Thermodynamic Casimir Effect in the large-$n$ limit

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We consider systems with slab geometry of finite thickness $L$ that undergo second order phase transitions in the bulk limit and belong to the universality class of $O(n)$-symmetric systems with short-range interactions. In these systems the critical fluctuations at the bulk critical temperature $T_{c,\infty}$ induce a long-range effective force called the “thermodynamic Casimir force”. We describe the systems in the framework of the $O(n)$-symmetric $\phi^4$-model, restricting us to the large-$n$ limit $n \to \infty$. In this limit the physically relevant case of three space dimensions $d = 3$ can be treated analytically in systems with translational symmetry as, e.g., in the bulk or slabs with periodic or antiperiodic boundary conditions. We consider Dirichlet and open boundary conditions at the surfaces that break the translational invariance along the axis perpendicular to the slab. From the broken translational invariance we conclude the necessity to solve the systems numerically. We evaluate the Casimir amplitudes for Dirichlet and open boundary conditions on both surfaces and for Dirichlet on one and open on the other surface. Belonging to the same surface universality class we find the expected asymptotic equivalence of Dirichlet and open boundary conditions. To test the quality of our method we confirm the analytical results for periodic and antiperiodic boundary conditions.

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I. INTRODUCTION

In a fluctuating medium confined between two surfaces long-range forces may arise. This effect was first predicted by H. B. G. Casimir [1] who considered a confinement of the electromagnetic vacuum fluctuations between two perfectly conducting metal plates. The boundary conditions imposed by the two plates modify these fluctuations in such a way that the energy of the system becomes dependent on the separation of the plates. From this energy gradient in the separation a long-range force, the so called Casimir force arises. This force was experimentally measured for the first time in 1998 by Mohideen and Roy [2]. After this breakthrough more measurements followed [3, 4], confirming Casimir’s prediction with high accuracy.

An analogous effect is the so called thermodynamic Casimir effect which was first proposed by Fisher and de Gennes [5]. It is caused by critical fluctuations of a medium near its bulk critical point $T_{c,\infty}$, where these fluctuations are correlated over an infinite range. The spatial confinement of such fluctuations also gives rise to a long-range Casimir force.

The thermodynamic Casimir effect was experimentally proven for the first time by Garcia and Chan in thin films of liquid $^4$He at its transition temperature to superfluidity [6]. They measured a characteristic dip of the film thickness at the critical temperature, that can be attributed to the thermodynamic Casimir force.

The experimental data are excellently reproduced by Monte Carlo simulations of the XY-model with open boundary conditions [7] which is in the same universality class as the superfluid transition in $^4$He.

Due to the presence of strong fluctuations in critical systems there are only a few exact results for the thermodynamic Casimir effect yet. These are usually restricted to the case of periodic boundary conditions along the slab. Though there are perturbation theory results up to second order for experimentally relevant boundary conditions as, e.g., Dirichlet boundary conditions [8], exact results for these are still lacking.

The remainder of this paper is organized as follows. In the next section we carry the elementary features of the thermodynamic Casimir effect together, and introduce the large-$n$ limit. In Section II the model considered in the present work will be defined and its excess free energy will be derived in Section III. This calculation leads to a self-consistent eigenvalue problem, which is solved numerically, providing the possibility for numerical estimation of the Casimir amplitudes. The paper is closed with a discussion of the achieved results.

A. Casimir effect

As predicted by finite-size scaling theory a statistical system confined between two parallel surfaces exhibits a dependence of the free energy on the separation $L$ of the surfaces [9]. This $L$-dependence leads to an effective force between the surfaces which is a typical example of a finite-size effect. This thermodynamic Casimir force is defined...
Hamiltonian of a second order phase transition. There are various classes of models that exhibit critical behavior but here we will only consider those with periodic boundary conditions. However, for systems with non-periodic boundary conditions, exact results are not available. This is the aim of the present work.

To investigate the thermodynamic Casimir effect, one needs a model that shows the characteristic critical properties of a second order phase transition. There are various classes of models that exhibit critical behavior, but here we restrict ourselves to the class of classical $O(n)$-invariant $n$-vector lattice models. These can be represented by the Hamiltonian

$$\mathcal{H}_n = -\frac{1}{2} J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

where $f_{\text{ex}}$ denotes the reduced excess free energy per unit area, which is given by $f_{\text{ex}} = f_L - L f_b$ with the total free energy per unit area $f_L$ and the reduced bulk free energy density $f_b$. The limit $A \to \infty$ of the cross-sectional area has been taken.

For temperatures away from the bulk critical point, the bulk correlation length $\xi(T)$ is much smaller than the macroscopic separation $L$. In this regime, the Casimir force decays exponentially for large $L$.

