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Casimir and Casimir-Polder forces with dissipation from first principles

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We consider Casimir-Polder and Casimir forces with finite dissipation by coupling heat baths to the dipoles introducing, this way, dissipation from first principles. We derive a representation of the free energy as an integral over real frequencies, which can be viewed as an generalization of the remarkable formula introduced by Ford *et al.* [Phys. Rev. Lett. **55**, 2273 (1985)]. For instance, we obtain a nonperturbative representation for the atom-atom and atom-wall interactions. We investigate several limiting cases. From the limit $T \to 0$ we show that the third law of thermodynamics cannot be violated within the given approach, where the dissipation parameter cannot depend on temperature by construction. We conclude that the given approach is insufficient to resolve the thermodynamic puzzle connected with the Drude model when inserted into the Lifshitz formula. Further, we consider the transition to the Matsubara representation and discuss modifications of the contribution from the zeroth Matsubara frequency.

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I. INTRODUCTION

Casimir and Casimir-Polder forces are the basic interaction between single atoms and macroscopic bodies at separations beyond the direct overlap of the electronic wave functions. Their range stretches from a few nanometers until macroscopic separations. In many areas of physics, and beyond, these are ubiquitous. Frequently, these are also called dispersion forces [1]. These forces are due to the quantum electromagnetic interaction between polarizable dipoles formed by the atoms and the polarization inside the bodies. There are several instructive explanations for these forces. One considers the influence of the dipoles or of the bodies on the vacuum of the electromagnetic field, generalizing the notion of zero point energy known long ago in quantum mechanics. The other considers the fluctuations, quantum and thermal, of the electromagnetic field in the presence of the polarizable bodies. The first was pioneered by Casimir for ideally reflecting bodies [2], the second by Lifshitz [3] for polarizable bodies. In a modern view, both have the same origin: the expectation value of the Hamiltonian (or the energy-momentum tensor) of the considered system taken in the vacuum or in a thermal state. Thereby the latter is usually described by the Matsubara formalism.

The dispersion force between macroscopic bodies is most frequently described by the Lifshitz formula (LF) [4]. All other cases can be obtained from here. For instance, for ideal conductors the original Casimir force follows, for rarified media the Casimir-Polder forces for atom-wall or atom-atom interactions follow (see [5] and citations therein). The LF is highly versatile for describing the interaction of real bodies as it uses the reflection coefficients of the bodies and the polarizability of the atoms as input. By using known theoretical models or experimental data for them, nearly any real situation can be handled. An impressive level of precision comparison between theoretical predictions and measurements has been reached [6]. In line with such progress, unresolved problems remained. On the theoretical side these manifest themselves, for instance, in a violation of the third law of thermodynamics (Nernst's heat theorem). As shown first in Ref. [7], inserting the Drude model permittivity into the LF, for a dissipation parameter γ, decreasing with temperature $T \to 0$ faster than the first power, $\gamma \sim T^{\alpha}$ ($\alpha > 1$), at $T = 0$ a nonzero entropy remains (see [6], Sec. II D, for details). On the experimental side, the use of the Drude model permittivity results in theoretical predictions, which are for some configurations in growing disagreement with measurements (see, for instance, [8]). There are similar problems for insulators with dc conductivity. There were also several attempts to resolve these problems, but all were not convincing, eventually.

One of the most controversial points is the question about the validity of the LF with Drude permittivity inserted. A main part of this discussion concerns the assumption of thermodynamic equilibrium assumed in deriving the LF, which may be violated in the case of dissipation of free charge carriers (electrons). On the other side, the LF is formulated in terms of reflection coefficients, which may be derived, or measured, independently. This way, it is not clear whether one is allowed to insert the Drude model permittivity, especially with a temperature-dependent dissipation parameter, into the LF.

In past years, several attempts have been undertaken to reach a derivation of the LF with Drude permittivity from first principles. In fact, this is possible by attaching heat baths (reservoirs) to the oscillators interacting with the electromagnetic field and allows one to generate a Drude permittivity in an effective equation for the electromagnetic field. As a result, the validity of the LF with Drude permittivity inserted could be verified. An early work in this direction was [4]; more recent are [9–13].

In the present paper we consider and then reconsider the heat bath approach. Thereby we give a direct derivation in simple terms of the involved fields and their Green's functions. We arrive at a simple and universal representation for the free energy of the considered configurations. These are atom-atom, atom-wall, and wall-wall configurations at some separation a. The first two are commonly named after Casimir and Polder [14] and the latter corresponds to the Casimir effect [2] and to the LF [3]. For all configurations we end up with a

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representation

$$F = \int_0^\infty \frac{d\omega}{\pi}\left(\frac{\hbar\omega}{2} + k_B T\ln(1-e^{-\beta\hbar\omega})\right)\frac{\partial}{\partial\omega}\delta(\omega) \tag{1}$$

for the free energy, where

$$\delta(\omega) = \frac{-1}{2i}\mathrm{tr}\ln\frac{L(\omega)}{L(\omega)^*} \tag{2}$$

(for details see below) is a kind of phase, the specific expression for depends on the considered configuration. In the case of no dissipation, $\delta(\omega)$ turns into the scattering phase shift (in the case of a continuous spectrum). For a recent example see eq. (96) in [21].

In fact, the representation (1) for the free energy can be viewed as a kind of generalization of the remarkable formula, derived in Ref. [15] for a single oscillator, where the role of $\delta(\omega)$ is played by a generalized susceptibility or the imaginary part of a Green's function. In the literature there are more generalizations and applications; one of the first can be found in Ref. [4], Eq. (16), and a more recent one in Ref. [16], which is in terms of modes.

As concerns the structure of Eq. (1), it must be mentioned that in the case of no dissipation the vacuum energy (at $T = 0$) can be expresses as a sum over modes

$$E_0 = \frac{\hbar}{2}\sum_J \omega_J, \tag{3}$$

where the ω_J are the eigenfrequencies of the Jth mode (dropping any ultraviolet regularization). In the case of a continuous spectrum, the sum must be substituted by a corresponding integral. In equilibrium, and with no losses, these frequencies are real. However, in the case of dissipation, these have an imaginary part and so does the vacuum energy (3), indicating an instability. In this context it is interesting to remark that (1) is an integral over a real variable ω having the meaning of a frequency. However, this frequency is not related to the frequencies ω_J in Eq. (3). Also, the physics behind (1) is different. Equation (1) is derived from the heat bath approach. It assumes the coupling of each oscillator (mode) to a reservoir. As a result, the motion of these oscillators is damped, but the damping is in equilibrium with the driving Langevin force. There are, in addition, the eigenmodes ω_J, but these die out with time and will not contribute in equilibrium. For this reason it would be misleading to call (1) a sum over modes.

Further in the present paper we check the limit of vanishing temperature $T \to 0$ and find in all configurations a decrease of the temperature-dependent part of the free energy $\Delta_T F \sim T^2$ at least, which ensures nonviolation of the third law of thermodynamics. This holds also for the case in which the intrinsic frequency of the oscillators is zero. It must be mentioned that the above-mentioned violation of the third law appears if the dissipation parameter itself depends on temperature $\gamma(T)$ and decreases sufficiently fast. We show that this violation happens in the heat bath approach too. In other words, the heat bath approach does not resolve the violation problem with thermodynamics either. The point is that the dissipation parameter, within the heat bath approach, does not depend on temperature by construction (it may only depend on frequency) and its temperature dependence is alien to this approach. It remains a kind of phenomenological input and does not follow from the first-principles approach taken here. Thus, the solution of the mentioned problem is beyond the approach taken in this paper and further work is necessary.

For the Casimir-Polder configurations we obtain formulas which are nonperturbative in the polarizability α of the dipole(s). The commonly considered case of large separations or small polarizability is then obtained by expansion in powers of α or $1/a$. This expansion has a finite radius of convergence which is determined by the onset of instability when decreasing the separation a. This instability corresponds to the spontaneous creation of photons. We assume that the corresponding states are occupied and exclude them from the statistical ensemble when doing the thermal averaging. A nonperturbative approach to the Casimir-Polder force, using a diagonalization of the corresponding Hamiltonian, was developed in Ref. [17], where also possible applications were discussed. Another nonperturbative approach to the Casimir-Polder force was taken in Ref. [18], where also a discussion of the instability was included. In electrodynamics, for the interaction of atoms, the instability would appear for separations a of order of the size of atoms, $a \sim \alpha^{-1/3}$, which is beyond the applicability of the dipole approximation. To conclude this topic, we mention that such an instability does not appear in the LF.

Further, in the present paper, we consider the transition from the representation (1) of the free energy to the Matsubara representation. This can be done by a kind of Wick rotation. For parameters, keeping the considered configuration below criticality and giving $L(0)$ a finite value, we obtain in each case the usual Matsubara representation. For the other cases we observe a transmutation of the contribution from the zeroth Matsubara frequency into a logarithmic term and an additional term in the case of criticality. Thereby we pay special attention to the case of vanishing intrinsic frequency of the oscillators and discuss the resulting modifications of the results.

Finally, in the present paper, we consider the relation of the considered model with the plasma model. As known, the permittivity of the plasma model follows from that of the Drude model by formally setting the dissipation parameter to zero $\gamma = 0$, whereas the free energy does not turn into that of the plasma model for $\gamma \to 0$. The difference can be traced back to contributions in Eq. (1) with ω, which are smaller than the frequencies in the spectrum of the modes of the plasma model.

Throughout the paper three- and two-dimensional vectors and matrices are denoted by bold letters. For instance, the coordinate is $\boldsymbol{x} = (x,y,z) = (\boldsymbol{x}_\parallel, z)$, where $\boldsymbol{x}_\parallel$ is a vector in the plane of an interface. We use units with $\hbar = c = k_B = 1$. We reserve the notation $\delta(\omega)$ for what is called phase in this paper. Spatial delta functions are always denoted by $\delta^{(1)}(x)$ or $\delta^{(3)}(\boldsymbol{x})$, in dependence on the dimensionality.

II. MODEL, BASIC FORMULAS, AND CONFIGURATIONS

In this section we collect the basic formulas for the considered model and configurations.

A. Model

The model consists of polarizable atoms and their interaction with the electromagnetic field and with heat baths. From the Maxwell equations we have

$$\left(\partial_t^2-\Delta+\nabla\circ\nabla\right)\boldsymbol{E}(t,\boldsymbol{x})=4\pi\,\partial_t\,\boldsymbol{j}(t,\boldsymbol{x}) \tag{4}$$

as the equation for the electric field in dyadic notation with the current density $\boldsymbol{j}(\boldsymbol{x})$ as the source. The magnetic field follows with rot$\boldsymbol{E}=-\partial_t\boldsymbol{B}$. The atoms are described by point dipoles and the interaction is taken in the dipole approximation. The ith atom is described by a dipole with the charge e at location $\boldsymbol{x}=\boldsymbol{a}_i$ and the displacement $\boldsymbol{\xi}_i(t)$ of its charge. Its dipole moment is $\boldsymbol{p}_i(t)=e\boldsymbol{\xi}_i(t)$ and this dipole is equipped with the dynamics of a harmonic oscillator

$$m\left(\partial_t^2+\gamma\partial_t+\Omega^2\right)\boldsymbol{\xi}_i(t)=e\boldsymbol{E}(t,\boldsymbol{a}_i)+\boldsymbol{F}_i(t), \tag{5}$$

where Ω is the intrinsic frequency of the oscillator, γ is the damping constant, and $\boldsymbol{F}(t)$ is the Langevin force. The current density generated by the atoms is

$$\boldsymbol{j}(t,\boldsymbol{x})=e\partial_t\sum_i\boldsymbol{\xi}_i(t)\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i). \tag{6}$$

The considered system has a Lagrangian

$$\begin{aligned}\mathcal{L}=&\int d\boldsymbol{x}\,\frac{1}{8\pi}[\boldsymbol{E}(t,\boldsymbol{x})^2-\boldsymbol{B}(t,\boldsymbol{x})^2]\\&+\sum_i\frac{m}{2}[\dot{\boldsymbol{\xi}}_i(t)^2-\Omega^2\boldsymbol{\xi}_i(t)^2]+\sum_i\boldsymbol{p}_i(t)\boldsymbol{E}(t,\boldsymbol{a}_i),\end{aligned} \tag{7}$$

where we did not show the heat bath part, and the classical energy is given by

$$E=E_{\mathrm{ED}}+E_{\mathrm{dipole}}, \tag{8}$$

with

$$\begin{aligned}E_{\mathrm{ED}}&=\frac{1}{8\pi}\int d^3\boldsymbol{x}[\boldsymbol{E}(t,\boldsymbol{x})^2+\boldsymbol{B}(t,\boldsymbol{x})^2],\\E_{\mathrm{dipole}}&=\sum_i\frac{m}{2}[\dot{\boldsymbol{\xi}}_i(t)^2+\Omega^2\boldsymbol{\xi}_i(t)^2]\end{aligned} \tag{9}$$

[see [19], p. 334, or [20], Eq. (9.37)]. The heat bath part, which we do not show here, as well as how it results in the damping term and the Langevin forces, was discussed in detail in the scalar example in Ref. [21] and also elsewhere in literature (see, for example, [22]). From the above Lagrangian (including the heat bath part), the equations of motion, Eqs. (4) and (5) for field and the oscillators, and the equations for the bath variables as well, can be derived. This way, the approach starts from first principles.

