (5.7)

Since, according to what already has been proven, \( y_L > y_\infty \), and \( K_{d,\sigma}(y_L) \) is a positive and monotonically decreasing function of \( y_L \) (the last follows from the explicit form of \( K_{d,\sigma}(y_L) \) given in Eq. 5.13, and the property 5.14 of \( E_{\alpha,1}(x) \) for \( n = 0 \) and \( n = 1 \)), from the above expression one immediately confirms the validity of statement D. In addition, from Eq. 5.12 it is easy to see that \( X_{\text{Casimir}}(x_1, x_2) < 0 \) also for \( \sigma < 1 \) if \( x_1 \leq 0 \), i.e. for \( T \geq T_c \). Furthermore, from Eqs. 5.15 and 5.12 it follows that
\[ \frac{\partial}{\partial x_1}X_{\text{Casimir}}(x_1 = 0, x_2 = 0) = -\frac{\sigma - 1}{2}y_L, \] (5.8)
where from we conclude, that at \( T = T_c \) the Casimir force is an increasing function of \( T \) for \( \sigma > 1 \) (see Fig. 4), and a decreasing function of \( T \) when \( \sigma < 1 \) (see Fig. 2). Therefore, at the critical point the monotonicity of the force changes as a function of \( \sigma \) at \( \sigma = 1 \) where we have an inflexion point.

VI. DISCUSSION

In the current article we consider the behavior of the excess finite-size free energy and the Casimir (solvation) force in a classical system with leading long range interactions in the limit \( n \to \infty \) of the \( O(n) \) models (i.e. within the spherical model). The dimensionality \( d \) and the parameters controlling the range of the interaction \( \sigma \) are chosen so, that the hyperscaling is valid, i.e. \( \sigma < d < 2\sigma \) is supposed. In this regime the critical exponents depend on \( \sigma \). We demonstrate that, despite of the choice of \( \sigma \), the excess free energy scaling function \( X_f \) (see Fig. 4 and FIG. 3) is a monotonic function of the temperature \( T \) and the magnetic field \( H \), with \( X_f \) being always a negative function. Surprisingly, to a given extend, the above properties do not hold in such a general fashion for the Casimir (solvation) force (see Fig. 5 and FIG. 4). This is in line with the results of Section VI where we show analytically that the force is attractive for any \( T \) and \( \sigma \geq 1 \), as well as for any \( T \geq T_c \) if \( \sigma < 1 \). The monotonicity of the force turns out to depend on \( \sigma \). For example, if \( \sigma > 1 \) at \( T = T_c \) and \( H = 0 \) the force is an increasing function of \( T \) and \( L^{-1} \), while for \( \sigma < 1 \) it is a decreasing function of both \( T \) and \( L^{-1} \) at this point (see Eq. 5.13 and FIG. 4).

In addition, one derives that for \( T = T_c \) the minimum of the force is not at \( H = 0 \) (see FIG. 4). Indeed, at \( T = T_c \) the minimum has been found to be at some finite value of the scaling field variable \( x_2 \sim H L^{2/\nu} \). For \( \sigma = 2, 1.5, 1 \) and 0.75 the minimum at \( T = T_c \) is found to be at \( x_2 \approx 0.084, 0.145, 0.263 \) and 0.416, respectively. Such an occurrence of a force minimum for a nonzero bulk field has also been reported for the case of \((+,-)\) boundary conditions [53, 54]. Here, in this Section, we provide more details for the universal finite-size scaling function of the Casimir force \( X_{\text{Casimir}}(x_1, x_2) \) presenting the numerical results for it as a function of both \( x_1 \) and \( x_2 \geq 0 \) in FIG. 5. There the effects due to both the temperature and the magnetic field are demonstrated (we recall that \( x_1 \sim (T - T_c)L^{1/\nu} \), \( x_2 \sim H L^{2/\nu} \)). We observe that for \( T < T_c \) and \( H \neq 0 \) a cavity shows up in the vicinity of the critical temperature that disappears for temperatures far away from the critical point. More precisely, one observes that there exists a finite value \( x_1^* \) of \( x_1 \), such that for any \( x_1^* > x_1 \geq 0 \) there is a local minimum of the force at some finite \( x_2 \), i.e. at \( H \neq 0 \). For \( x_1 > x_1^* \) there is no such minimum at nonzero \( H \). In FIG. 5 the last is shown for the cases \( \sigma = 0.75, 1, 1.5 \) and \( \sigma = 2 \) (the short-range case). Note, that for \( \sigma = 0.75 \) one needs to go deeply in the under critical region to find out where exactly the cavity vanishes. In the short-range case \( \sigma = 2 \) we established that \( x_1^* \approx 0.28 \).

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APPENDIX A: SOME PROPERTIES OF THE MITTAG-LEFFLER TYPE FUNCTIONS

The Mittag-Leffler type functions are defined by the power series [12]:
\[ E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad \alpha, \beta > 0. \] (A1)
They are entire functions of finite order of growth. The functions are named after Mittag-Leffler who first considered the particular case \( \beta = 1 \). These function are very popular in the field of fractional calculus (for a recent review see Ref. [12]).