As it is generally known, $\xi(T)$ diverges as $|T - T_{c,\infty}|^{-\nu}$ at the bulk critical temperature $T_{c,\infty}$, with critical exponent $\nu$, so in the vicinity of $T_{c,\infty}$ the bulk correlation length has the same order as $L$. This implies that the Casimir force $F_C(T, L)$ extends to distances much larger than the microscopic scale $a \approx \text{lattice constant}$. In this regime, the Casimir force decays algebraically for large $L$.

Examining the excess free energy more precisely, one finds that it can be decomposed into two contributions

$$f_{\text{ex}}(T, L) = f_s(T) + f_{\text{res}}(T, L) .$$

The first one is the $L$-independent nonlocal surface excess free energy $f_s(T) \equiv f_{\text{ex}}(T, \infty)$ [13]. The second one is the residual finite-size contribution $f_{\text{res}}(T, L)$ which contains the whole information about the $L$-dependence of the free energy.

At the bulk critical point $T_{c,\infty}$ the finite-size contribution has the characteristic algebraic behavior [31]

$$f_{\text{res}}(T_{c,\infty}, L) \sim L^{-(d-1)} \Delta_C L^{-\nu} .$$

leading to a long-range effective Casimir force

$$\frac{F_C(T_{c,\infty}, L)}{k_B T_{c,\infty}} \sim L^{-\nu} \Delta_C L^{-d} .$$

The quantity $\Delta_C$ is an universal finite-size quantity, called the Casimir amplitude [5]. Universal means that it depends only on the bulk universality class of the phase transition and the surface universality class of the boundary planes [13]. It is in particular independent of microscopic details of the system, such as, e.g., the lattice structure.

Near the bulk critical point, the residual free energy density and the Casimir force obey the scaling forms

$$f_{\text{res}}(T, L) \sim L^{-(d-1)} \Theta(L/\xi(T))$$

and

$$\frac{F_C(T, L)}{k_B T} \sim L^{-d} \vartheta(L/\xi(T)) ,$$

where $\Theta(x)$ and $\vartheta(x)$ are universal functions with the scaling argument $x = L/\xi$. At $T_{c,\infty}$, where $L/\xi = 0$, they take the values $\Theta(0) = \Delta_C$ and $\vartheta(0) = (d-1)\Delta_C$.

There is no complete analytic theory for the thermodynamic Casimir effect joining the regimes above and below $T_{c,\infty}$, but second-order perturbative calculations up to second order for different boundary conditions at and above $T_{c,\infty}$ were performed. There are also exact results for the spherical model with periodic [12] and antiperiodic [17] boundary conditions. However, for slab systems with non-periodic boundary conditions, no exact results are available. This is the aim of the present work.

### B. The large-$n$ limit and the spherical model

To investigate the thermodynamic Casimir effect one needs a model that shows the characteristic critical properties of a second order phase transition. There are various classes of models that exhibit critical behavior, but here we restrict ourselves to the class of classical $O(n)$-invariant $n$-vector lattice models. These can be represented by the Hamiltonian
where the $S = (s_1, ..., s_n)$ are $n$-component vector spin variables, restricted to the local constraint $|S|^2 = 1$. The exchange coupling $J$ is assumed to have a positive nonzero value and the sum runs over all nearest neighbors.

In the limit $n \to \infty$, which is called the large-$n$ limit this model can be solved analytically for the bulk or for systems of finite size [18]. This case is connected to the so called the spherical model, which was first introduced and solved by Berlin and Kac [19] and is defined by the Hamiltonian

$$\mathcal{H}_{SM} = -\frac{1}{2} J' \sum_{i,j} s_i s_j.$$  \hfill (1.8)

Here the $s_i$ are scalar spin variables fulfilling a global constraint $\sum_i s_i^2 = N$ called “spherical constraint”, where $N$ is the number of lattice sites.

This model is even more easy to handle if one uses the constraint $\langle \sum_i s_i^2 \rangle = N$ where one takes the statistical mean over the sum. It is then called the “mean spherical model” but the both formulations are equivalent in translationally invariant systems.

It was found by Stanley [20] that these spherical models are equivalent to the large-$n$ limit for translationally invariant systems as e.g. the bulk case or systems with periodic boundary conditions.

To hold this equivalence in non-translationally invariant systems the spherical constraint has to be modified [21]. In the case of a slab where the boundary conditions are non periodic one needs a spherical constraint for each layer parallel to the surfaces. These multiple constraints make the analytical treatment impossible so that numerical calculations are needed. This is the challenge we are going to face here.