Since our setup keeps the translation invariance in time, it is meaningful to apply the Fourier transform in time. For the electric field we have

$$\begin{aligned}\boldsymbol{E}(t,\boldsymbol{x})&=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\tilde{\boldsymbol{E}}_\omega(\boldsymbol{x}),\\\tilde{\boldsymbol{E}}_\omega(\boldsymbol{x})&=\int_{-\infty}^{\infty}dt\,e^{i\omega t}\boldsymbol{E}(t,\boldsymbol{x}),\end{aligned} \tag{10}$$

and similar for all other time-dependent quantities. The transformed quantities are always denoted by a tilde. After the Fourier transform (10), we get from Eq. (4) for the electric field and from Eq. (5) for the displacements the set of equations

$$\begin{aligned}(-\omega^2-\Delta+\nabla\circ\nabla)\tilde{\boldsymbol{E}}_\omega(\boldsymbol{x})&=4\pi e\omega^2\sum_i\tilde{\boldsymbol{\xi}}_{\omega,i}\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i),\\m(-\omega^2-i\gamma\omega+\Omega^2)\tilde{\boldsymbol{\xi}}_{\omega,i}&=e\tilde{\boldsymbol{E}}_\omega(\boldsymbol{a}_i)+\tilde{\boldsymbol{F}}_{\omega,i},\end{aligned} \tag{11}$$

which is the starting point for the following.

As said above, we assume an individual continuous heat bath coupled to each oscillator. As known, a heat bath, or reservoir, can be represented as a continuous set of harmonic oscillators. In simple terms this procedure is described in detail for a one-dimensional case in Ref. [21]. In [23], the most general formulation and its relation to the oscillator model are discussed along with different couplings between the bath and oscillator. The procedure goes as follows. First one solves the Heisenberg equation of motion of the bath operators. As a result, in the equations of motions of the dipole oscillators [the second of Eqs. (11)], the friction term $-i\gamma\omega$ and the Langevin force $\tilde{\boldsymbol{F}}_{\omega,i}$, on the right side, appear. The damping parameter γ may depend on frequency, being a positive function, but we restrict ourselves to a constant $\gamma>0$. The Langevin force $\tilde{\boldsymbol{F}}_\omega$ can be expressed in terms of the heat bath operators. Here we need only their thermal averages

$$\langle\tilde{\boldsymbol{F}}_{\omega,i}\tilde{\boldsymbol{F}}_{\omega',j}\rangle=\frac{\gamma m\omega}{\pi}\delta(\omega+\omega')\delta_{ij}\coth\frac{\beta\omega}{2}. \tag{12}$$

Below we consider the following thermodynamic potentials. The internal energy U is the thermal average of the Hamiltonian (6),

$$U=\langle H\rangle. \tag{13}$$

It will be calculated by solving Eqs. (4) and (5) for the corresponding configuration, expressing the electric field and the displacement fields in terms of the Langevin forces and using the averages (12). Further, by means of the thermodynamic relations

$$U=\frac{\partial}{\partial\beta}(\beta F),\quad S=-\frac{\partial}{\partial T}F, \tag{14}$$

the free energy F and the entropy S can be calculated.

B. Solutions for the electric field and the displacements

In this section we solve the system (11). As discussed in Ref. [21], two ways are possible. The first starts with solving first the equation for the displacements, the second of Eqs. (11), which then will be inserted into the equation for the electric field, the first of Eqs. (11). The second way, which we will follow now, goes in inverse order. We start by solving the equation for the electric field from (11),

$$\tilde{\boldsymbol{E}}_\omega(\boldsymbol{x})=4\pi e\omega^2\sum_i\boldsymbol{G}_\omega^{(0)}(\boldsymbol{x}-a_i)\tilde{\boldsymbol{\xi}}_{\omega,i}, \tag{15}$$

where we introduced the free-space Green's function $\boldsymbol{G}_\omega^{(0)}(\boldsymbol{x})$, obeying the equation

$$(-\omega^2-\Delta+\nabla\circ\nabla)\boldsymbol{G}_\omega^{(0)}(\boldsymbol{x}-\boldsymbol{x}')=\delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}'). \tag{16}$$

It has the representation

$$\boldsymbol{G}_\omega^{(0)}(\boldsymbol{x})=\left(1+\frac{\nabla\circ\nabla}{\omega^2}\right)G_\omega^{(0)}(\boldsymbol{x}), \tag{17}$$

where $G^{(0)}_\omega(\boldsymbol{x})$ is the scalar Green's function

$$G^{(0)}_\omega(\boldsymbol{x}) = \int \frac{d\boldsymbol{k}}{(2\pi)^3}\,\frac{e^{i\boldsymbol{k}\boldsymbol{x}}}{-\omega^2+\boldsymbol{k}^2+i0} = \frac{e^{i\omega|\boldsymbol{x}|}}{4\pi|\boldsymbol{x}|}. \tag{18}$$

Carrying out the derivatives in Eq. (68), we get

$$\boldsymbol{G}^{(0)}_\omega(\boldsymbol{x}) = \left(\boldsymbol{A} - \frac{1-i\omega|\boldsymbol{x}|}{(\omega|\boldsymbol{x}|)^2}\boldsymbol{B}\right)\frac{e^{i\omega|\boldsymbol{x}|}}{4\pi|\boldsymbol{x}|}, \tag{19}$$

with

$$\boldsymbol{A} = 1 - \frac{\boldsymbol{x}\circ\boldsymbol{x}}{|\boldsymbol{x}|^2}, \quad \boldsymbol{B} = 1 - 3\frac{\boldsymbol{x}\circ\boldsymbol{x}}{|\boldsymbol{x}|^2}. \tag{20}$$

Equation (19) is the well-known retarded potential of a dipole.

The solution (15) for the electric field can be inserted into the second equation in Eq. (11), which gives

$$\sum_j \left[m(-\omega^2 - i\gamma\omega + \Omega^2)\delta_{ij} - 4\pi e^2\omega^2\boldsymbol{G}^{(0)}_\omega(\boldsymbol{a}_i-\boldsymbol{a}_j)\right]\tilde{\boldsymbol{\xi}}_{\omega,j} = \tilde{\boldsymbol{F}}_{\omega,i}. \tag{21}$$

This is an algebraic equation. Its solution can be written in the form

$$\tilde{\boldsymbol{\xi}}_{\omega,i} = \frac{1}{mN(\omega)}\sum_j \boldsymbol{L}^{-1}_{ij}(\omega)\tilde{\boldsymbol{F}}_{\omega,j}, \tag{22}$$

where $\boldsymbol{L}^{-1}_{ij}(\omega)$ is the inverse of

$$\boldsymbol{L}_{ij}(\omega) = \delta_{ij} - \alpha(\omega)\omega^2\boldsymbol{G}^{(0)}_\omega(\boldsymbol{a}_i-\boldsymbol{a}_j) \tag{23}$$

and where we defined

$$N(\omega) = -\omega^2 - i\gamma\omega + \Omega^2, \quad \alpha(\omega) = \frac{4\pi e^2}{mN(\omega)}. \tag{24}$$

Finally, we insert (22) into (15),

$$\tilde{\boldsymbol{E}}_\omega(\boldsymbol{x}) = \frac{\alpha(\omega)\omega^2}{e}\sum_{i,j}\boldsymbol{G}^{(0)}_\omega(\boldsymbol{x}-\boldsymbol{a}_i)\boldsymbol{L}^{-1}_{ij}(\omega)\tilde{\boldsymbol{F}}_{\omega,j}, \tag{25}$$

and have with Eqs. (22) and (25) the solutions of the inhomogeneous equations (11) for the displacements and for the electric field, expressed in terms of the Langevin forces.

For the relation of the free energy with the vacuum energy, which will be discussed below, it is meaningful to consider the first way too. We solve the second equation in Eq. (11),

$$\tilde{\boldsymbol{\xi}}_{\omega,i} = \frac{1}{mN(\omega)}[e\tilde{\boldsymbol{E}}_\omega(\boldsymbol{a}_i) + \tilde{\boldsymbol{F}}_{\omega,i}], \tag{26}$$

and insert the result into the first equation,

$$\left(-\omega^2 - \Delta + \nabla\circ\nabla - \alpha(\omega)\omega^2\sum_i\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i)\right)\tilde{\boldsymbol{E}}_\omega(\boldsymbol{x}) = \frac{\alpha(\omega)\omega^2}{e}\sum_i\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i)\tilde{\boldsymbol{F}}_{\omega,i}\,. \tag{27}$$

This is an effective equation for the electric field. It is like a Schrödinger equation with δ-function potentials. This problem, especially equations like (27), were recently discussed in Ref. [24]. The δ functions in this equation are three dimensional and therefor the equation is ill defined. All known methods to handle this situation were discussed in Ref. [24]. In terms of electrodynamics, one needs to exclude from the solution of Eq. (27) the action of the electric field created from a dipole acting on the dipole itself, i.e., its self-field. With these remarks, Eq. (27) can be easily solved. For that we introduce the corresponding Green's function $\boldsymbol{G}_\omega(\boldsymbol{x},\boldsymbol{x}')$, obeying

$$\left(-\omega^2 - \Delta + \nabla\circ\nabla - \alpha(\omega)\omega^2\sum_i\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i)\right)\boldsymbol{G}_\omega(\boldsymbol{x},\boldsymbol{x}') = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}'). \tag{28}$$

This Green's function is related to the T operator by

$$\boldsymbol{G}_\omega(\boldsymbol{x},\boldsymbol{x}') = \boldsymbol{G}^{(0)}_\omega(\boldsymbol{x}-\boldsymbol{x}') + \sum_{i,j}\boldsymbol{G}^{(0)}_\omega(\boldsymbol{x}-\boldsymbol{a}_i) \times \boldsymbol{T}_{ij}(\omega)\boldsymbol{G}^{(0)}_\omega(\boldsymbol{a}_j-\boldsymbol{x}'), \tag{29}$$

with the free Green's function defined in Eq. (16). Inserting (29) into (28), one obtains the equation

$$\sum_k\left[\delta_{ij} - \alpha(\omega)\omega^2\boldsymbol{G}^{(0)}_\omega(\boldsymbol{a}_i-\boldsymbol{a}_k)\right]\boldsymbol{T}_{kj}(\omega) = \alpha(\omega)\omega^2\delta_{ij} \tag{30}$$

for the T operator. Returning to Eq. (23), we note its relation to the $\boldsymbol{L}_{ij}(\omega)$,

$$\boldsymbol{T}_{ij}(\omega) = \alpha(\omega)\omega^2\boldsymbol{L}^{-1}_{ij}(\omega), \tag{31}$$

which allows for the expression

$$\begin{aligned}\tilde{\boldsymbol{E}}_\omega(\boldsymbol{x}) &= \frac{1}{e}\sum_{i,jj}\boldsymbol{G}^{(0)}_\omega(\boldsymbol{x},\boldsymbol{a}_i)\boldsymbol{T}_{ij}(\omega)\tilde{\boldsymbol{F}}_{\omega,j},\\ \tilde{\boldsymbol{\xi}}_{\omega,i} &= \frac{1}{4\pi e^2\omega^2}\sum_j\boldsymbol{T}_{ij}(\omega)\tilde{\boldsymbol{F}}_{\omega,j}\end{aligned} \tag{32}$$

of the electric field and the displacements in terms of the T operator.

These formulas will represent the correct solution only if we account for the remark on the self-field. It can be excluded by writing the T operator in the form

$$T^{-1}_{ij}(\omega) = \frac{1}{\alpha(\omega)\omega^2}\left[\delta_{ij} - \alpha(\omega)\omega^2\boldsymbol{G}^{(0)}_{\omega,ij}\right], \tag{33}$$

where

$$\boldsymbol{G}^{(0)}_{\omega,ij} = \begin{cases}0, & i=j\\ \boldsymbol{G}^{(0)}_\omega(\boldsymbol{a}_i-\boldsymbol{a}_j), & i\neq j,\end{cases} \tag{34}$$

i.e., where the diagonal terms were dropped. This way, Eqs. (32) and (33) describe the solutions for the electric field and for the displacements in the case of dissipation.

C. Thermal averages and the free energy

In this section we calculate the internal energy U by taking the thermal averages of the Hamiltonian (8). We insert (32) and use the averages (12). In these averages we have to insert the corresponding time-dependent quantities, i.e., we have to go back using (10). Now suppose a field $A(t)$ has the Fourier representation

$$\hat{A}(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\sum_i h_i(\omega)\tilde{\boldsymbol{F}}_{\omega,i}. \tag{35}$$

The corresponding thermal average, using (12), is then

$$\begin{aligned}\langle \hat{A}(t)\hat{A}(t)\rangle &= \int_0^\infty \frac{d\omega}{2\pi}\int_0^\infty \frac{d\omega'}{2\pi} e^{i(\omega+\omega')t}\\ &\quad\times \sum_{i,j} h_i(\omega)h_j(\omega')\langle \tilde{\boldsymbol{F}}_{\omega,i}\tilde{\boldsymbol{F}}_{\omega',j}\rangle\\ &= \int_0^\infty \frac{d\omega}{\pi}\,\gamma m\hbar\omega \coth\frac{\beta\omega}{2}\sum_i h_i(\omega)h_i(-\omega).\end{aligned} \tag{36}$$

With these formulas, substituting $h_i(\omega) \to \frac{1}{e}\sum_i \boldsymbol{G}^{(0)}_\omega(\boldsymbol{x},\boldsymbol{a}_j)\boldsymbol{T}_{ji}(\omega)$ for the electric field and $\alpha_i(\omega) \to \frac{1}{m\omega_p^2\omega^2}\boldsymbol{T}_{ji}(\omega)$ for the displacement field, we get

$$U = \int_0^\infty \frac{d\omega}{\pi}\,\gamma m\omega \coth\frac{\beta\omega}{2}\sum_i M_{ii}, \tag{37}$$

with

$$\begin{aligned}M_{ij} &= \mathrm{tr}\sum_{k,l} \boldsymbol{T}_{ik}(\omega)\bigg[\frac{1}{8\pi e^2}\int d\boldsymbol{x}\,\boldsymbol{G}^{(0)}_\omega(\boldsymbol{a}_k,\boldsymbol{x})\\ &\quad\times\left(1+\frac{-\Delta+\nabla\circ\nabla}{\omega^2}\right)\boldsymbol{G}^{(0)}_\omega(\boldsymbol{x},\boldsymbol{a}_l)\\ &\quad+\frac{m}{2}\frac{\omega^2+\Omega^2}{(4\pi e^2\omega^2)^2}\delta_{kl}\bigg]\boldsymbol{T}_{lj}(-\omega),\end{aligned} \tag{38}$$

and the trace is over the spatial structure. In the first term, which results from E_{ED} [Eq. (9)], the second term in the square bracket results from the magnetic field.

