Casimir energy in spherical cavities

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Abstract
We calculate the Casimir energy at spherical cavities within a host made up of an arbitrary material described by a possibly dispersive and lossy dielectric response. To that end, we add to the coherent optical response a contribution that takes account of the incoherent radiation emitted by the host in order to guarantee the detailed balance required to keep the system at thermodynamic equilibrium in the presence of dissipation. The resulting boundary conditions allow a conventional quantum mechanical treatment of the radiation within the cavity from which we obtain the contribution of the cavity walls to the density of states, and from it, the thermodynamic properties of the system. The contribution of the cavity to the energy diverges as it incorporates the interaction energy between neighbor atoms in a continuum description. The change in the energy of an atom situated at the center of the cavity due to its interaction with the fluctuating cavity field is however finite. We evaluate the latter for a simple case.

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1. Introduction
Motivated by his finding that zero-point fluctuations may induce an attractive force between parallel conducting plates [1], Casimir proposed in 1956 that the zero-point force could be the Poincaré stress involving a semiclassical model of the electron [2]. In that model the electron was considered as a spherical charge distribution stabilized by vacuum fluctuations. However, Boyer [3] showed in 1968 that the stress for a spherical conducting shell of radius $a$ is indeed repulsive, since the Casimir energy turns out to be positive: $E = \frac{0.09235}{2a}$. Subsequent calculations based on a Green’s function method [4] and on a multiple scattering formalism [5] confirmed Boyer’s calculation. The more general problem of the Casimir effect of a dielectric ball was first considered by Milton [6] in the absence of dispersion, and later on by Candelas
Candelas argued that in the presence of boundaries vacuum energies depend on a cutoff on transverse momenta, independent of the dielectric properties of the media. Therefore, Boyer’s result should be corrected by terms associated to surface and curvature tensions. The Casimir forces for a dilute dielectric and diamagnetic sphere was studied by Brevik and Kolventvedt [8], and more recently by Klich [9], while the role of dispersion in this problem was discussed in [10–12]. In this case, the Casimir stress may be attractive, but very sensitive to the specific values of the parameters characterizing the electric and magnetic response of the materials. An excellent review of different approaches to the Casimir effect of spherical regions, together with applications to QCD bag models, higher dimensional spaces, or sonoluminescence can be found in [13].

In a series of papers [14–16] an expression for the Casimir force within planar cavities was derived without making particular models or assumptions about the nature of the walls. By considering that the system is in a thermodynamic equilibrium, we obtained the energy and the stress tensor in a closed ancillary system that has the same optical response as the original system. This approach consistently incorporates evanescent fields and allows a fully quantum–mechanical treatment of the electromagnetic degrees of freedom. Unlike the calculations presented in [14–16] the fictitious system was eliminated in [17], keeping only its essential property that detailed balance should hold in thermodynamic equilibrium: for each photon that is not coherently reflected at the cavity walls and is therefore either absorbed or transmitted beyond the system, an identical photon has to be incoherently injected back into the cavity with no phase relation with the lost photon. In this paper we show that approach may be straightforwardly generalized to study the Casimir effect of spherical cavities with arbitrary dielectric properties. We then apply the formalism to calculate the energy shift for a polarizable atom placed at the center of a cavity.

2. Theory

Consider a system made up of an empty spherical cavity of radius $R$ carved out of an arbitrary material and with a scatterer situated at its center (figure 1). Within the empty space of the cavity there are outgoing ($o$) and ingoing ($i$) electromagnetic waves with transverse electric (TE) and transverse magnetic (TM) polarizations, described by the field

$$F_{d\xi}^{d\xi}(\vec{r}) = \int_{l=0}^{\infty} f_{d\xi}^{l\xi} h_{d}^{l}(kr) Y_{lm}(\hat{r}),$$

where $d = o, i$ describes the propagation direction, $\xi = TE, TM$ describes the polarization, $l = 0, 1, 2, \ldots$ denotes the angular momentum, $m = -l \ldots l$ its projection along the $z$-axis, $h_{o}^{l} \equiv h_{o}^{l(1)}$ and $h_{i}^{l} \equiv h_{i}^{l(2)}$ are the outgoing and the ingoing spherical Hankel functions respectively, $k = \omega/c$ is the wavenumber within vacuum, and we choose the scalar field $F_{d\xi}^{TE} \equiv \vec{B}_{d\xi}^{TE} \cdot \vec{r}$ to describe the TE electromagnetic field $(\vec{E}_{d\xi}^{TE}, \vec{B}_{d\xi}^{TE})$ and $F_{d\xi}^{TM} \equiv \vec{E}_{d\xi}^{TM} \cdot \vec{r}$ to describe the TM electromagnetic field $(\vec{E}_{d\xi}^{TM}, \vec{B}_{d\xi}^{TM})$ [18]. When the outgoing radiation reaches the boundary of the cavity it is partially scattered back into the cavity with an amplitude $s_{h\xi}^{l\xi}$, and when the ingoing radiation hits the scatterer at the center it is scattered back toward the cavity with an amplitude $s_{c\xi}^{l\xi}$, that is,