The large-$n$ limit can also be understand as the zeroth order of a systematical expansion in $1/n$ [22]. This connects our theory to the physical relevant case of e.g. three order parameter components known as the Heisenberg model. But this expansion is more useful for formal studies than to comparison to experimental observations.

## II. DEFINITION OF THE MODEL

In the last chapter we have discussed $O(n)$-symmetrical lattice models but now we turn to the description of the universal critical behavior in the framework of an $O(n)$-symmetrical $\phi^4$-model. The connection between both is that the $n$-vector lattice model can be mapped on the $n$-vector $\phi^4$-model by means of coarse graining [23].

We consider a $d$-dimensional slab of finite thickness $L$, which occupies the volume $\mathcal{Q} = \mathbb{R}^{d-1} \times [0, L]$. Let the $x_j$ with $j = 1, ..., d$, be cartesian coordinates and we write $x_d = z$ to denote the coordinate of the finite direction called the perpendicular direction. The full position vector is given by $x = (y, z)$, where $y = (x_1, \ldots, x_{d-1})$ denotes the coordinates of the directions along the slab called parallel directions.

As discussed in detail in [13] the general Hamiltonian of $\phi^4$-models with surfaces is given by

$$\mathcal{H}[\phi(x)] = \int_\mathcal{Q} \mathcal{L}_{\mathcal{Q}}[\phi(x)] \, dV + \int_{\partial \mathcal{Q}} \mathcal{L}_{\partial \mathcal{Q}}[\phi(x)] \, dA.$$  \hfill (2.1)

The densities $\mathcal{L}_{\mathcal{Q}}(x)$ and $\mathcal{L}_{\partial \mathcal{Q}}(x)$ depend on the $n$-component order parameter field $\phi(x)$ and its derivatives. This order parameter field is a classical $n$-component vector field that, using the language of magnetism, can be interpreted as the local spin density. The first part is the bulk Hamiltonian and the second is the additional surface Hamiltonian. The latter is taken in account because the coupling at the surface might deviate from that in the bulk.

The bulk density $\mathcal{L}_{\mathcal{Q}}(x)$ is given by

$$\mathcal{L}_{\mathcal{Q}}[\phi(x)] = \frac{1}{2} \sum_{\alpha=1}^n (\nabla \phi_\alpha(x))^2 + \frac{\tilde{\tau}}{2} \phi^2(x) + \frac{\tilde{u}}{4!n} (\phi^2(x))^2,$$  \hfill (2.2)

where $\tilde{\tau}$ is the temperature variable often called mass and $\tilde{u}$ is the coupling constant.

Note that in contrast to $\phi^4$-theories with a finite number of order parameter field components there is an additional $1/n$ in front of the $\phi^4$-term, which is needed to make the limit $n \to \infty$ well defined [24].

The general boundary density $\mathcal{L}_{\partial \mathcal{Q}}(x)$ reads

$$\mathcal{L}_{\partial \mathcal{Q}}[\phi(x)] = \frac{\tilde{c}(x)}{2} \phi^2(x).$$  \hfill (2.3)

The $\tilde{c}(x)$ is the surface enhancement that controls the additional couplings at the surface. It may have different values on the two boundaries $\partial \mathcal{B}_1$ and $\partial \mathcal{B}_2$, i.e.,

$$\tilde{c}(x) = \begin{cases} \tilde{c}_1(x) & \text{for } x \in \partial \mathcal{B}_1, \\ \tilde{c}_2(x) & \text{for } x \in \partial \mathcal{B}_2. \end{cases}$$  \hfill (2.4)
In our framework these boundary terms need not to be taken into account any longer because they give no contribution to the finite size energy that we are interested in and one can take account for the boundary conditions on the surface without those additional terms. The boundary conditions will be taken into account in the calculation of the eigensystem of the system. How this is done will be described in the next section.

III. THE FREE ENERGY

We now want to derive the exact expression for the free energy of the system. In the large-\( n \) limit such an expression can be obtained in different ways. One can use e.g. variational techniques as well as the saddle-point approximation \([25]\). Both become exact in the limit \( n \to \infty \). In the following we resort on the saddle-point approximation method.