The first term in Eq. (38) can be simplified by taking the Green's functions in the momentum representation (17) and (18),

$$\begin{aligned}&\int d\boldsymbol{x}\,\boldsymbol{G}^{(0)}_\omega(\boldsymbol{a}_k,\boldsymbol{x})\left(1+\frac{-\Delta+\nabla\circ\nabla}{\omega^2}\right)\boldsymbol{G}^{(0)}_\omega(\boldsymbol{x},\boldsymbol{a}_l)\\ &\quad= \int \frac{d\boldsymbol{k}}{(2\pi)^3}\, e^{i\boldsymbol{k}(\boldsymbol{a}_k-\boldsymbol{a}_l)}m(k)\\ &\quad= \frac{1}{\omega^4}(-1+\omega\partial_\omega)\omega^2\boldsymbol{G}^{(0)}_\omega(\boldsymbol{a}_k-\boldsymbol{a}_l),\end{aligned} \tag{39}$$

where we used the calculation

$$\begin{aligned}m(k) &= \frac{1-\frac{\boldsymbol{k}\circ\boldsymbol{k}}{\omega^2}}{-\omega^2+k^2+i0}\left(1+\frac{k^2-\boldsymbol{k}\circ\boldsymbol{k}}{\omega^2}\right)\frac{1-\frac{\boldsymbol{k}\circ\boldsymbol{k}}{\omega^2}}{-\omega^2+k^2+i0}\\ &= \frac{1}{\omega^4}(-1+\omega\partial_\omega)\omega^2\frac{1-\frac{\boldsymbol{k}\circ\boldsymbol{k}}{\omega^2}}{-\omega^2+k^2+i0},\end{aligned} \tag{40}$$

carried out in momentum space. Inserting (39) into (38) delivers

$$\begin{aligned}M_{ij} &= \frac{1}{2m\left(\omega_p^2\omega^2\right)^2}\,\mathrm{tr}\sum_{k,l}\boldsymbol{T}_{ik}(\omega)\big[(\omega^2+\Omega^2)\delta_{kl}\\ &\quad+\omega_p^2(-1+\omega\partial_\omega)\omega^2\boldsymbol{G}^{(0)}_{\omega,ij}\big]\boldsymbol{T}_{lj}(-\omega),\end{aligned} \tag{41}$$

where we used (34) to exclude the self-field. At this point it is meaningful to switch completely to matrix notation. We have to pay attention to the fact that we have two matrix structures, one structure resulting from the dipoles, corresponding to the indices i and j, and a 3×3 structure resulting from the spatial structures and that we must consider their tensor product. Matrixes in the corresponding space are denoted by a circumflex. In this sense, Eq. (41) can be written in the form

$$\begin{aligned}\sum_i M_{ii} &= \frac{m}{2(4\pi e^2\omega^2)^2}\mathrm{tr}\hat{\boldsymbol{T}}(\omega)\big[\omega^2+\Omega^2\\ &\quad+\omega_p^2(-1+\omega\partial_\omega)\omega^2\hat{\boldsymbol{G}}^{(0)}_\omega\big]\hat{\boldsymbol{T}}(-\omega),\end{aligned} \tag{42}$$

where the trace is now over the whole space.

The expression (42) can be rewritten in a more compact form. From (31) and (23), we can write the inverse of the T operator in the form

$$\frac{4\pi e^2}{m}\omega^2\hat{\boldsymbol{T}}^{-1}(\omega) = -\omega^2 - i\gamma\omega + \Omega^2 - \frac{4\pi e^2}{m}\omega^2\hat{\boldsymbol{G}}^{(0)}_\omega \tag{43}$$

and for its derivative

$$\partial_\omega\left(\frac{4\pi e^2}{m}\omega^2\hat{\boldsymbol{T}}^{-1}(\omega)\right) = -2\omega - i\gamma - \frac{4\pi e^2}{m}\partial_\omega\left(\omega^2\hat{\boldsymbol{G}}^{(0)}_\omega\right) \tag{44}$$

holds. We compose

$$\begin{aligned}&\partial_\omega\left(\frac{4\pi e^2}{m}\omega^2\hat{\boldsymbol{T}}^{-1}(\omega)\right)\left(\frac{4\pi e^2}{m}\omega^2\hat{\boldsymbol{T}}^{-1}(-\omega)\right)\\ &\quad-\left(\frac{4\pi e^2}{m}\omega^2\hat{\boldsymbol{T}}^{-1}(\omega)\right)\partial_\omega\left(\frac{4\pi e^2}{m}\omega^2\hat{\boldsymbol{T}}^{-1}(-\omega)\right)\\ &\quad= -2i\gamma\left[\omega^2+\Omega^2-\frac{4\pi e^2}{m}(-1+\omega\partial_\omega)\left(\omega^2\hat{\boldsymbol{G}}^{(0)}_\omega\right)\right].\end{aligned} \tag{45}$$

This relation allows us to represent $\sum_i M_{ii}$ [Eq. (42)] in the form

$$\sum_i M_{ii} = \frac{1}{2m\gamma}\delta(\omega), \tag{46}$$

with

$$\delta(\omega) = \frac{1}{2i}\mathrm{tr}\ln\frac{\hat{\boldsymbol{T}}(\omega)}{\hat{\boldsymbol{T}}(-\omega)}. \tag{47}$$

This way, from (37) we get, for the internal energy,

$$U = \frac{1}{2}\int_0^\infty \frac{d\omega}{\pi}\,\omega\coth\frac{\beta\omega}{2}\,\partial_\omega\delta(\omega) \tag{48}$$

and, using (14), for the free energy

$$F = \int_0^\infty \frac{d\omega}{\pi}\left(\frac{\omega}{2}+T\ln(1-e^{-\beta\omega})\right)\partial_\omega\delta(\omega). \tag{49}$$

With Eqs. (49) and (47), we have a representation of the free energy in terms of the T operator related to the effective equation (28) for the electric field.

On a formal level (at least), it is possible to establish also a relation to the Green's function $\boldsymbol{G}_\omega(\boldsymbol{x},\boldsymbol{x}')$, defined by Eq. (28). In matrix notation, we have from (28) a formal solution

$$\hat{\boldsymbol{G}}_\omega = \hat{\boldsymbol{G}}^{(0)}_\omega\left(1-\hat{\boldsymbol{V}}\hat{\boldsymbol{G}}^{(0)}_\omega\right)^{-1} = \hat{\boldsymbol{G}}^{(0)}_\omega\left[1+\hat{\boldsymbol{T}}(\omega)\hat{\boldsymbol{G}}^{(0)}_\omega\right], \tag{50}$$

where the last equality follows from (29). Written in matrix form, Eq. (30) reads $(1-\hat{\boldsymbol{V}}\hat{\boldsymbol{G}}^{(0)}_\omega)\hat{\boldsymbol{T}} = \hat{\boldsymbol{V}}$ and can be rewritten in the form

$$\hat{\boldsymbol{V}}\left[1+\hat{\boldsymbol{G}}^{(0)}_\omega\hat{\boldsymbol{T}}(\omega)\right] = \hat{\boldsymbol{T}}. \tag{51}$$

The potential $\hat{\boldsymbol{V}}$ is in our case $V(\boldsymbol{x}) = \alpha(\omega)\omega^2 \sum_i \delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i)$, which was the result of the interaction with the dipoles. Now we use the chain of relations

$$\begin{aligned}\operatorname{tr}\ln \hat{\boldsymbol{T}}(\omega) &= \operatorname{tr}\ln \hat{\boldsymbol{V}}\big[1+\hat{\boldsymbol{G}}^{(0)}_{\omega}\hat{\boldsymbol{T}}(\omega)\big]\\ &= \operatorname{tr}\ln \hat{\boldsymbol{G}}_{\omega} - \operatorname{tr}\ln \hat{\boldsymbol{G}}^{(0)}_{\omega} + \operatorname{tr}\ln \hat{\boldsymbol{V}}.\end{aligned} \tag{52}$$

On the formal level, we did not care about the existence of the individual contributions, especially about the ultraviolet divergences which are there. Next we drop the last two terms as giving a constant contribution to the free energy. This is justified, especially if we have in mind as the final goal the Casimir or Casimir-Polder forces. If doing so, we can write, in place of (47),

$$\delta(\omega) = \frac{1}{2i}\operatorname{tr}\ln\frac{\hat{\boldsymbol{G}}_{\omega}}{\hat{\boldsymbol{G}}_{-\omega}}. \tag{53}$$

Also, provided $\hat{\boldsymbol{G}}_{-\omega} = \hat{\boldsymbol{G}}^{*}_{\omega}$ holds, a further rewriting delivers

$$\delta(\omega) = \operatorname{Im}\operatorname{tr}\ln \hat{\boldsymbol{G}}_{\omega}. \tag{54}$$

Inserted into the free energy (49), the relation to the remarkable formula, mentioned in the Introduction, is more direct.

D. Configurations considered

We are going to apply the formulas developed above for a generic collection of dipoles, represented by their displacements $\tilde{\boldsymbol{\xi}}_{\omega,i}$, to three specific configurations, which we describe in this section. These configurations are the following.

The atom-atom (AA) configuration. Here we consider two atoms at positions $\boldsymbol{a}_i$ $(i=1,2)$. Each atom is modeled as a dipole with dipole moment $\boldsymbol{p}_i(t) = e\boldsymbol{\xi}_i(t)$ and has its own displacement vector $\boldsymbol{\xi}_i(t)$ $(i=1,2)$. The corresponding current density is

$$\boldsymbol{j}(\boldsymbol{x}) = e\sum_{i=1}^{2}\partial_t\boldsymbol{\xi}_i(t)\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i). \tag{55}$$

This is basically the same equation as (6), only the index i is now restricted to $i=1,2$. In a similar way, we get, for Eqs. (11),

$$\begin{aligned}(-\omega^2-\Delta+\nabla\circ\nabla)\tilde{\boldsymbol{E}}_{\omega}(\boldsymbol{x}) &= 4\pi e\omega^2\sum_{i=1}^{2}\tilde{\boldsymbol{\xi}}_{\omega,i}\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i),\\ m(-\omega^2-i\gamma\omega+\Omega^2)\tilde{\boldsymbol{\xi}}_{\omega,i} &= e\tilde{\boldsymbol{E}}_{\omega}(\boldsymbol{a}_i)+\tilde{\boldsymbol{F}}_{\omega,i}\quad (i=1,2).\end{aligned} \tag{56}$$

At this point we mention that, in general, the parameters of the atoms, for instance, their intrinsic frequency Ω or their mass, can be chosen individually for each. However, in order to keep formulas as simple as possible, we take these parameters to be equal for both atoms and do the same in the other configurations too.

The atom-wall (AW) configuration. For the atom we have a single dipole, which we give the number $i=0$, at location $\boldsymbol{a}_0$ with $a_z>0$, i.e., in the half space above the (x,y) plane, and with displacement $\boldsymbol{\xi}_0(t)$. We give its parameters entering (24) an index 0, i.e., we use γ_0, Ω_0, and $\omega_{p,0}$. For the wall we assume a collection of dipoles with $i=1,2,\ldots$, which are distributed homogeneously in the half space $z<0$, i.e., below the (x,y) plane. Further, we increase their density to form a continuous distribution of dipoles such that their displacements turn into a displacement field $\boldsymbol{\xi}_i(t)\to\boldsymbol{\xi}(t,\boldsymbol{x})$. Accordingly, the dipole moments turn into a continuous polarization $\boldsymbol{p}_i(t)\to\boldsymbol{p}(t,\boldsymbol{x})$. In all formulas for this transition we use

$$\begin{aligned}&\boldsymbol{a}_i\to\boldsymbol{x},\quad \sum_{i=1}^{\infty}\to\rho\int d\boldsymbol{x}\,\Theta(-z),\\ &\delta_{ij}\to\rho\delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}'),\end{aligned} \tag{57}$$

where ρ is the density (number per unit volume) of the dipoles in the wall. In this configuration, the equations for the electric field and for the displacements are, again after Fourier transform in time,

$$\begin{aligned}(-\omega^2-\Delta+\nabla\circ\nabla)\tilde{\boldsymbol{E}}_{\omega}(\boldsymbol{x}) &= 4\pi e\omega^2\tilde{\boldsymbol{\xi}}_{\omega,0}\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_0)\\ &\quad +4\pi e\rho\omega^2\tilde{\boldsymbol{\xi}}_{\omega}(\boldsymbol{x})\Theta(-z),\\ m\big(-\omega^2-i\gamma_0\omega+\Omega_0^2\big)\tilde{\boldsymbol{\xi}}_{\omega,0} &= e\tilde{\boldsymbol{E}}_{\omega}(\boldsymbol{a}_0)+\tilde{\boldsymbol{F}}_{\omega,0},\\ m(-\omega^2-i\gamma\omega+\Omega^2)\tilde{\boldsymbol{\xi}}_{\omega}(x) &= e\tilde{\boldsymbol{E}}_{\omega}(\boldsymbol{x})+\tilde{\boldsymbol{F}}_{\omega}(x)\quad (z<0),\end{aligned} \tag{58}$$

which in fact constitute a special case of (11). Again, we have a Langevin force $\tilde{\boldsymbol{F}}_{\omega,0}$ for the atom and a continuum of these $\tilde{\boldsymbol{F}}_{\omega}(\boldsymbol{x})$ for the polarization of the medium.