One of the most useful property of these functions is
the identity \[42\]
\[
\frac{1}{1+z} = \int_0^\infty dx e^{-x} x^{\beta-1} E_{\alpha,\beta} (-x^\alpha z),
\]
which is obtained by means of term-by-term integration of the series \[41\]. The integral in Eq. \(A2\) converges in the complex plane to the left of the line \(\text{Re } z^{1/\alpha} = 1\), \(|\arg z| \leq \frac{1}{2}\alpha\pi\). The identity \(A2\) lies in the basis of the mathematical investigation of finite-size scaling in the spherical model with algebraically decaying long-range interaction (see Ref. \[3\] and references therein).

In some particular cases the functions \(E_{\alpha,\beta}(z)\) reduce to known functions. For example, in the case corresponding to the short range case we have
\[
E_{1,1}(z) = \exp(z).
\]

Setting \(z = y^{-\alpha}\), \(y > 0\), and \(x = ty\), we obtain the Laplace transform
\[
\frac{y^\alpha - 1}{1 + y^\alpha} = \int_0^\infty dt e^{-y t^{\beta-1}} E_{\alpha,\beta} (-t^\alpha)
\]
from which we derive the useful identity
\[
\frac{1}{1 + z^\alpha} = \int_0^\infty dx \exp (-x z) x^{\alpha-1} E_{\alpha,\alpha} (-x^\alpha),
\]
by setting \(\beta = \alpha\).

The asymptotic behavior for large arguments of the Mittag-Leffler functions is given by the Lemma \[55\]:

Let \(0 < \alpha < 2\), \(\beta\) be an arbitrary complex number, and \(\gamma\) be a real number obeying the condition
\[
\frac{1}{2} \alpha \pi < \gamma < \min\{\pi, \alpha \pi\}.
\]

Then for any integer \(p \geq 1\) the following asymptotic expressions hold when \(|z| \to \infty\):

- At \(|\arg z| \leq \gamma\),
  
  \[
  E_{\alpha,\beta}(z) = \frac{1}{\alpha} z^{(1-\beta)/\alpha} e^{-z^{1/\alpha}} - \sum_{k=1}^\infty \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + \mathcal{O}(|z|^{-p-1}).
  \]

- At \(\gamma \leq |\arg z| \leq \pi\),
  
  \[
  E_{\alpha,\beta}(z) = - \sum_{k=1}^\infty \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + \mathcal{O}(|z|^{-p-1}).
  \]

### APPENDIX B: ASYMPTOTICS OF THE FUNCTION \(K_{d,\sigma}(y)\)

Here we will evaluate the asymptotic behaviors of the auxiliary function \(K_{d,\sigma}(y)\) used in the expression of the free energy and the quantities descending from it. It is defined by:
\[
K_{d,\sigma}(y) = \frac{\sigma}{2(4\pi)^{d/2}} \int_0^\infty dx x^{-d/2-1} \left[ A \left( \frac{1}{4x} \right) - 1 \right] \times E_{\frac{d}{2}+1} (-x^{\frac{d}{2}} y),
\]
where
\[
A(u) = \sum_{l=-\infty}^{\infty} e^{-u^2}.
\]

Using the identity
\[
E_{\alpha,1}(-z) = 1 - z E_{\alpha,\alpha+1}(-z),
\]
it is possible to write down Eq. \(B1a\) in a more convenient form, which will allow us to extract the asymptotics of the function under investigation. After some algebra one obtains
\[
K_{d,\sigma}(y) = \frac{\sigma}{2(4\pi)^{d/2}} \int_0^\infty dx x^{-d/2} \left[ A \left( \frac{1}{4x} \right) - 1 \right] \times E_{\frac{d}{2}+1} (-x^{\frac{d}{2}} y),
\]
where we have introduced the auxiliary function
\[
I_{d,\sigma}(y) = \frac{y}{(4\pi)^{d/2}} \int_0^\infty dx x^{-d/2} \left[ A \left( \frac{1}{4x} \right) - 1 \right] \times E_{\frac{d}{2}+1} (-x^{\frac{d}{2}} y).
\]

Now, setting \(x = z(2\pi)^{-2}\) and with the help of the identity
\[
A(u) = \sqrt{\frac{\pi}{u}} A \left( \frac{\pi^2}{u} \right),
\]
we rewrite equation \(B3a\) (after some algebra) in the form
\[
I_{d,\sigma}(y) = y^{(d-1)/2} (2\pi)^{\sigma} \left[ A(x) - \sqrt{x \frac{\pi}{x} - 1} \right] E_{\frac{d}{2}+1} (-y^{\frac{d}{2}} (2\pi)^{\sigma})
\]
\[
+ y^{(d-1)/2} (2\pi)^{\sigma} \int_0^\infty dx x^{-d/2} E_{\frac{d}{2}+1} (-y^{\frac{d}{2}} (2\pi)^{\sigma}).
\]

\[B5\]
The integral in the second term of the right-hand side of (B5) can be evaluated exactly with the help of the identities

\[ \int_0^\infty dt e^{-\pi t} = \frac{1}{\Gamma(\nu)} \int_0^{\infty} dt t^{\nu-1} e^{-ut} \quad (B6) \]

and

\[ \int_0^\infty u^{\nu-1} \ln(a + bu) = \left( \frac{\nu}{b} \right) \frac{\pi}{\sin(\pi \nu/\nu)} \quad (B7) \]

to yield the result

\[ 2(d - 1)^{-1} D_{d-1,\sigma} y^{(d-1)/\sigma}. \quad (B8) \]