We start the calculation by computing the canonical partition function \( Z \) of the system. It is given by the functional integral over all possible configurations of the order parameter field \( \phi(x) \). We write

\[
Z = \int \mathcal{D}[\phi] e^{-\mathcal{H}[\phi]} = \int \mathcal{D}[\phi] \exp \left\{ - \int d^d x \left[ \frac{1}{2} \sum_{\alpha=1}^{n} (\nabla \phi_\alpha)^2 + \frac{\tilde{\tau}}{2} \phi^2 + \frac{\hat{u}}{4\bar{n}} (\phi^2)^2 \right] \right\}. \tag{3.1}
\]

To determine the partition function with the saddle-point approximation we transform the last expression by applying the Hubbard Stratonovich decoupling technique \([26]\) and introducing an additional parameter \( \psi \). This leads to

\[
Z = C \int \mathcal{D}[\phi] \int \mathcal{D}[\psi] \exp \left\{ - \int d^d x \left[ \phi(x)(-\nabla^2 + \tilde{\tau} - \psi(z))\phi(x) - \frac{3n}{\bar{u}} \psi^2(z) \right] \right\}. \tag{3.2}
\]

The constant pre-factor \( C \) is irrelevant since it does not contribute to the excess free energy. The introduced variational parameter \( \psi \) is chosen to depend on \( z \) because the boundary conditions break the translational invariance along that axis.

The integration over \( \phi(x) \) is now Gaussian and can be carried out (see e.g. \([27]\)). This leads us to the expression

\[
Z = \tilde{C} \int \mathcal{D}[\psi] \exp \left\{ -\frac{n}{2} \text{Tr} \log(-\nabla^2 + \tilde{\tau} - \psi_0(z)) - \frac{3n}{2\bar{u}} A \int_0^L dz \psi_0^2(z) \right\}. \tag{3.3}
\]

The remaining functional integral can be evaluated by the saddle-point approximation. This means that we take the value of the integrand at its saddle point as solution of the integral. The number of order parameter components \( n \) serves as large parameter in the exponential function that makes the saddle-point a sharp peak as required for this approximation. With growing \( n \) the peak becomes sharper so that the approximation gets better and will become exact in the limit \( n \to \infty \). So we conclude that the partition function is given by

\[
Z = \tilde{C} \exp \left\{ -\frac{n}{2} \text{Tr} \log(-\nabla^2 + \tilde{\tau} - \psi_0(z)) - \frac{3n}{2\bar{u}} A \int_0^L dz \psi_0^2(z) \right\}. \tag{3.4}
\]

From the partition function we obtain the reduced free energy using its definition \( F(L) = \mathcal{F}/k_B T = -\log Z \). It is useful to consider the reduced free energy density per cross sectional area and order parameter component, \( f_L = F/An \) with \( A \to \infty \), that comes out as

\[
f_L = f_0 + \frac{1}{2} \int_p^{(d-1)} \text{Tr}_z \log(-\partial_z^2 + p^2 + \tilde{\tau} - \psi_0(z)) - \frac{3}{2\bar{u}} A \int_0^L dz \psi_0^2(z). \tag{3.5}
\]

Note that we have set \( \psi = \psi_0 \) in equations (3.4) and (3.4) where \( \psi_0 \) is the saddle-point value. It is defined by requiring that at the saddle-point the integrand must be extremal in \( \psi \), and obeys the self-consistent equation

\[
\psi_0(z) = -\frac{\hat{u}}{6} \int_p^{(d-1)} \text{Tr}_z \left[ -\partial_z^2 + p^2 + \tilde{\tau} - \psi_0(z) \right]. \tag{3.6}
\]

We now examine this self-consistent equation and determine the saddle-point value and the eigensystem along the \( z \) axis.

But first we want to remark the following: The problem can also be approached with the help of diagrammatic perturbation theory. From this theory one obtains the Dyson equation

\[
\left[ G(k) \right]^{-1} = k + \tilde{\tau} - \tilde{\Sigma}(k). \tag{3.7}
\]
for the two point correlation function of the system often named propagator \(\hat{G}(k)\). The contributions from all orders of perturbation theory are summed in the mass-operator \(\Sigma(k)\). Usually this cannot be done without approximation but, in the large-\(n\) limit the contributions to the mass operator can be summed up exactly (see [24, 28]). That mass-operator has the same self-consistent structure as \(\psi_0(z)\) in equation (3.6). So in comparison we can identify \(\psi_0(z) = \Sigma(z)\) and we will use \(\Sigma(z)\) instead of \(\psi_0(z)\) the following.

For simplicity we write the mass-operator \(\Sigma(z)\) in the mixed \(p\)-\(z\)-representation

\[
\Sigma(z) = -\frac{\hat{u}}{6} \int_p^{(d-1)} \sum_\nu \frac{\hat{\varphi}_\nu(z) \hat{\varphi}_\nu^*(z)}{\epsilon_\nu + p^2 + \hat{\tau}}.
\]

Here we define

\[
\int_p^{(d-1)} \equiv \prod_{i=1}^d \int_{-\infty}^{\infty} \frac{dp_i}{2\pi}
\]

and use this notation in the following.