The wall-wall (WW) configuration. Here we assume two half spaces, one at $z<0$ and the other at $z>a$, both filled with a medium having the same properties as in the AW configuration. The displacement field $\tilde{\boldsymbol{\xi}}_{\omega}(\boldsymbol{x})$ exists in the two half spaces $z<0$ and $z>a$. The gap between the half spaces has width a and is assumed to be empty. Equations (11) take here the form

$$\begin{aligned}&(-\omega^2-\Delta+\nabla\circ\nabla)\tilde{\boldsymbol{E}}_{\omega}(\boldsymbol{x})\\ &\quad = 4\pi e\rho\omega^2\tilde{\boldsymbol{\xi}}_{\omega}(\boldsymbol{x})[\Theta(-z)+\Theta(z-a)],\\ &m(-\omega^2-i\gamma\omega+\Omega^2)\tilde{\boldsymbol{\xi}}_{\omega}(x)\\ &\quad = e\tilde{\boldsymbol{E}}_{\omega}(\boldsymbol{x})+\tilde{\boldsymbol{F}}_{\omega}(x)\quad (z<0,\ z>a)\end{aligned} \tag{59}$$

and $\tilde{\boldsymbol{F}}_{\omega}(x)$ is the continuum of the Langevin forces.

The first two configurations AA and AW correspond to the Casimir-Polder force [14] and the third one WW corresponds to the Casimir effect [2] for ideal conductors and [3] for dielectric slabs.

III. ATOM-ATOM CONFIGURATION

In this section we investigate in detail the AA configuration, i.e., the interaction of two dipoles at separation $a=|\boldsymbol{a}_1-\boldsymbol{a}_2|$, as introduced in Sec. II D. The relevant equations are (56). The calculation of the free energy goes literally the same way as in Sec. II C, with the restriction of the indices to the values $i=1,2$. This way, the free energy is given by (49) and (47), together with (31) and (23). With these formulas we express $\delta(\omega)$ in the form

$$\delta(\omega) = \frac{-1}{2i}\operatorname{tr}\ln\frac{\hat{\boldsymbol{L}}(\omega)}{\hat{\boldsymbol{L}}(-\omega)}, \tag{60}$$

which is rewritten as compared to (47) using (31), dropping contributions, which do not depend on the separation between the atoms. The matrix $\hat{\boldsymbol{L}}(\omega)$ is now 2×2 in the indices i and j and, using (33), it can be rewritten in the form

$$\hat{\boldsymbol{L}}(\omega) = 1 - \alpha(\omega)\omega^2 \boldsymbol{\sigma}_1 \boldsymbol{G}^{(0)}_\omega, \tag{61}$$

where with (34) we defined $\boldsymbol{G}^{(0)}_\omega = \boldsymbol{G}^{(0)}_{\omega,12}$ (i.e., excluding the self-field) and $\boldsymbol{\sigma}_1 = \left(\begin{smallmatrix}0,1\\1,0\end{smallmatrix}\right)$.

The trace in Eq. (60) can be calculated in two steps. First, we consider the 2×2 structure related to the two atoms. It gives simply

$$\operatorname{tr}\ln \hat{\boldsymbol{L}}(\omega) = \sum_{\sigma=\pm 1} \operatorname{tr}\ln\left[1 - \sigma\alpha(\omega)\omega^2 \boldsymbol{G}^{(0)}_\omega\right]. \tag{62}$$

The terms with $\sigma = \pm 1$ correspond to symmetric and antisymmetric solutions of Eq. (27), which is a result of the symmetry under exchanging the two dipoles. In (62), the remaining trace is over the spatial 3×3 structure. Now $\boldsymbol{G}^{(0)}_\omega$ is given by (18) with $\boldsymbol{x} = \boldsymbol{a}_1 - \boldsymbol{a}_2$ and we can use the explicit formula (19) with $|\boldsymbol{x}| = a$. For the trace we use the formula

$$\operatorname{tr}\ln(1 + p\boldsymbol{A} + q\boldsymbol{B}) = 2\ln(1 + p + q) + \ln(1 - 2q), \tag{63}$$

where p and q are some numbers and $\boldsymbol{A}$ and $\boldsymbol{B}$ are the matrices given by (20). This way, and carrying out the sum over $\sigma = \pm 1$, we get

$$\delta(\omega) = 2\delta_1(\omega) + \delta_2(\omega), \tag{64}$$

with

$$\delta_i(\omega) = \frac{-1}{2i} \ln \frac{L_i(\omega)}{L_i(-\omega)}, \tag{65}$$

where we defined

$$\begin{aligned} L_1(\omega) &= 1 - \left[\frac{\alpha(\omega)e^{i\omega a}}{4\pi a^3}(1 - i\omega a - (\omega a)^2)\right]^2, \\ L_2(\omega) &= 1 - \left[\frac{2\alpha(\omega)e^{i\omega a}}{4\pi a^3}(1 - i\omega a)\right]^2. \end{aligned} \tag{66}$$

With these formulas, and inserting the representation (64) for $\delta(\omega)$ into F [Eq. (49)], we have explicit formulas for the free interaction energy of two atoms in the case of dissipation. It should be remarked that these expressions constitute a nonperturbative generalization of the Casimir-Polder interaction potential, which can be obtained backward by expanding in powers of the coupling $\alpha(\omega)$.

In the following, we consider limiting cases of the free energy and the transition to the Matsubara representation.

A. Limiting cases

In this section we consider the limiting cases of vanishing dissipation parameter and the relation to the vacuum energy and check the low-temperature expansion.

1. Vanishing dissipation parameter and vacuum energy

We split the free energy (49) according to the phase (64),

$$F = 2F_1 + F_2, \tag{67}$$

with

$$F_i = \int_0^\infty \frac{d\omega}{\pi}\left(\frac{\omega}{2} + T\ln(1 - e^{-\beta\omega})\right) \sum_{\sigma=\pm 1} \partial_\omega \delta_i(\omega). \tag{68}$$

The $\delta_i(\omega)$ are given by (65). Instead, we use

$$\delta_i(\omega) = -\frac{1}{2i} \ln \frac{\Phi_i(\omega) - i\gamma\omega}{\Phi_i(\omega) + i\gamma\omega}, \tag{69}$$

where

$$\begin{aligned} \Phi_1(\omega) &= -\omega^2 + \Omega^2 - \sigma\frac{e^2}{ma^3}e^{i\omega a}, \\ \Phi_2(\omega) &= -\omega^2 + \Omega^2 - 2\sigma\frac{e^2}{ma^3}e^{i\omega a}, \end{aligned} \tag{70}$$

and, again using (24), we dropped a factor, resulting in a contribution to the free energy which does not depend on the separation.

Next we consider the limit $\gamma \to 0$ and apply the Sokhotski-Plemelj theorem to

$$\partial_\omega \delta_i(\omega) = -\frac{1}{2i}\left(\frac{\partial_\omega \Phi_i(\omega) - i\gamma}{\Phi_i(\omega) - i\gamma\omega} - \frac{\partial_\omega \Phi_i(\omega) + i\gamma}{\Phi_i(\omega) + i\gamma\omega}\right), \tag{71}$$

which results in

$$\lim_{\gamma\to 0} \partial_\omega \delta_i(\omega) = -\pi\delta(\Phi_i(\omega))\partial_\omega(\Phi_i(\omega)). \tag{72}$$

Inserting into (68) gives, for the free energy at vanishing dissipation,

$$\begin{aligned} F_{i\,|_{\gamma=0}} = -\int_0^\infty d\omega\left(\frac{\omega}{2} + T\ln(1 - e^{-\beta\omega})\right) \\ \times \delta(\Phi_i(\omega))\partial_\omega(\Phi_i(\omega)). \end{aligned} \tag{73}$$

Using the δ function, the integration can be carried out. Let ω_J be the zeros of the equation $\Phi_i(\omega) = 0$, i.e., the eigenfrequencies of the system of two dipoles interacting with the electromagnetic field without dissipation. Then the integral can be written as a sum

$$F_{|_{\gamma=0}} = \sum_J \left(\frac{\omega_J}{2} + T\ln(1 - e^{-\beta\omega_J})\right). \tag{74}$$

Here we assumed the sum over σ and over the two contributions $2F_1 + F_2$ being included in the sum over J and we accounted for $\partial_\omega(\Phi_i(\omega)) < 0$, which can be seen from (70) at least for small ω_p^2. The vacuum energy can now be obtained from (74) by simply taking $T \to 0$,

$$E_0 = (F_{|_{\gamma=0}})_{|_{T=0}} = \frac{1}{2}\sum_s \omega_s, \tag{75}$$

in agreement with (3), again ignoring the necessary regularization.

At this point another remark concerning the sum over the eigenfrequencies ω_s is in order. As discussed in detail in [21], the considered system of two dipoles does not have real eigenfrequencies in empty space, since any excitation would be radiated away. The way out is to put the system, including the electromagnetic field, into a box. Then the eigenfrequencies are real and the sum in Eq. (75) makes sense. Afterward the volume may tend to infinity and the vacuum energy (75) is obtained.

Another way to get the vacuum energy from the free energy is to let $\gamma \to 0$ directly in Eq. (68). Thereby one has to pay attention to the singularities of $\Phi_i(\omega) - i\gamma\omega$ being in the lower half plane and from $-i\gamma$ one has to keep a $+i0$ prescription. This can be done in the following way:

$$E_0 = (F_{|_{\gamma=0}})_{|_{T=0}} = -\frac{1}{2}\int_0^\infty \frac{d\omega}{\pi}\omega\partial_\omega \times \frac{1}{2i}\mathrm{tr}\left(2\ln\frac{L_1(\omega-i0)}{L_1(\omega+i0)} + \ln\frac{L_2(\omega-i0)}{L_2(\omega+i0)}\right). \tag{76}$$

In this representation, it makes sense to integrate by parts and to make the Wick rotation. One arrives at

$$E_0 = \frac{1}{2}\int_0^\infty \frac{d\xi}{\pi}[2\ln L_1(i\xi) + \ln L_2(i\xi)], \tag{77}$$

with, explicitly,

$$\begin{aligned} L_1(i\xi) &= 1 - \left[\frac{\alpha(i\xi)e^{-a\xi}}{a^3}(1 + a\xi + (a\xi)^2)\right]^2, \\ L_2(i\xi) &= 1 - \left[\frac{2\alpha(i\xi)e^{-a\xi}}{a^3}(1 + a\xi)\right]^2, \end{aligned} \tag{78}$$

with $\alpha(i\xi) = \frac{\omega_p^2}{\xi^2+\Omega^2}$. These formulas constitute the nonperturbative formulation of the Casimir-Polder interaction energy of two dipoles (without dissipation). We mention that the functions $L_i(i\xi)$ $(i = 1,2)$ may have zeros and change sign. This is the criticality mentioned in the Introduction. It happens with L_2 for $\alpha/4\pi a^3 < 1/4$ and with L_1 for $\alpha/4\pi a^3 < 1$ for constant α and for e^2/Ω^2 in place of α for $\alpha(\omega)$ given by (24), provided $\Omega \neq 0$. In the case $\Omega = 0$, there is criticality for all values of the parameters. This instability was mentioned in the literature earlier, for example, in Ref. [18], which also mentioned that the onset of criticality coincides with the radius of convergence of the long separation expansion.

At this point it is easy the check that (78) gives the correct long separation expansion. Expanding (78) in powers of α and substituting $\xi \to \xi/a$, we get

$$E_0 \cong -\frac{1}{a}\int_0^\infty \frac{d\xi}{\pi}\left(\frac{\alpha(i\xi)}{4\pi a^3}\right)^2(3 + 6\xi + 5\xi^2 + 2\xi^3 + \xi^4)\,e^{-2\xi}, \tag{79}$$

and carrying out the integration for constant α, $E_0 \cong -\frac{23}{4\pi a^7}(\frac{\alpha}{4\pi})^2$ holds, in agreement with Eq. (57) in Ref. [14].

2. *Low-temperature expansion*

For the expansion for $T \to 0$ of the temperature-dependent part of the free energy,

$$\Delta_T F = T\int_0^\infty \frac{d\omega}{\pi}\ln(1 - e^{-\beta\omega})\partial_\omega\delta(\omega), \tag{80}$$

which results from the second term in large parentheses in (49), we need the expansions of the phases $\delta_i(\omega)$ for $\omega \to 0$. From (66) we get, with (24), for $\Omega \neq 0$,

$$\begin{aligned} L_1(\omega) &= 1 - \left(\frac{e^2}{ma^3\Omega^2}\right)^2 + O(\omega), \\ L_2(\omega) &= 1 - \left(\frac{2e^2}{ma^3\Omega^2}\right)^2 + O(\omega), \end{aligned} \tag{81}$$

and for the phase

$$\delta(\omega) = \frac{6(\gamma + 2a\Omega^2)\left[8\pi^2a^6\Omega^4 - \left(\frac{4\pi e^2}{m}\right)^2\right]}{\left[\omega_p^8 - 20\pi^2\left(\frac{4\pi e^2}{m}\right)^2\Omega^4 + 64\pi^4a^{12}\Omega^8\right]\Omega^2}\omega + O(\omega^3) \tag{82}$$

holds. We note that formulas (81) do not depend on the dissipation parameter γ. In (82) one may set $\gamma = 0$ without principal changes.