For the evaluation of the first integral in the right hand side of (B5), we note that the two terms in the square brackets in (B5) cannot be integrated separately, since they diverge. Nevertheless, it is possible to outwit this divergence, by transforming further (B5) by adding and subtracting from the function \( E_{\alpha,\alpha+1}(z) \) its asymptotic behavior at small arguments, leading, after some algebra, to

\[ \frac{2\pi y^{(d-1)/2}}{\sigma} C_{d,\sigma} - 2d^{-1} D_{d,\sigma} y^{d/\sigma} + R_{d,\sigma}(y). \quad (B9a) \]

Here we introduced the notations

\[ C_{d,\sigma} = \int_0^\infty dxx^{\frac{d}{2}} - \frac{\sigma}{2} \left[ \sum_{l=1}^\infty e^{-x} \right], \quad d - 1 < \sigma, \quad (B9b) \]

and

\[ R_{d,\sigma}(y) = 2y \pi^{(d-1)/2} \frac{(2\pi)^\sigma}{\sigma} \sum_{l=1}^\infty \int_0^\infty dxx^{\frac{d}{2}} - \frac{\sigma}{2} e^{-x} \]
\[ \times \left[ E_{\frac{d}{2},\frac{d}{2}+1} \left( -y \right) - \frac{1}{\Gamma[\frac{d}{2}+1]} \right]. \quad (B9c) \]

Collecting the above results, we obtain

\[ K_{d,\sigma}(y) = \sigma \pi^{-d/2} \Gamma \left( \frac{d}{2} \right) \zeta(d) \]
\[ -\sigma(d - 1)^{-1} D_{d-1,\sigma} y^{(d-1)/\sigma} - y \sigma^{d/2} \frac{(2\pi)^\sigma}{\Gamma[\sigma/2]} \]
\[ + \sigma d^{-1} D_{d,\sigma} y^{d/\sigma} - \frac{\sigma}{2} R_{d,\sigma}(y). \quad (B10) \]

The constant \( C_{d,\sigma} \) introduced in Eq. (B9a) is the so called Madelung constant (see e.g. [54, 57]).

\[ C_{d,\sigma} = \lim_{\delta \to 0} \left\{ \sum_{l=1}^\infty \frac{\Gamma((\sigma - d + 1)/2)}{\Gamma[(\sigma - d + 1)/2]} \right\} \frac{\delta^{d-1}}{d^{\sigma + d}}, \quad d - 1 < \sigma, \quad (B11) \]

where \( \Gamma[\alpha, x] \) is the incomplete gamma function. It has been shown that this constant has a remarkable property of symmetry [57], which relates its values in the case \( d - 1 < \sigma \) to those in the case \( d - 1 > \sigma \). On the other hand, it has been shown that \( C_{d,\sigma} \) can be expressed in terms of the analytic continuation, over \( d - 1 < \sigma \), of (for details see [57]).

\[ C_{d,\sigma} = 2\pi^{\frac{d}{2} + \sigma - d/2} \Gamma \left( \frac{d}{2} \right) \zeta(d - \sigma), \quad d - 1 > \sigma. \quad (B12) \]

Eq. (B10) is the general form of the functions \( K_{d,\sigma}(y) \). According to Eqs. (B11) and (B12), it can be used to investigate the critical behavior of the system for any dimension less than \( d \).

For small \( y \) the asymptotic behavior of the function \( K_{d,\sigma}(y) \) is easily deduced from equation (B14). It is given by

\[ K_{d,\sigma}(y) \approx \frac{2\pi^{\frac{d}{2}} \Gamma \left( \frac{d}{2} \right)}{\sigma^{d/2}} \zeta(d + \sigma), \quad \sigma = d - 1, \quad (B13) \]

For large \( y \) the asymptotic behavior of the function \( K_{d,\sigma}(y) \) is obtained by substituting the large \( x \) behavior of the functions \( E_{\alpha,\beta}(x) \) (given in Eq. (A7)) in the definition (B14a). After some calculations one ends up with

\[ K_{d,\sigma}(y) \approx a_{d,\sigma} y^{-1}, \quad (B14a) \]

where

\[ a_{d,\sigma} = \frac{2^{1+\sigma} \Gamma \left[ (d + \sigma)/2 \right]}{\Gamma \left[ -\sigma/2 \right]} \zeta(d + \sigma). \quad (B14b) \]
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