The \(\hat{\varphi}_\nu(z)\) and the \(\epsilon_\nu\) are the eigenfunctions and the eigenvalues used to expand the \(z\)-dependence and are given by the equation

\[
\left[-\partial_z^2 + \Sigma(z)\right] \hat{\varphi}_\nu(z) = \epsilon_\nu \hat{\varphi}_\nu(z).
\]

Obviously the quantity \(\Sigma(z)\) is not well defined because the \(p\)-integration is UV-divergent. Usually one would have to deal with the procedures of regularization and renormalization to give the divergent expression a physical meaning. But our case is much simpler because we are not interested in the mass-operator itself. Thus we define another quantity which is UV-convergent by taking the difference of \(\Sigma(z)\) and a quantity which is UV-divergent to the same order.

For this purpose we decompose the mass \(\hat{\tau}\) into \(\hat{\tau} = \hat{\tau}_c + \delta\hat{\tau}\). The \(\hat{\tau}_c\) gives the value of \(\hat{\tau}\) at which the corresponding bulk system reaches criticality and \(\delta\hat{\tau}\) gives the deviation from this critical value. The \(\hat{\tau}_c\) is given by the expression [24]

\[
\hat{\tau}_c = -\frac{\hat{u}}{6} \int_p^{(d-1)} \int_{-\infty}^{\infty} \frac{dq}{2\pi} \frac{1}{p^2 + q^2}.
\]

It is UV-divergent to the same order as \(\Sigma(z)\). From the sum of both we now obtain a UV-convergent expression. We define the new quantity

\[
U(z) = \Sigma(z) + \hat{\tau}_c = \frac{\hat{u}}{6} \int_p^{(d-1)} \left( \sum_\nu \frac{\varphi_\nu(z) \varphi_\nu^*(z)}{\epsilon_\nu + p^2 + \hat{\tau}} - \int_{-\infty}^{\infty} \frac{dq}{2\pi} \frac{1}{p^2 + q^2} \right).
\]

Introducing this quantity the eigensystem is given by

\[
\left[-\partial_z^2 + U(z)\right] \varphi_\nu(z) = \epsilon_\nu \varphi_\nu(z).
\]

To simplify the further discussion we will interpret the two terms on the right hand side of equation (3.12) analogue to Ref. [28]. The first term on the right hand side is the propagator of the slab system for temperature deviations from the critical point defined by \(\delta\hat{\tau}\). The second term is the propagator of the corresponding bulk system at criticality where \(\delta\hat{\tau} = 0\). With this definitions one may write equation (3.12) in the following form

\[
U(z) = \frac{\hat{u}}{6} \int_p^{(d-1)} \left( \hat{G}(p; z, z) - \hat{G}_{\text{bulk}}(p; q) \right).
\]

Equations (3.12) and (3.13) form a self-consistent eigenvalue problem similar to the one dimensional Schrödinger equation of a particle in a potential \(U(z)\). The numerical solution of this problem is the content of the following subsection.
A. Discretization of the problem

Using a numerical method we now calculate the potential $U(z)$ and the corresponding eigensystem self-consistently. Therefore the model needs to be discrete along the $z$-axis. We introduce a discretization of the $z$-direction with $N$ points and the lattice constant $a$ in the sense that $z \to z_i$ with $z_i \in \{a, 2a, 3a, \ldots, Na\}$. The lattice constant is chosen to be $a = 1$ without loss of generality.

This discretization leads to some more changes. At first the number of eigenvalues $\epsilon_\nu$ and functions $\varphi_\nu$ is restricted to the number of discrete points $N$. At second there is also a change of the dispersion relation in the corresponding bulk model. The $q^2$ in the second term of the right hand side of equation (3.12) has to be replaced by the dispersion relation

$$
\epsilon(q) = \frac{4}{a^2} \sin^2\left(\frac{qa}{2}\right),
$$

of a lattice theory. Due to the periodicity of (3.15) the integration with respect to $q$ is restricted to the first Brillouin zone.

Implementing these modifications the potential $U(z)$ displayed in (3.12) becomes

$$
U(z_i) = \frac{\hat{u}}{6} \int_p^{(d-1)} \left[ \sum_{\nu=1}^{N} \frac{\varphi_\nu(z_i)\varphi^*_\nu(z_i)}{\epsilon_\nu + p^2 + \delta} \int_0^{2\pi} \frac{dq}{2\pi} \frac{1}{p^2 + \frac{4}{a^2} \sin^2\left(\frac{qa}{2}\right)} \right],
$$

where the corresponding eigenvalue equation (3.13) now reads

$$
[-\partial^2_{z_i} + U] \varphi_\nu = \epsilon_\nu \varphi_\nu.
$$

Here the $\partial^2_{z_i}$ and $U$ are finite $N \times N$ matrices and the $\varphi_\nu$ are the corresponding finite $N$-component vectors. We specify these objects now: The $\partial^2_{z_i}$ stands for the symmetric differentiation operator for the second derivative of a
discrete function. Usually this operator is defined by
\[
\partial^2_{z_i} \varphi_\nu(z_i) = \frac{\varphi_\nu(z_{i+1}) - 2\varphi_\nu(z_i) + \varphi_\nu(z_{i-1})}{a^2}.
\] (3.18)