If we set $\Omega = 0$, these expressions simplify and the L_i become more singular,

$$\begin{aligned} L_1(\omega) &= \left(\frac{e^2}{ma^3\gamma}\right)^2\frac{1}{\omega^2} + O\left(\frac{1}{\omega}\right), \\ L_2(\omega) &= \left(\frac{2e^2}{ma^3\gamma}\right)^2\frac{1}{\omega^2} + O\left(\frac{1}{\omega}\right), \end{aligned} \tag{83}$$

and for the phase,

$$\delta(\omega) = -\frac{6(1 + 2\gamma a)}{\gamma}\omega + O(\omega^3) \tag{84}$$

holds. Finally, if we set, in addition, also $\gamma = 0$, we get an even more singular behavior,

$$\begin{aligned} L_1(\omega) &= -\left(\frac{e^2}{ma^3}\right)^2\frac{1}{\omega^4} + O\left(\frac{1}{\omega^3}\right), \\ L_2(\omega) &= \left(\frac{2e^2}{ma^3}\right)^2\frac{1}{\omega^4} + O\left(\frac{1}{\omega^3}\right), \end{aligned} \tag{85}$$

and for the phase,

$$\delta(\omega) = -12a\omega + O(\omega^3) \tag{86}$$

holds. Below we need, for $\Omega \neq 0$ the values $L_i(0)$, which are finite, and for $\Omega = 0$ the derivatives, which are, for $\gamma \neq 0$,

$$\partial_\omega \ln L_i(\omega) = -\frac{2}{\omega} + O(1), \tag{87}$$

and, in addition, for $\gamma = 0$,

$$\partial_\omega \ln L_i(\omega) = -\frac{4}{\omega} + O(1). \tag{88}$$

It must be mentioned that the leading orders of the expansions of the phases for the cases considered result from the next-order contributions in the expansions of $L_i(\omega)$, which are not shown. Also we mention that the phases $\delta(\omega)$ always start from the first order in ω since any constant contribution disappears under the derivative ∂_ω in Eq. (80).

Summarizing, introducing the notation c_1 for the coefficient in the expansion (82), (84), and (86),

$$\delta(\omega) = c_1\omega + O(\omega^3), \tag{89}$$

we get in the temperature-dependent part of the free energy (80), after the substitution $\omega \to \omega T$,

$$\Delta_T F = T^2\int_0^\infty \frac{d\omega}{\pi}\ln(1 - e^{-\hbar\omega})\partial_\omega(c_1\omega + O(T^2\omega^3)), \tag{90}$$

which gives

$$\Delta_T F = -\frac{c_1\zeta(2)}{\pi\hbar}T^2 + O(T^4), \tag{91}$$

where $\zeta(2)=\pi^2/6$ is the Riemann zeta function. In this formula, c_1 is first nonzero coefficient in the expansion of the phase for $\omega\to 0$ for all values of the parameters. Thus, the low-temperature behavior of the entropy (16),

$$S=2c_1T+O(T^2),\tag{92}$$

never violates the third law of thermodynamics. We mention that the same holds if we allow for a temperature dependence of the dissipation parameter $\gamma(T)$ with a low-T behavior $\gamma(T)\underset{T\to 0}{\sim}\gamma_1T^{\alpha}$ $(\alpha>1)$. With $\Omega=0$ we get, after the substitution $\omega\to\omega T$,

$$\alpha(\omega T)=\frac{4\pi e^2}{m(-\omega^2T^2-i\gamma_1T^{\alpha+1})}.\tag{93}$$

Now, for $\alpha<1$ this is equivalent to the case (83) and (84), and for $\alpha>1$ it is equivalent to (85) and (86). This way, in the AA configuration, also the temperature dependence of the dissipation parameter does not result in thermodynamic problems.

B. Transition to Matsubara frequencies

The starting point for the transition to Matsubara frequencies is the free energy

$$\begin{aligned}F=&\int_0^\infty\frac{d\omega}{\pi}\left[\frac{\omega}{2}+T\ln(1-e^{-\beta\omega})\right]\\&\times\partial_\omega\frac{-1}{2i}\left(2\ln\frac{L_1(\omega)}{L_1(-\omega)}+\ln\frac{L_2(\omega)}{L_2(-\omega)}\right),\end{aligned}\tag{94}$$

which follows from (80), (64), and (66). We mention that $L_i(\omega)$ has no singularities in the upper half plane (at least for sufficiently small γ). Thus we write the logarithms of the quotients as the differences of two logarithms and turn the integration path upward towards the imaginary axis in the first term and in the second term correspondingly downward, which is in fact a Wick rotation.

Below we will need the simple relation

$$\frac{\beta\omega}{2}+\ln(1-e^{-\beta\omega})=\ln\left(2\sinh\frac{\beta\omega}{2}\right)\tag{95}$$

and its continuation

$$\ln\left(2\sinh\frac{i\beta\xi}{2}\right)=\ln\left|2\sin\frac{\beta\xi}{2}\right|+i\pi{\sum_{l=0}^{\infty}}'\Theta(\xi-\xi_l),\tag{96}$$

where $\xi_l=2\pi Tl$ are the Matsubara frequencies. This relation follows since the logarithm has cuts starting in $\xi=\xi_l$. The prime on the sum symbol denotes, as usual, that the contribution from $l=0$ must be taken with a factor $1/2$.

However, in doing the Wick rotation, we must split the integral over the difference into the difference of two integrals. In doing so, the integration over ω will not converge at $\omega=0$ in the cases with $\Omega=0$ because of the singular behavior in (83) and (85). We note that this is not the case for $\Omega\neq 0$, as can be seen from (81).

The difficulty arising at $\omega=0$ can be handled by introducing a lower integration boundary $\varepsilon>0$ and taking the limit $\varepsilon\to 0$ after the rotations. This way we get

$$\begin{aligned}F_i=&-\frac{1}{2\pi i}\lim_{\varepsilon\to 0}\left[\int_\varepsilon^\infty d\omega\left(\frac{\hbar\omega}{2}+T\ln(1-e^{-\beta\hbar\omega})\right)\partial_\omega\ln L_i(\omega)\right.\\&\left.-\int_\varepsilon^\infty d\omega\left(\frac{\hbar\omega}{2}+T\ln(1-e^{-\beta\hbar\omega})\right)\partial_\omega\ln L_i(-\omega)\right],\end{aligned}\tag{97}$$

where we have split the free energy $F=2F_1+F_2$ in accord with the split (64) of the phase.

Now we split the integration pathes into two parts each. The first part is a half circle of radius ε, given by $\omega=\varepsilon e^{i\varphi}$ in the first integral and $\omega=\varepsilon e^{-i\varphi}$ in the second one, with $\varphi=0,\dots,\frac{\pi}{2}$ in both cases. The second part is a straight line along the imaginary axis with $\omega=i\xi$ in the first integral and $\omega=-i\xi$ in the second one, with $\xi\in[\varepsilon,\infty)$ in both cases. From the integrals along the straight lines, using (96), we have

$$\begin{aligned}F_i^{\text{lin}}=&-\frac{T}{2\pi i}\left[\int_\varepsilon^\infty d\xi\left(\ln\left|2\sin\frac{\beta\xi}{2}\right|-i\pi{\sum_{l=0}^{\infty}}'\Theta(\xi-\xi_l)\right)\right.\\&\times\partial_\xi(\ln|L_i(i\xi)|+i\pi\Theta(\xi_*-\xi))\\&-\int_\varepsilon^\infty d\xi\left(\ln\left|2\sin\frac{\beta\xi}{2}\right|+i\pi{\sum_{l=0}^{\infty}}'\Theta(\xi-\xi_l)\right)\\&\left.\times\partial_\xi(\ln|L_i(-i\xi)|-i\pi\Theta(\xi_*-\xi))\right].\end{aligned}\tag{98}$$

An additional feature appears here in the case where the functions $L_i(-i\xi)$ have a zero, i.e., there is a real $\xi_*>0$ such that $L_i(-i\xi_*)=0$ holds, as discussed in Sec. III A. For this reason, the logarithms of L_i acquire imaginary parts as shown in the above formula. The signs follow from $L_i(i\xi)>0$ for sufficiently large ξ and the side on which the branch point of the logarithm is passed.

After simplifying in Eq. (98), we integrate by parts. In the contribution with $l=0$, accounting for $\Theta(\xi-\xi_0)=1$ for $\xi>0$, we get $\frac{T}{2}\ln|L(i\varepsilon)|$. In all other contribution we can set $\varepsilon=0$. This way, from (98),

$$F_i^{\text{lin}}=\frac{T}{2}\ln|L_i(i\varepsilon)|+T\sum_{l=1}^{\infty}\ln|L_i(i\xi_l)|-T\ln\left|2\sin\frac{\beta\xi_*}{2}\right|\tag{99}$$

follows. Indeed, this expression is divergent for $\varepsilon\to 0$ in the case of $\Omega=0$. For $\Omega\neq 0$, Eqs. (81) show finite $L_i(0)$. For $\Omega=0$, using (83), we get, for $\gamma\neq 0$,

$$\frac{T}{2}\ln|L_1(i\varepsilon)|=-T\ln\varepsilon+T\ln\left(\frac{e^2}{ma^3\gamma}\right)+O(\varepsilon),\tag{100}$$

and for $\gamma=0$, using (85),

$$\frac{T}{2}\ln|L_1(i\varepsilon)|=-2T\ln\varepsilon+T\ln\left(\frac{e^2}{ma^3}\right)+O(\varepsilon).\tag{101}$$

The corresponding expressions for $L_2(i\varepsilon)$ can be obtained from these by the substitution $\omega_p^2\to 2\omega_p^2$. We see that in these cases, i.e., for $\Omega=0$, there is a logarithmic divergence.

It remains to calculate the contribution from the half circles. Restricted to contributions not vanishing for $\varepsilon\to 0$, we note that

$$\frac{\hbar\omega}{2}+T\,\ln(1-e^{-\beta\hbar\omega})\sim T\,\ln(\beta\varepsilon e^{i\varphi})$$

in the first contribution in Eq. (97) and the complex conjugate of that in the second. Using the leading contribution in Eq. (87) or (88), we get, from (97),

$$\begin{aligned}F_i^{\text{half circ}}&=-\frac{T}{\pi}\int_0^{\pi/2}d\varphi(\,\ln(\beta\varepsilon e^{i\varphi})+\ln(\beta\varepsilon e^{-i\varphi}))\\&=T\,\ln(\beta\varepsilon)+O(\varepsilon)\end{aligned}\tag{102}$$

for $\gamma\neq0$ and

$$\begin{aligned}F_i^{\text{half circ}}&=-\frac{T}{\pi}\int_0^{\pi/2}d\varphi(\,\ln(\beta\varepsilon e^{i\varphi})+\ln(\beta\varepsilon e^{-i\varphi}))\\&=2T\,\ln(\beta\varepsilon)+O(\varepsilon)\end{aligned}\tag{103}$$

for $\gamma=0$. We see that the divergence for $\varepsilon\to0$ compensates just that in Eq. (100) or (101), as expected, and we get for the sum of (99) and (103), for $\gamma\neq0$,

$$\begin{aligned}F_i&=T\,\ln\left(\frac{c_i\omega_p^2\beta}{4\pi a^3\gamma}\right)+T\sum_{l=1}^{\infty}\ln|L_1(i\xi_l)|\\&\quad-T\,\ln\left|2\sin\frac{\beta\xi_*}{2}\right|\quad(i=1,2),\end{aligned}\tag{104}$$

with $c_1=1$ and $c_2=2$, and from (99) and (101), for $\gamma=0$, we get

$$\begin{aligned}F_i&=2T\,\ln\left(\frac{c_i\omega_p^2\beta}{4\pi a^3}\right)+T\sum_{l=1}^{\infty}\ln|L_1(i\xi_l)|\\&\quad-T\,\ln\left|2\sin\frac{\beta\xi_*}{2}\right|\quad(i=1,2).\end{aligned}\tag{105}$$

With these formulas we derive the Matsubara representation of the complete free energy $F=2F_1+F-2$ for the nonperturbative Casimir-Polder interaction of two dipoles with dissipation in the case of vanishing intrinsic frequency $\Omega=0$. For $\Omega\neq0$, the same formulas hold with the usual terms corresponding to the zeroth Matsubara frequency $L_i(i\xi_{|l=0})$ in place of the first logarithmic contributions. In other words, the modifications, coming in for $\Omega=0$, can be formulated in terms of the formal substitutions of the contributions from the zeroth Matsubara frequency according to, for $\gamma\neq0$,

$$L_1(i\xi_{|_{l=0}})\to\left(\frac{e^2\beta}{ma^3\gamma}\right)^2,\quad L_2(i\xi_{|_{l=0}})\to\left(\frac{2e^2\beta}{ma^3\gamma}\right)^2,\tag{106}$$

and, for $\gamma=0$,

$$L_1(i\xi_{|_{l=0}})\to\left(\frac{e^2\beta}{ma^3}\right)^4,\quad L_2(i\xi_{|_{l=0}})\to\left(\frac{2e^2\beta}{ma^3}\right)^4.\tag{107}$$

The other modification in Eqs. (104) and (105), i.e., the second logarithmic contributions, comes from the critical behavior, which may be present for $\Omega\neq0$ and will be present for $\Omega=0$. We mention that for $\Omega=0$ the contributions from the zeroth Matsubara frequency has, for $T\to0$, a logarithmic behavior $F\sim-T\,\ln T$.

IV. ATOM-WALL CONFIGURATION

In this section we investigate in detail the AW configuration, i.e., the interaction of a single dipole with a dielectric half space, as introduced in Sec. II D. As before, the free energy is given by Eq. (49). The phase $\delta(\omega)$ is given, in general notation, by (47). Using (31), we express $\delta(\omega)$ through $\hat{\boldsymbol{L}}(\omega)$,

$$\delta(\omega)=-\frac{1}{2i}\text{tr}\ln\frac{\hat{\boldsymbol{L}}(\omega)}{\hat{\boldsymbol{L}}(\omega)^*},\tag{108}$$

dropping terms which would not contribute to the Casimir-Polder force. In this formula we also used $\hat{\boldsymbol{L}}(-\omega)=\hat{\boldsymbol{L}}(\omega)^*$. With (31) and (33) we have

$$\boldsymbol{L}_{ij}(\omega)=\delta_{ij}-\alpha(\omega)\omega^2\boldsymbol{G}^{(0)}_{\omega,ij}\tag{109}$$

for the matrix elements of $\hat{\boldsymbol{L}}(\omega)$.

For the AW configuration, the index $i=0$ describes the atom and the indices $i=1,2,\ldots$ describe the dipoles in the half space $z<0$. The separation between the atom and the wall is $a=(\boldsymbol{a}_0)_z$.

For the subsequent derivations we return for a moment to Eq. (28) for the Green's function

$$[-\omega^2-\Delta+\nabla\circ\nabla-V(\boldsymbol{x})]\boldsymbol{G}_\omega(\boldsymbol{x},\boldsymbol{x}')=\delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}'),\tag{110}$$

where we introduced the notation

$$V(\boldsymbol{x})=V_s(\boldsymbol{x})+V_1(\boldsymbol{x}),\tag{111}$$

with

$$\begin{aligned}V_s(\boldsymbol{x})&=\alpha(\omega)\omega^2\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_0),\\V_1(\boldsymbol{x})&=\alpha(\omega)\omega^2\sum_{i=1}^{\infty}\delta^{(3)}(\boldsymbol{x}-\boldsymbol{a}_i).\end{aligned}\tag{112}$$

Here $V_s(\boldsymbol{x})$ is the potential from the single atom with $\alpha(\omega)$ given by Eq. (24) and $V_1(\boldsymbol{x})$ is the potential from the dipoles in the half space. Next we switch to the operator and matrix notations as used already at the end of Sec. II C. From Eqs. (109) and (112) we have

$$\text{tr}\ln\hat{\boldsymbol{L}}(\omega)=\text{tr}\ln\left[1-(\hat{\boldsymbol{V}}_s+\hat{\boldsymbol{V}}_1)\hat{\boldsymbol{G}}^{(0)}_\omega\right].\tag{113}$$

We continue by rewriting

$$\begin{aligned}\text{tr}\ln\hat{\boldsymbol{L}}(\omega)&=\text{tr}\ln\left(1-\hat{\boldsymbol{V}}_1\hat{\boldsymbol{G}}^{(0)}_\omega\right)\\&\quad+\text{tr}\ln\left[1-\left(1-\hat{\boldsymbol{V}}_1\hat{\boldsymbol{G}}^{(0)}_\omega\right)^{-1}\hat{\boldsymbol{V}}_s\hat{\boldsymbol{G}}^{(0)}_\omega\right],\end{aligned}\tag{114}$$

where the first term does not depend on the atom-wall separation and will be dropped as not contributing to the Casimir-Polder force. In the other term, we use the cyclic property of the trace and an equation which is analogous to (50) with $V_1(\boldsymbol{x})$ in place of $V(\boldsymbol{x})$, defining the Green's function $\hat{\boldsymbol{G}}^{(1)}_\omega(\boldsymbol{x},\boldsymbol{x}')$, which is the Green's function in the presence of the dipoles in the half space alone, and arrive at

$$\text{tr}\ln\hat{\boldsymbol{L}}(\omega)=\text{tr}\ln\left(1-\hat{\boldsymbol{V}}_s\hat{\boldsymbol{G}}^{(1)}_\omega\right)+\cdots,\tag{115}$$

which we will use in the following. The next step is the limiting transition $\boldsymbol{a}_i\to\boldsymbol{x}$ with $i=1,2,\ldots$ to a continuous medium in $z<0$. Thereby the potential $V_1(\boldsymbol{x})$ turns into

$$V_1(\boldsymbol{x})=[\varepsilon(\omega)-1]\omega^2\Theta(-z)\tag{116}$$

and we introduced the permittivity

$$\varepsilon(\omega) = 1 + \frac{\omega_p^2}{N(\omega)}, \quad \omega_p^2 = \frac{4\pi e^2}{m}\rho, \tag{117}$$

where ρ is the density (number of atoms per unit volume). Representing

$$\hat{\boldsymbol{G}}_\omega^{(1)} = \hat{\boldsymbol{G}}_\omega^{(0)} + \Delta\hat{\boldsymbol{G}}_\omega^{(1)} \tag{118}$$

as a sum of the free space Green's function (17) and an addendum from the half space, we note that

$$\boldsymbol{G}_\omega^{(1)}(\boldsymbol{x},\boldsymbol{x}') = \lim_{\substack{\boldsymbol{a}_i\to\boldsymbol{x}\\ \boldsymbol{a}_j\to\boldsymbol{x}'}} \left[\boldsymbol{G}_\omega^{(0)}(\boldsymbol{a}_i-\boldsymbol{a}_j) + \Delta\boldsymbol{G}_\omega^{(1)}(\boldsymbol{a}_i-\boldsymbol{a}_j)\right]. \tag{119}$$

Now, in Eq. (115), the arguments $\boldsymbol{x}$ and $\boldsymbol{x}'$ will be set equal to one another due to the potential $V_s(\boldsymbol{x})$ [Eq. (112)]. Thus, the free Green's function $\boldsymbol{G}_\omega^{(0)}(\boldsymbol{a}_i-\boldsymbol{a}_j)$ must be set equal to zero in order to avoid self-fields and we are left with the addendum and arrive at

$$\operatorname{tr}\ln\hat{\boldsymbol{L}}(\omega) = \operatorname{tr}\ln\left(1-\hat{\boldsymbol{V}}_s\Delta\hat{\boldsymbol{G}}_\omega^{(1)}\right) + \cdots. \tag{120}$$

After performing the transition to the continuum, the Green's function $\boldsymbol{G}_\omega^{(1)}(\boldsymbol{x},\boldsymbol{x}')$ obeys the equation

$$\begin{aligned}&\{-\omega^2 - \Delta + \nabla\circ\nabla - [\varepsilon(\omega)-1]\omega^2\Theta(-z)\}\boldsymbol{G}_\omega^{(1)}(\boldsymbol{x},\boldsymbol{x}')\\ &\quad = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}').\end{aligned} \tag{121}$$

Here, in view of the translational invariance in the (x,y) plane, we perform the corresponding Fourier transform

$$\boldsymbol{G}_\omega^{(1)}(\boldsymbol{x},\boldsymbol{x}') = \int\frac{dk_\parallel}{(2\pi)^2}e^{i\boldsymbol{k}_\parallel(\boldsymbol{x}_\parallel-\boldsymbol{x}'_\parallel)}\boldsymbol{g}_\Gamma(z,z'), \tag{122}$$

with $\Gamma = \sqrt{\omega^2-k_\parallel^2+i0}$, and the equation

$$\begin{aligned}&\left\{-\Gamma^2-\partial_z^2+\nabla\circ\nabla-[\varepsilon(\omega)-1]\omega^2\Theta(-z)\right\}\boldsymbol{g}_\Gamma(z,z')\\ &\quad = \delta^{(1)}(z-z')\end{aligned} \tag{123}$$

holds. In this representation, the gradient is $\nabla = (i\boldsymbol{k}_\parallel,\partial_z)$. This Green's function is well known (see, for example, Appendix A in Ref. [25] or Chap. 13 in Ref. [20]). We use its decomposition into polarizations

$$\boldsymbol{g}_\Gamma(z,z') = \boldsymbol{E}_{\rm TE}g_\Gamma^{\rm TE}(z,z')\boldsymbol{E}_{\rm TE}^\dagger + \boldsymbol{E}_{\rm TM}g_\Gamma^{\rm TM}(z,z')\boldsymbol{E}_{\rm TM}^\dagger, \tag{124}$$

with the polarization vectors

$$\boldsymbol{E}_{\rm TE} = \begin{pmatrix}-k_2\\ k_1\\ 0\end{pmatrix}\frac{1}{k_\parallel}, \quad \boldsymbol{E}_{\rm TM} = \begin{pmatrix}-ik_1\partial_z\\ ik_2\partial_z\\ -k_\parallel^2\end{pmatrix}\frac{1}{k_\parallel\omega} \tag{125}$$

and we dropped the δ-function contribution at $z=z'$ since it results from the free space part in Eq. (118), which we drop.

For the scalar functions $g_\Gamma^X(z,z')$ with $X=\mathrm{TE}$ or $X=\mathrm{TM}$, we use the representation

$$g_\Gamma^X(z,z') = \frac{u_X(z_<)v_X(z_>)}{w}, \tag{126}$$

with

$$\begin{aligned}v_X(z) &= (e^{ikz}+r_Xe^{-ikz})\Theta(-z)+t_Xe^{iqz}\Theta(z),\\ u_X(z) &= \bar{t}_Xe^{-ikz}\Theta(-z)+(e^{-iqz}+\bar{r}_Xe^{iqz})\Theta(z),\\ w &= -2iqt_X,\end{aligned} \tag{127}$$

and the well-known reflection coefficients

$$r_{\rm TE} = \frac{q-k}{q+k}, \quad r_{\rm TM} = \frac{\varepsilon(\omega)q-k}{\varepsilon(\omega)q+k}. \tag{128}$$

The momenta are related by

$$\omega^2 = k_\parallel^2+q^2, \quad \varepsilon(\omega)\omega^2 = k_\parallel^2+k^2. \tag{129}$$

Now, since the polarization vectors are the same for the free space part $\boldsymbol{G}_\omega^{(0)}$ and for the addendum in Eq. (118), we get the free space part from the above formulas with $r_X\to0$ and $t_X\to1$. Therefore, we get, at $z=z'=a$,

$$\begin{aligned}\Delta g_\Gamma^X(a,a) &= \frac{\bar{t}_Xe^{iqa}(e^{-iqa}+r_Xe^{iqa})}{-2iq\bar{t}_X}-\frac{1}{-2iq}\\ &= \frac{r_X}{-2iq}\,e^{2iqa}.\end{aligned} \tag{130}$$

Further, using (122), we arrive at

$$\Delta\boldsymbol{G}_\omega^{(1)}(\boldsymbol{a},\boldsymbol{a}) = \int\frac{d\boldsymbol{k}_\parallel}{(2\pi)^2}\sum_{X=\mathrm{TE,TM}}\operatorname{tr}E_X\frac{r_X}{-2iq}\,e^{2iqa}E_X^\dagger, \tag{131}$$

where the trace is over the spatial structure. Inserting into (115) and using (125) for the polarization vectors, under the trace we arrive at

$$\operatorname{tr}\ln\hat{\boldsymbol{L}}(\omega) = \ln[1-\alpha(\omega)\omega^2\Delta G^{(1)}] \equiv \ln L(\omega), \tag{132}$$

with

$$\Delta G^{(1)} = \int\frac{d\boldsymbol{k}_\parallel}{(2\pi)^2}\left(r_{\rm TE}+\frac{-q^2+k_\parallel^2}{\omega^2}r_{\rm TM}\right)\frac{e^{2iqa}}{-2iq}. \tag{133}$$

We take (132) as the definition for $L(\omega)$, which we will use in the following. For convenience, we recall here the formulas (49) and (108),

$$\begin{aligned}F &= \int_0^\infty\frac{d\omega}{\pi}\left(\frac{\omega}{2}+T\ln(1-e^{-\beta\omega})\right)\partial_\omega\delta(\omega), \quad \delta(\omega)\\ &= -\frac{1}{2i}\ln\frac{L(\omega)}{L(-\omega)},\end{aligned} \tag{134}$$

which, together with (132), give the distance-dependent part of the free energy.

In the following sections we analyze the limiting cases and the transition to the Matsubara representation. It will turn out that this analysis goes much in parallel to that in the AA configuration in Secs. III A and III B.

A. Limiting cases

1. *Vanishing dissipation parameter and vacuum energy*

Here we restrict ourself to the second way mentioned in Sec. III A using the $+i0$ prescription and take vanishing both $\gamma\to0$ and $\gamma_0\to0$. We start from the representation (134) for $T=0$,

$$E_0 = (F_{|_{\gamma=0}})_{|_{T=0}} = \frac{1}{2}\int_0^\infty\frac{d\omega}{\pi}\omega\partial_\omega\frac{-1}{2i}\ln\frac{L(\omega-i0)}{L(\omega+i0)}, \tag{135}$$

where $L(\omega)$ is given by (132) with $\gamma=\gamma_0=0$. Doing the Wick rotation and integrating by parts we get

$$E_0 = \frac{1}{2\pi}\int_0^\infty d\xi\,\ln L(i\xi), \tag{136}$$

where we assumed that criticality is absent. The explicit formulas are

$$L(i\xi) = 1 + \alpha(i\xi)\xi^2 \Delta G^{(1)}(i\xi), \tag{137}$$

with

$$\Delta G^{(1)}(i\xi) = \int \frac{d\boldsymbol{k}_{\parallel}}{(2\pi)^2}\left[r_{\rm TE} + \left(1 - \frac{2\eta^2}{\xi^2}\right) r_{\rm TM}\right]\frac{e^{-2a\eta}}{2\eta}. \tag{138}$$

Under the Wick rotation, the momenta turn into $q = i\eta$ and $k = i\kappa$ and from the relations (129) one arrives at

$$\eta = \sqrt{\xi^2 + k_{\parallel}^2}, \quad \kappa = \sqrt{(\varepsilon(i\xi) - 1)\xi^2 + \eta^2}. \tag{139}$$

Expressed in these momenta, the reflection coefficients are now

$$r_{\rm TE} = \frac{\eta - \kappa}{\eta + \kappa}, \quad r_{\rm TM} = \frac{\varepsilon(i\xi)\eta - \kappa}{\varepsilon(i\xi)\eta + \kappa}. \tag{140}$$

In the integration in Eq. (138), it is meaningful to change the variable for η and the final formula for $L(i\xi)$ is

$$L(i\xi) = 1 + \frac{\alpha(i\xi)}{4\pi}\xi^2 \int_{\xi}^{\infty} d\eta \left[r_{\rm TE} + \left(1 - \frac{2\eta^2}{\xi^2}\right) r_{\rm TM}\right] e^{-2a\eta}, \tag{141}$$

with $\alpha(i\xi) = \frac{\omega_p^2}{\xi^2 + \Omega_0^2}$. With this notation, E_0 [Eq. (136)] gives the Casimir-Polder vacuum interaction energy in the AW configuration. We mention that this E_0 is nonperturbative in the polarizability.