Setting the lattice constant \(a = 1\) explicitly we can represent this operator as the matrix
\[
\partial^2_{z_i} = \begin{pmatrix}
-x & 1 & 0 & \ldots & 0 & y \\
1 & -2 & 1 & \ldots & 0 \\
0 & 1 & -2 & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & -2 & 1 & y \\
y & 0 & \ldots & \ldots & 1 & -x
\end{pmatrix}.
\] (3.19)

At this stage the boundary conditions of the system come into play. We can control them by choosing adequate values for \(x\) and \(y\). The reader can convince himself that if one chooses \(x = 1\) [\(x = 2\)] and \(y = 0\) this corresponds to open [Dirichlet] boundary conditions. If one sets \(y = 1\) [\(y = -1\)] and \(x = 2\) one gets periodic [antiperiodic] boundary conditions.

The matrix \(U\) is the diagonal matrix of the \(U(z_i)\)
\[
U = \text{diag}[U(z_i)]
\] (3.20)

and the eigenfunctions of the discrete model are represented as vectors where the components are given by
\[
\varphi_\nu(z_i) = \varphi_{\nu,i}.
\] (3.21)
FIG. 3: Numerical data of the potential for a system with open boundary conditions on one side and Dirichlet on the other side.

In this discrete form the self-consistent eigenvalue problem can be implemented into an iterative routine to determine the eigensystem and the matrix $U$. The calculations were carried out with build-in functions of the program Mathematica [29].

The iteration starts from an initial guess for the potential. From this guess the associated eigensystem is computed. With the eigensystem one computes again the potential for the next iteration step. This procedure is repeated until the difference between the steps is small enough to fulfill a certain termination condition.

Figures 1, 2 and 3 show the numerical results for the potential $U(z_i)$ plotted over the scaling variable $z_i/L$. We show system sizes $L$ in powers $2^n$ from $L = 256a$ to $L = 4096a$.

Figure 1 shows the results for the systems with Dirichlet boundary conditions on both surfaces. The potential as anticipated diverges at the boundaries to ensure that the eigenfunctions fall to zero on the surface. In the middle of the slab the potential tends with a characteristic algebraic behavior to its bulk value which is zero at criticality (see [22]). This tendency is more and more distinct for bigger systems because the influence of the boundaries in the middle of the slab decays with increasing system size.

Figure 2 shows the results for open boundary conditions. In the middle of the slab the potential approaches the behavior of systems with Dirichlet boundary conditions. This approach becomes stronger for larger systems. But next to the surfaces the evolution differs very strongly from the Dirichlet case. The most remarkable difference is that the potential has now a finite, positive value at the surface.

When there are both boundary conditions mixed in one system as it is shown in Figure 3 we find the diverging behavior on the Dirichlet side and the finite values on the open side. The values of the potential in the middle of the slab are still converging to the bulk value with increasing system size.

The Dirichlet and the open system are that similar because they are in the same surface universality class [13]. This means that their asymptotical behavior for large $L$ and large values of $z$ far away from the surface is identical.

To test the quality of our method we have also computed the potential $U(z)$ for the known cases of periodic and antiperiodic boundary conditions with our numerical method. We found that our results are in excellent agreement.
with the analytical results. A comparison between our results for the Casimir amplitude calculated from this potentials and the analytic results is shown in the next section.

IV. EXCESS FREE ENERGY AND CASIMIR AMPLITUDES

Now that the $U(z)$ is determined we can calculate the Casimir amplitudes. But first we have to modify the expression of the free energy by using the definitions $\tau = \tau_c + \delta \tau$ and $\Sigma(z) = \tau_c - U(z)$ to have only well defined quantities in it.

As we are not interested in the free energy itself but in the difference of the free energy of the slab and the bulk, called excess free energy we need an expression for the free energy of the bulk. We obtain this expression from a calculation analogous to that in the last chapter. The translational invariance of the bulk allows one to obtain its free energy analytically [22].