We check the above formula by considering the case of an ideally conducting wall. In that case the reflection coefficients are $r_{\rm TE} = -1$ and $r_{\rm TM} = 1$ and the integration over η can be carried out. Then the vacuum energy simplifies

$$E_0 = \frac{1}{2\pi}\int_0^{\infty} d\xi \times \ln\left(1 - \frac{2\alpha(i\xi)}{4\pi(2a)^3}[2 + 2(2a\xi) + (2a\xi)^2]e^{-2a\xi}\right).$$

Making here an expansion for small $\alpha(i\xi)$ or for large separation a in leading order one arrives at

$$E_0 = -\frac{3}{8\pi a^4}\frac{\alpha(0)}{4\pi}, \tag{142}$$

in agreement with Eq. (25) in Ref. [14] or Eq. (16.28) in Ref. [5].

At this point it should be mentioned that the onset of criticality follows from (141) to be at $\frac{\alpha(0)}{4\pi(2a)^3} > \frac{1}{4}$ for $\Omega_0 \neq 0$ and that criticality is always present for $\Omega_0 = 0$. These are the same relations as in the AA configuration.

2. Low-temperature expansion

We start from the representation (80) for the temperature-dependent part of the free energy and Eq. (132) for $L(\omega)$. However, we distinguish now between $\alpha(\omega)$ [Eq. (24)] for the atom [this is $i = 0$ in Eq. (112)] and $\varepsilon(\omega)$ [Eq. (117)] for the half space, by giving an index 0 to the parameters entering $\alpha(\omega)$,

$$\alpha(\omega) = \frac{4\pi e^2}{m\left(-\omega^2 - i\gamma_0\omega + \Omega_0^2\right)}. \tag{143}$$

This way we will be able to trace the origin of different behavior.

Again, we need the expansion for $\omega \to 0$. From (132) and (133) we get, for $\Omega_0 \neq 0$,

$$L(\omega) = 1 - \frac{\alpha(0)\omega_p^2}{\pi(2a)^3\left(\omega_p^2 + 2\Omega^2\right)} + O(\omega), \tag{144}$$

and for the phase,

$$\delta(\omega) = \left(\frac{2\gamma}{\omega_p^2 + 2\Omega^2} + \frac{\gamma_0}{\Omega_0^2}\right)\omega + O(\omega^3). \tag{145}$$

In the case $\Omega_0 = 0$ we get

$$\begin{aligned} L(\omega) &= \frac{ie^2\omega_p^2}{2ma^3\gamma_0\left(\omega_p^2 + 2\Omega^2\right)}\frac{1}{\omega} + O(1), \\ \delta(\omega) &= \left(\frac{2\gamma}{\omega_p^2 + 2\Omega^2} + \frac{1}{\gamma_0}\right)\omega + O(\omega^3). \end{aligned} \tag{146}$$

If, in addition, we have $\gamma_0 = 0$, we get

$$\begin{aligned} L(\omega) &= \frac{ie^2\omega_p^2}{2ma^3\left(\omega_p^2 + 2\Omega^2\right)}\frac{1}{\omega^2} + O(1), \\ \delta(\omega) &= \frac{2\gamma}{\omega_p^2 + 2\Omega^2}\omega + O(\omega^3). \end{aligned} \tag{147}$$

In the derivation of these formulas, in Eq. (133) the expansion is straightforward and, after that, the integration over $k_{\parallel}$ is simple.

From (144) we see that a vanishing Ω does not change the behavior essentially, whereas $\Omega_0 = 0$ changes the behavior of $L(\omega)$. The phases are not affected and start with the first power in ω. Also we see that vanishing dissipation may increase only the power of the leading order. Thus, using Eqs. (88)–(92), we see a T^2 behavior of the temperature-dependent part of the free energy (at least) and, consequently, no violation of the third law is possible. This holds also for a dissipation parameter vanishing with temperature due to the factor ω^2 in front of $\Delta G^{(1)}(\omega)$ in Eq. (132) (see also the discussion in Sec. 16.3.3 in Ref. [5]). We do not consider problems reported for dc conductivity (see Secs. 12.6.3 and 16.4.3 in Ref. [5]), where the TM polarization becomes important, in this paper.

B. Transition to the Matsubara representation

The starting point for the transition to the Matsubara representation is Eq. (134) for the free energy. Further, we can use a number of formulas from Sec. III B by dropping the index i, namely, (95)–(99). For $\Omega_0 \neq 0$ and without criticality, we get simply

$$F = T\sum_{l=0}^{\infty}{}' \ln L(i\xi_l). \tag{148}$$

For $\Omega_0 = 0$, $L(0)$ is not finite and we need to go through the limiting procedure like in Sec. III B. However, all calculations go completely in parallel. The difference starts from (100), in place of which we get

$$\frac{T}{2}\ln|L_1(i\varepsilon)| = -\frac{T}{2}\ln\varepsilon + \frac{T}{2}\ln\left(\frac{e^2\omega_p^2}{2ma^3\gamma_0(\omega_p^2+2\Omega^2)}\right) + O(\varepsilon). \tag{149}$$

For the contributions from the half circles first we need

$$\partial_\omega \ln L(\omega) = -\frac{1}{\omega} + O(1) \tag{150}$$

in place of (146) and similar to (102) we have now

$$F^{\text{half circ}} = \frac{T}{2}\ln(\beta\varepsilon) + O(\varepsilon). \tag{151}$$

Again, the divergent logarithmic terms cancel as expected and we get finally

$$F_i = \frac{T}{2}\ln\left(\frac{e^2\omega_p^2\beta}{2ma^3\gamma_0(\omega_p^2+2\Omega^2)}\right) + T\sum_{l=1}^{\infty}\ln|L_1(i\xi_l)| - T\ln\left|2\sin\frac{\beta\xi_*}{2}\right|. \tag{152}$$

This way, for $\Omega_0 = 0$ we have the formal substitution

$$L(i\xi_{|l=0}) \to \frac{e^2\omega_p^2\beta}{2ma^3\gamma_0(\omega_p^2+2\Omega^2)}. \tag{153}$$

A similar result can be obtained if we have $\gamma_0 = 0$ in addition.

V. WALL-WALL CONFIGURATION

In this section we consider the WW configuration. As set up in Sec. IV B, it consists of two half spaces filled with a medium and a gap of width a between them. This is just the setup of the Casimir effect. The free energy is given by Eq. (49) with $\delta(\omega)$ given by Eq. (108) and $\boldsymbol{L}(\omega)$ by (23). We act in parallel to the preceding section and introduce a potential

$$V(\boldsymbol{x}) = V_1(z) + V_2(z), \tag{154}$$

with

$$\begin{aligned} V_1(z) &= [\varepsilon(\omega)-1]\omega^2\Theta(-z),\\ V_2(z) &= [\varepsilon(\omega)-1]\omega^2\Theta(z-a), \end{aligned} \tag{155}$$

where $\varepsilon(\omega)$ is given by (117). Next we consider

$$\operatorname{tr}\ln\hat{\boldsymbol{L}}(\omega) = \operatorname{tr}\ln\left\{1-[V_1(z)+V_2(z)]\hat{\boldsymbol{G}}^{(0)}_\omega\right\}. \tag{156}$$

This expression can be split into

$$\operatorname{tr}\ln\hat{\boldsymbol{L}} = \operatorname{tr}\ln\left[1-V_1(z)\hat{\boldsymbol{G}}^{(0)}_\omega\right] + \operatorname{tr}\ln\left[1-V_2(z)\hat{\boldsymbol{G}}^{(0)}_\omega\right] + \operatorname{tr}\ln(1-\mathcal{M}), \tag{157}$$

where

$$\mathcal{M} = \left(1-V_1\hat{\boldsymbol{G}}^{(0)}_\omega\right)^{-1}\hat{\boldsymbol{V}}_1\hat{\boldsymbol{G}}^{(0)}_\omega\left(1-V_2\hat{\boldsymbol{G}}^{(0)}_\omega\right)^{-1}\hat{\boldsymbol{V}}_1\hat{\boldsymbol{G}}^{(0)}_\omega = \hat{\boldsymbol{T}}_1\hat{\boldsymbol{G}}^{(0)}_\omega\hat{\boldsymbol{T}}_2\hat{\boldsymbol{G}}^{(0)}_\omega. \tag{158}$$

Here $\hat{\boldsymbol{T}}_1$ and $\hat{\boldsymbol{T}}_2$ are the T operators for the potentials $V_1(\boldsymbol{x})$ and $V_2(\boldsymbol{x})$ taken separately. Further, in deriving this equation, formulas like (50) and (51) were used as well as the cyclic property of the trace. Equation (157) is nothing but the well-known transition to the $TGTG$ formula [26]. Equivalent formulas can be found also in the so-called scattering approach [27]. The first two terms in Eq. (157) give contributions to the free energy, which will not depend on the width of the gap and we drop them. This way, we have to consider

$$\operatorname{tr}\ln\hat{\boldsymbol{L}} = \operatorname{tr}\ln(1-\mathcal{M}), \tag{159}$$

which is a well-known expression in connection with the Casimir effect (see, for instance, Sec. 10.1.2 in Ref. [5]). At this point it should be mentioned that the known formulas are very similar to those derived here, which, however, follow from the heat bath approach.

Continuing from Eq. (159), we can use the known explicit formulas (see, for example, Sec. 12.1 in Ref. [5]) (however, with slightly different notation). This way we get

$$\operatorname{tr}\ln\hat{\boldsymbol{L}} = \int\frac{d\boldsymbol{k}_\parallel}{(2\pi)^2}\sum_{X=\text{TE,TM}}\ln\left(1-r_X^2e^{2iaq}\right), \tag{160}$$

where the reflection coefficients r_{TE} and r_{TM} are defined in Eq. (128), the momenta q and k are defined in Eq. (129), and $\varepsilon(\omega)$ is defined in Eq. (117).

For the convenience of the following, we rewrite the above representation of the free energy in the form

$$F = \frac{1}{4\pi^2}\int_0^\infty d\omega\left(\frac{\omega}{2}+T\ln(1-e^{-\beta\omega})\right)\partial_\omega\phi(\omega), \tag{161}$$

where

$$\phi(\omega) = \frac{-1}{2i}[\varphi(\omega)-\varphi(\omega)^*], \tag{162}$$

with

$$\varphi(\omega) = \int_0^\infty dk_\parallel k_\parallel\sum_{X=\text{TE,TM}}\ln\left(1-r_X^2e^{2iaq}\right). \tag{163}$$

With formulas (161)–(163) we have in fact a representation of the Lifshitz formula with finite dissipation γ in terms of real frequencies. In fact, it is not really new. A similar formula was obtained in Ref. [28], however starting from the Matsubara representation with Drude permittivity inserted and applying the Abel-Plana formula [Eq. (58) in Ref. [28]]. Equations (62) and (63) in Ref. [28] correspond to the above (161)–(163), however with slightly different notations. Also we mention that the analysis done in Ref. [28] contains nearly all calculations which are needed here to investigate the limiting cases of the free energy (161) and its relation to the Matsubara representation.

We mention that the representation (161) for the free energy can also be rewritten using the same notation as in Eq. (49) and (47), with a different definition for $\hat{\boldsymbol{T}}(\omega)$ and the trace. However, because we take over a number of formulas from [28], it is meaningful also to use the notation from there.

A. Limiting case $T \to 0$

In fact, the limiting case for $T \to 0$ was calculated in Ref. [28] (and earlier; see literature cited therein). For this reason we restrict ourselves here to a short review of the methods used and display the results.

The first step of the method is the same as in Sec. III A, Eqs. (89)–(91). One derives an expansion of $\delta(\omega)$ for $\omega \to 0$ and inserting this expansion into the free energy gives its expansion for $T \to 0$. In order to get the expansion for $\omega \to 0$, it is meaningful to divide the integration region in Eq. (163) into two regions, (a) with $\omega > k_\parallel$ and (b) with $\omega < k_\parallel$, splitting $\varphi(\omega)$ accordingly,

$$\varphi(\omega) = \varphi_a(\omega) + \varphi_b(\omega), \tag{164}$$

with

$$\begin{aligned} \varphi_a(\omega) &= \int_0^\omega dk_\parallel k_\parallel \sum_{X=\mathrm{TE},\mathrm{TM}} \ln\left(1 - r_X^2 e^{2iaq}\right), \\ \varphi_b(\omega) &= \int_\omega^\infty dk_\parallel k_\parallel \sum_{X=\mathrm{TE},\mathrm{TM}} \ln\left(1 - r_X^2 e^{2iaq}\right). \end{aligned} \tag{165}$$

In this division, the first part $\varphi_a(\omega)$ is irrelevant for the leading orders in ω since it decreases not slower than $\sim\omega^2$ because of the integration interval. In $\varphi_b(\omega)$, where we have $q = \sqrt{-\omega^2 + k_\parallel^2} \equiv i\eta$ with $\eta = \sqrt{\omega^2 + k_\parallel^2}$ real, it is meaningful to change the integration variable for η. Then the relevant formulas are

$$\begin{aligned} k = i\kappa, &\quad \kappa = \sqrt{\eta^2 - (\varepsilon(\omega) - 1)\omega^2}, \\ r_{\mathrm{TE}} = \frac{\eta - \kappa}{\eta + \kappa}, &\quad r_{\mathrm{TM}} = \frac{\varepsilon(\omega)\eta - \kappa}{\varepsilon(\omega)\eta + \kappa} \end{aligned} \tag{166}$$

and we have

$$\varphi_b(\omega) = \int_0^\infty d\eta\, \eta \sum_{X=\mathrm{TE},\mathrm{TM}} \ln\left(1 - r_X^2 e^{-2a\eta}\right). \tag{167}$$

We insert the permittivity (117) and $N(\omega)$ [Eq. (24)] into κ [Eq. (166)],

$$\kappa = \sqrt{\eta^2 - \omega_p^2 \frac{\omega^2}{-\omega^2 - i\gamma\omega + \Omega^2}}. \tag{168}$$

Now, for $\Omega \neq 0$, one may obtain a power-series expansion in ω for $\omega \to 0$ and this case is not really interesting. It is largely equivalent to a fixed permittivity, considered in Sec. 4.2 in Ref. [28]. Therefore, we continue with the case $\Omega = 0$. In this case, $\varepsilon(\omega)$ [Eq. (117)] is that of the Drude model,

$$\varepsilon^{\mathrm{Dr}}(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}. \tag{169}$$

The calculation of $\varphi_b(\omega)$ for $\omega \to 0$ requires the expansion of integrals like that in Eq. (165). Partly corresponding formulas can be found in the literature. The most complete expansion is given in Appendix A in Ref. [28]. Using these results, the following expansions were obtained. From Eqs. (165) and (171) in Ref. [28] we get

$$\begin{aligned} \phi_{\mathrm{TE}}(\omega) &= \frac{2\ln 2 - 1}{2} \frac{\omega_p^2}{\gamma^2}\omega - \frac{1}{6\sqrt{2}} \left(\frac{\omega_p^2}{\gamma}\right)^3 \omega^{3/2} + O(\omega^2), \\ \phi_{\mathrm{TM}}(\omega) &= -\frac{4\pi^2\gamma}{3\omega_p^2}\omega + O(\omega^2), \end{aligned} \tag{170}$$

and from (275) in Ref. [28]

$$\begin{aligned} \Delta_T F = &\left(\frac{(2\ln 2 - 1)\omega_p^2}{\gamma} - \frac{2\pi^2\gamma}{3a^2\omega_p^2}\right)\frac{T^2}{48} \\ &- \frac{\zeta(5/2)\omega_p^2}{16\sqrt{2}\gamma^{3/2}} a T^{5/2} + O(T^3) \end{aligned} \tag{171}$$

follows. This way, the expansion of the free energy starts with T^2 and the third law of thermodynamics is respected.

B. Limiting case $\gamma \to 0$ and relation to the plasma model

For $\Omega = 0$, the limit $\gamma \to 0$ of the vanishing dissipation parameter is the most interesting one since it causes the problems with the third law. There are two aspects. One is the limit $\gamma \to 0$ at fixed T and the other is the limit $T \to 0$ with a temperature-dependent dissipation parameter $\gamma(T)$, having the property

$$\gamma(T) \underset{T \to 0}{\sim} \gamma_1 T^\alpha \quad (\alpha > 1), \tag{172}$$

where γ_1 is some constant, i.e., vanishing faster than the first power of the temperature.

On a formal level, setting $\gamma = 0$ turns the permittivity (169) of the Drude model into that of the plasma model,

$$\varepsilon^{\mathrm{pl}}(\omega) = 1 - \frac{\omega_p^2}{\omega^2}, \tag{173}$$

and the same holds for the reflection coefficients. However, the free energy does not do the same and an additional contribution appears. This can be seen in the following way. First, we remark that the additional contribution appears from the TE polarization to the function $\varphi_b(\omega)$ in Eq. (167),

$$\varphi_b^{\mathrm{TE}}(\omega) = \int_0^\infty d\eta\, \eta \ln\left(1 - r_{\mathrm{TE}}^2 e^{-2a\eta}\right). \tag{174}$$

Here the dissipation parameter enters through the momentum κ [Eq. (168)], which using (169) now reads

$$\kappa = \sqrt{\eta^2 + \frac{\omega_p^2\omega}{\omega + i\gamma}}. \tag{175}$$

This way, the dependence on γ enters only through the quotient ω/γ and we define

$$\varphi_b^{\mathrm{TE}}(\omega) \equiv \psi\left(\frac{\omega}{\gamma}\right). \tag{176}$$

For considering $\gamma \to 0$, we make the substitution $\omega \to \omega\gamma$ in the corresponding part of the free energy (161) and get

$$\begin{aligned} \Delta_T F_b^{\mathrm{TE}} = &\frac{T}{4\pi^2} \int_0^\infty d\omega \ln(1 - e^{-\beta\gamma\omega}) \\ &\times \partial_\omega \frac{1}{2i}[\psi(\omega) - \psi(\omega)^*]. \end{aligned} \tag{177}$$

Now, because $\psi(\omega)$ is decreasing for $\omega \to 0$, as follows from (170), and for $\omega \to \infty$, as can be shown easily, we can take $\gamma \to 0$ in the logarithm, $\ln(1 - e^{-\beta\gamma\omega}) = \ln\omega + \ln(\beta\gamma) + \cdots$. The term $\ln(\beta\gamma)$ does not contribute to $\Delta_T F$ and from the first term we get

$$\Delta_T F \underset{\gamma\to 0}{=} \frac{T}{4\pi^2}\int_0^\infty d\omega \ln\omega\, \partial_\omega \frac{1}{2i}[\psi(\omega)-\psi(\omega)^*]. \tag{178}$$

The integral over ω can be carried out, as shown in Appendix B in Ref. [28], and one arrives at [see Eq. (183) in Ref. [28]]

$$\lim_{\gamma\to 0}\Delta_T F = \Delta_T F^{\text{pl}} + \mathcal{F}_1 T, \tag{179}$$

with

$$\mathcal{F}_1 = \frac{-1}{4\pi^2}\int_0^\infty d\eta\, \eta \ln\left[1-\left(r_{\text{TE}}^{\text{pl}}\right)^2 e^{-2a\eta}\right], \tag{180}$$

where

$$r_{\text{TE}}^{\text{pl}} = \frac{\eta-\sqrt{\eta^2+\omega_p^2}}{\eta+\sqrt{\eta^2+\omega_p^2}} \tag{181}$$

is the reflection coefficient of the TE polarization in the plasma model and $\Delta_T F^{\text{pl}}$ is the free energy of the plasma model, i.e., the free energy with $\gamma=0$ taken from the very beginning.

The observation that the limit $\gamma\to 0$ delivers an additional contribution linear in T was made already in Ref. [29] (see also the discussion in Sec. 4.4.2 in Ref. [28] or in Sec. 14.1 in Ref. [5]) for the representation of the free energy in terms of Matsubara frequencies, which we will consider in the next section. Here we mention only that now this behavior follows also within the heat bath approach.

Using the above formulas, it is easy to consider the second aspect, i.e., the limit $T\to 0$ with $\gamma(T)$ decreasing as shown in Eq. (172). The relevant contribution comes again from (177). Inserting (172) we get

$$\Delta_T F_b^{\text{TE}} = \frac{T}{4\pi^2}\int_0^\infty d\omega \ln[1-\exp(-\gamma_1\omega T^{\alpha-1})] \times \partial_\omega \frac{1}{2i}[\psi(\omega)-\psi(\omega)^*]. \tag{182}$$

Now, for $\alpha>1$, $T\to 0$ calls, like $\gamma\to 0$ in Eq. (176), for an expansion of the logarithm and using the same arguments one arrives at

$$\Delta_T F = T\mathcal{F}_1 + O(T^2), \tag{183}$$

where $\mathcal{F}_1$ is the same as in Eq. (177). This way, a temperature-dependent dissipation parameter with the property (172) delivers for small T a linear contribution, which violates the third law.

Let us consider the relation to the free energy calculated within the plasma model in more detail. We have seen that an additional contribution comes from the TE polarization and the frequency region (b), defined in Eq. (165), i.e., from a region where $\omega\leqslant k_\|$ holds. In general, as discussed in detail in Ref. [30] (see, in particular, Fig. 2), there are frequency regions corresponding to waveguide and scattering modes. These have $\omega>k_\|$ [region (a)]. For $\omega<k_\|$ [region (b)], there are surface modes, however only in the TM polarization. This way, the additional contribution comes from the frequency region (b), where in the plasma model there are no modes.

We add a comment on the limit $\gamma\to 0$. Before the substitution $\omega\to\gamma\omega$, resulting in Eq. (177), the contribution from the region (b) to the temperature-dependent part of the free energy, following from (161), reads

$$\Delta_T F_b^{\text{TE}} = \frac{T}{4\pi^2}\int_0^\infty d\omega\, \ln(1-e^{-\beta\omega}) \times \partial_\omega \frac{1}{2i}\left[\psi\left(\frac{\omega}{\gamma}\right)-\psi\left(\frac{\omega}{\gamma}\right)^*\right]. \tag{184}$$

If we set $\gamma=0$ here directly in the integrand we get zero since $\psi(\infty)$ is real. This can be seen from (175), which turns into $\kappa=\sqrt{\eta^2+\omega_p^2}$, which is the same as in Eq. (181). However, as we have seen above, this result is incorrect. Indeed, interchanging the limit $\gamma\to 0$ and the integration in the representation (184) is not allowed in distinction to the representation (177).

C. Transition to the Matsubara representation

In the WW configuration, the transition to the Matsubara representation can be done the same way as is in the two preceding sections; however now it is even easier since $\phi_X(\omega=0)=0$ [see (170)] and no problems may appear in dividing the integral in Eq. (161) into two integrals according to (162). This way, from (161)–(163), we arrive at the known formulas for the free energy in the Matsubara representation, i.e., to the Lifshitz formula with finite dissipation γ. These formulas read

$$F = \frac{1}{4\pi^2} T \sum_{l=0}^{\infty}{}' \varphi(i\xi_l) \quad (\xi_l = 2\pi T L), \tag{185}$$

with

$$\varphi(i\xi) = \int_{\xi_l}^\infty d\eta\, \eta \sum_{X=\text{TE,TM}} \ln\left(1-r_X^2 e^{-2a\eta}\right) \tag{186}$$

and the reflection coefficients

$$r_{\text{TE}} = \frac{\eta-\kappa}{\eta+\kappa}, \quad r_{\text{TM}} = \frac{\varepsilon(i\xi)\eta-\kappa}{\varepsilon(i\xi)\eta+\kappa}, \tag{187}$$

which are the same as in Eq. (166) except for momentum and permittivity,

$$\kappa = \sqrt{\eta^2+\omega_p^2\frac{\xi^2}{\xi^2+\xi\gamma+\Omega^2}}, \quad \varepsilon(i\xi) = 1+\frac{\omega_p^2}{\xi^2+\xi\gamma+\Omega^2}. \tag{188}$$

Here several comments are in order. In the Lifshitz formula (185), criticality never appears. This can be seen in Eq. (186), where we have $r_X\leqslant 1$ since all quantities entering (187) are non-negative. For $\Omega=0$, which makes the permittivity (188) like that of a metal, for $l=0$ a peculiarity appears. In general, for $\xi\to 0$ we note $\varepsilon(i\xi)\to\infty$, and the reflection coefficients turn into

$$r_{\text{TE}}\to 0, \quad r_{\text{TM}}\to 1, \tag{189}$$

i.e., only the reflection coefficient for the TM polarization turns into that of an ideal conductor and that of the TE polarization turns into zero. This way, the contribution from the TE polarization to the zeroth Matsubara frequency is missing. This is counterintuitive, especially since $l=0$ determines the behavior of the free energy for $T\to\infty$. This problem is well known and has discussed, for instance, in Chap. 14.1 in Ref. [5]. A similar problem was observed earlier for fixed permittivity ε [for $\varepsilon \to \infty$ we have also (189)] and resolved by the Schwinger prescription in Ref. [31]. Here we have to state that this problem appears in the heat bath approach too.

We mention that the linear term $\mathcal{F}_1 T$ in Eq. (179) can be seen in the Matsubara representation more easily since it simply describes the difference between the Drude model for $\gamma \to 0$ and the plasma model at $\gamma = 0$, which in the Matsubara representation shows up in the zeroth Matsubara frequency, $l = 0$, and $\xi_0 = 0$. As seen from (181), the reflection coefficient for the plasma model does not depend on ξ and $\xi = 0$ gives $r_{\text{TE}} \neq 0$, whereas from (187) and (188), for $\Omega = 0$ and $\gamma \neq 0$, (189) follows for $\xi = 0$. This way, $l = 0$ turns (182) just into $\mathcal{F}_1 T$ with $\mathcal{F}_1$ given by (180).

VI. CONCLUSION

In the foregoing sections we considered dipoles interacting with the electromagnetic field and with heat baths. The aim is to describe, in this system, dissipation from first principles. Indeed, and this was in principle known before, this is possible using known formulas. We got a general representation (49) for the free energy.

This representation is similar to the remarkable formula in Ref. [15] and one may expect that it reflects some more general underlying structure. For our system, we have with (47) a specific expression in terms of the T operator of the effective equation (27) for the electric field.

We applied the general formula to three configurations: AA and AW, which correspond to the Casimir-Polder force, and WW, which corresponds to the Casimir effect. In each case, we obtain a representation of the free energy in terms of an integral over real frequencies in the presence of dissipation. For the AA and AW configurations, we obtain formulas which are nonperturbative in the polarizability, i.e., include all orders. Of course, from here the known expansions (79) and (142), for small polarizability or large separation, follow. It should be mentioned that in this sense the WW configuration, i.e., the Lifshitz formula, is always nonperturbative.

In the nonperturbative treatment of the AA and AW configurations, criticality may appear. As a result, the transition to the Matsubara representation becomes modified. Another modification of the Matsubara representation occurs if the intrinsic frequency of the atoms in the AA and AW configurations vanishes. This modification results in a change of the contribution from the zeroth Matsubara frequency, Eqs. (106), (107), and (153).

The main motivation for the present paper was to look at the problems with thermodynamics known in connection with the Casimir effect for the temperature-dependent dissipation parameter, decreasing faster than the first power of the temperature. First of all, the dissipation parameter γ, as it appears in Eq. (11) from the heat bath, does not depend on temperature (it may depend on frequency), so to say, by construction. The temperature dependence comes in solely through the averages (12). We show that in all cases, for a constant γ, the laws of thermodynamics are respected. If, however, inserting by hand a temperature dependence into the dissipation parameter as given by Eq. (172), the known problems appear, now also in the heat bath approach. We conclude that the heat bath approach, at least in the present form, is insufficient to solve the mentioned problems. In calling for another approach one should bear in mind that the temperature dependence (172) follows from the behavior of real metals and this way cannot be ignored.

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