Now the exact expression for the excess free energy defined in Sec. I can be written in the form

$$f_{ex} = \frac{1}{2} \int_{p}^{(d-1)} \sum_{\nu} \log(\epsilon_{\nu} + p^2 + \delta \tau) - \frac{3}{2u} \int_{0}^{L} dz (\tau_c - U(z))^2$$

$$- \frac{L}{2} \int_{p}^{(d-1)} \frac{dq}{2\pi} \log(\tau_c - U_{bulk}) - \frac{3L}{2u} (\tau_c - U_{bulk})^2. \quad (4.1)$$

Because of the discrete numerical evaluation of the potential $U(z)$ all $z$ dependences in the last expression have to be discrete. This is what will be done the next section.

A. Discrete form of $f_{ex}$

We now obtain the form of the excess free energy with a discretized $z$ dependence. This means substituting $z \rightarrow z_i$ like in Sec. III. With this change we have to replace the dispersion relation of the continuum by that of the lattice and restrict the $q$ momentum integrations to the first Brillouin zone (see also Sec. III).

Finally the real space integration along the $z$-axis has to be turned into a sum. This is achieved by following the rule $\int_{0}^{L} dz \rightarrow a \sum_{i=1}^{N}$.

From this changes we obtain the excess free energy in the discrete form given by

$$f_{ex} = \frac{1}{2} \int_{p}^{(d-1)} \sum_{\nu=1}^{N} \log \left( \epsilon_{\nu} + p^2 + \delta \tau \right) - \frac{3}{2u} \sum_{i=1}^{N} (\tau_c - U(ia))^2$$

$$- \frac{L}{2} \int_{p}^{(d-1)} \left[ \frac{2\pi}{a^2} \log \left( p^2 + \frac{4}{a^2} \sin^2 \left( \frac{qa}{2} \right) + \delta \tau + U_{bulk} \right) \right] - \frac{3L}{2u} (\tau_c - U_{bulk})^2. \quad (4.2)$$

Since we are interested in the Casimir amplitude we limit the following discussion to the case $T = T_{c,\infty}$ and set the temperature variable $\delta \tau = 0$. In the following we use the result that the $U_{bulk}$ equals zero at $T_{c,\infty}$ (see [22]).

After evaluating the momentum integrals we get the expression

$$f_{ex} = \frac{1}{8} \pi^{\frac{d}{2}} \sum_{\nu=1}^{N} \left[ \frac{a^{2-d} \sum_{i=1}^{N} U(ia) \Gamma(d-1)}{\Gamma^2(d-2)} \right] - \frac{a^{4-d} \sqrt{\pi} \epsilon_{\nu}^{d-1}}{a(d-1) \Gamma(d-2)} + \frac{4a^{d-1} \Gamma(\frac{2}{4})}{\Gamma^2(4d-1)} \right] \sec \left( \frac{d\pi}{2} \right)$$

$$- \frac{3}{2u} \sum_{i=1}^{N} U^2(ia). \quad (4.3)$$

Examining the term “$\sec(d\pi/2)$” in this expression one recognizes that it has a remaining pole term in $d = 3$ space dimensions. This pole term can be understood by realizing that the $q$-integration is carried out but the corresponding summation over the eigenvalues is left unevaluated. The pole term needs to be removed to set $d = 3$ because the evaluation of the remaining sum in arbitrary dimensions is not feasible.

To make the pole-term visible and isolate it we expand $f_{ex}$ in the space dimension around $d = 3$. In this expansion we find a term from order $O(1/(d - 3))$

$$\sum_{\nu=1}^{N} \frac{2 + a^2 \sum_{i=1}^{N} U(ia) - a^2 \epsilon}{4a^{3}(d - 3)\pi} \quad (4.4)$$
which is singular at \( d = 3 \). But if we carry out the sums over \( \nu \) an \( i \) this pole-term becomes zero in the range of numerical accuracy. In other words: The pole-term is just an artifact of the non exact summation of numerically calculated objects. The zeroth order of the expansion contains the whole information of the excess free energy at \( d = 3 \) so we restrict us to the discussion of this term.

If the lattice constant \( a \) is explicitly taken to be unity, without loss of generality, we obtain the expression

\[
\begin{align*}
\mathcal{F}_{\text{ex}} &= \frac{1}{8\pi} \sum_{\nu=1}^{N} \left\{ \left[ \left( \sum_{i=1}^{N} U(i) + \epsilon_{\nu} \right) + 2 \right] \log(4\pi) \\
&\quad + \left[ \epsilon_{\nu} \left( \sum_{i=1}^{N} U(i) \right) - 2 \right] \log(\epsilon_{\nu}) \right\} - \frac{3}{2\pi} \sum_{i=1}^{N} U^2(i) \\
&= a_0 + a_2 L^{-2} + a_3 L^{-3} + a_4 L^{-4} + \ldots
\end{align*}
\]

where \( \gamma \) is the Euler-Gamma constant. In this expression the remaining sums can be evaluated to obtain the excess free energies for the given system sizes.

To compute the Casimir amplitude from the evolution of the numerical evaluated excess free energy with increasing system size we fit the data using the \textit{ansatz}

\[
f_{\text{ex}} = a_0 + a_2 L^{-2} + a_3 L^{-3} + a_4 L^{-4} + \ldots
\]

where the factor \( a_2 \) will later be interpreted as the Casimir amplitude. This fitting \textit{ansatz} is justified by the following: From fundamental arguments one knows that the order \( O(L^{-1}) \) is absent and the leading order is the order \( O(L^{-2}) \) [5, 8]. Higher orders are caused by corrections to the leading scaling behavior (for details see [30]). Here we restrict ourselves to orders up to \( O(L^{-4}) \). The constant term \( a_0 \) is caused by surface contributions introduced by the considered boundary conditions and is absent in the case of periodic and antiperiodic boundary conditions. The numerical data and the associated fits are shown in Figure 4 and the results for the fitting parameters are assembled in Table I.

Interpreting the fit parameter \( a_2 \) as the Casimir amplitude we estimate the following values:

\[
\begin{align*}
\Delta C_{\text{OO}} &= -0.012(1) \\
\Delta C_{\text{DO}} &= -0.012(3) \\
\Delta C_{\text{DD}} &= -0.012(3)
\end{align*}
\]

where the numbers in brackets give the error bars.

As anticipated the numerical values of the Casimir amplitudes lie all together in a small range. They are equal up to the third decimal place when we take the adjusted error bar into account. We see that due to the fact that the boundary conditions are all in the same surface universality class the evolutions of the excess free energies of the three systems are asymptotically equivalent for large \( L \). Looking at the non-universal corrections to the leading scaling behavior namely the terms of order \( O(1/L^3) \) and \( O(1/L^4) \) we see that their weights are much higher in the DD and DO case compared to the OO case.

We checked the accuracy of our method by computing results for the periodic and the antiperiodic case and comparing them to the analytical results. Our fit parameters are also shown in Fig. I and the numerical result are

| \( a_0 \) | \( a_2 \) | \( a_3 \) | \( a_4 \) |
|---|---|---|---|
| OO | 0.0297 | -0.0122 | 0.0106 | -6.06 |
| DO | -0.0466 | -0.0119 | -2.97 | 441 |
| DD | 0.0309 | -0.0115 | -4.53 | 427 |
| PBC | - | -0.1530 | -1.23 | 51.0 |
| APBC | - | 0.2742 | -27.4 | 3390 |

\textbf{TABLE I}: Fit parameters for the excess free energy, Eq. (4.6). OO means open boundary conditions on both sides, DD means the same with Dirichlet boundary conditions, and DO means the mix of both.
compared to the analytic results in Fig. 5. The analytical results for the Casimir amplitudes [12, 17] are given by

\[ \Delta_{C,\text{PER}} = -\frac{2\zeta(3)}{5\pi} = -0.153 \ldots \]  
\[ \Delta_{C,\text{APER}} = \frac{\text{Cl}_2(\pi/3)}{3} - \frac{\zeta(3)}{6\pi} = 0.274 \ldots . \]

where \( \text{Cl}_2 \) denotes the Clausen function. For the case of periodic boundary conditions we find a perfect agreement with the analytic results. For the case of antiperiodic boundary conditions we find an asymptotic agreement for large \( L \) because there are more corrections due to the inhomogeneity introduced by this boundary condition.

V. SUMMARY AND CONCLUDING REMARKS

We showed a new method for the computation of Casimir amplitudes in the large-\( n \) limit. This method can be applied to the case of slabs with non translationally invariant boundary conditions as well as for those with periodic and antiperiodic boundary conditions. We evaluated the Casimir amplitudes for the cases of Dirichlet-Dirichlet, open-open and Dirichlet-open boundary conditions and reproduced their asymptotical equivalence in the limit of large systems. We find that the non-universal corrections to the leading scaling behavior in the open-open case are much smaller than in the other cases. From this we conclude that evaluations of Casimir amplitudes following our method in this universality class are simpler in this open-open case. We also confirmed the known analytic result for the Casimir amplitudes in the case of periodic and antiperiodic boundary conditions.
FIG. 5: Comparison between analytic and numeric results for periodic and antiperiodic boundary conditions

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[31] ∼ means “asymptotically equal”, i.e. \( f(x) \sim g(x) \Leftrightarrow \lim_{x \to \infty} f(x)/g(x) = 1 \)