$$f_{o}^{i} = s_{b} f_{o}^{o},$$

$$f_{o}^{o} = s_{c} f_{i}^{i},$$

where we removed the indices $l, m$ and $\xi$ to simplify our notation. From equations (2) and (3) we immediately obtain the normal modes of the system, given by

$$1 - s_{b}s_{c} = 0.$$
Taking into account the frequency ($\omega$) dependence of $s_b$ and $s_c$, we may solve equation (4) to obtain the frequency spectrum $\omega_n$ for each value of $l$, $m$ and $\zeta$. However, in the presence of absorbing materials or even of transparent, leaky materials, $\omega_n$ would turn out to be complex. The system would be open and ordinary quantum mechanics would not be applicable to the radiation field, i.e., $\hbar \omega_n$ would not be an energy quantum.

The coefficients $s_b$ and $s_c$ describe the amplitude and the phase of the radiation that is coherently scattered back into the cavity. The energy that is not coherently scattered back into the cavity, described by $1 - |s_c|^2$ and $1 - |s_b|^2$, is absorbed or it leaves the system through its external boundary. Nevertheless, in thermodynamic equilibrium, an absorbing scatterer or an absorbing enclosure has to eventually radiate back any radiation that it absorbs. The system should also admit photons from the vacuum that surrounds it to replenish those photons that were transmitted away. Detailed balance must hold and in the average, for each photon with numbers $l$, $m$ and $\zeta$ that leaves the cavity, an identical photon, with the same numbers but having no phase relation with the original photon, has to be injected back into the cavity. We mimic this incoherent radiation by a coherent field that is delayed a large time $T_\chi$ ($\chi = b, c$).

To avoid interference with the coherently scattered field, we take the limit $T_{\chi} \rightarrow \infty$. Thus, the incoherent radiation may be taken into account by replacing the scattering coefficients $s_b$ and $s_c$ by total scattering coefficients

$$s_\chi \rightarrow S_\chi = \frac{s_\chi + a_\chi e^{i\omega T_\chi}}{1 + b_\chi e^{i\omega T_\chi}}, \quad \chi = b, c.$$  \hfill (5)

Here, $\exp(i\omega T_\chi)$ is the phase acquired during the large delay $T_\chi$ and is an extremely fast varying function of the frequency $\omega$, so that for any finite bandwidth interference effects would disappear. We assume that $a_\chi$ and $b_\chi$ are relatively slowly varying functions of frequency which are to be determined. The term $s_\chi$ in the numerator corresponds to the coherent scattering. The term $a_\chi e^{i\omega T_\chi}$ corresponds to re-radiation by the central scatterer ($\chi = c$), re-radiation by the walls of the cavity ($\chi = b$) or to photons that enter the system from outside to replenish the cavity losses. Finally, it may happen that a re-radiated photon fails to reach the cavity on its first attempt, as it may be re-absorbed or scattered away. Thus, we should allow for multiple injection attempts. These are accounted for by the term $b_\chi e^{i\omega T_\chi}$ in the denominator.

As all the energy that leaves the cavity has to enter again in an equilibrium situation, the total scattering amplitudes must obey

$$|S_\chi|^2 = 1,$$ \hfill (6)

which yields

$$|s_\chi|^2 + |a_\chi|^2 + 2 \Re s_\chi^* a_\chi e^{i\omega T_\chi} = 1 + |b_\chi|^2 + 2 \Re b_\chi e^{i\omega T_\chi}.$$ \hfill (7)
Separating the slowly from the rapidly varying terms,
\[ |s_x|^2 + |a_x|^2 = 1 + |b_x|^2, \]
we obtain
\[ a_x = e^{i\delta_x}, \quad b_x = s_x^* e^{i\delta_x}, \]
where \( \delta_x \) are slowly varying phases. The normal modes of the system in equilibrium are not given by equation (4) but by
\[ D = 1 - S_b S_c = 0, \]
which may be recast as
\[ 2\text{arg}(1 + s_b e^{i\delta_b} e^{i\omega T_b}) + 2\text{arg}(1 + s_c e^{i\delta_c} e^{i\omega T_c}) + (\delta_b + \delta_c) + \omega (T_b + T_c) = 2\pi n, \]
with integer \( n \). The first two terms on the LHS of equation (11) oscillate rapidly, but are bounded within the interval \((-\pi, \pi)\), while the third term varies slowly. Thus, the separation between nearby modes \( \omega_n \) is close to 
\[ \Delta \omega = \frac{2\pi}{(T_b + T_c)}, \]
and the density of modes diverges in the limit \( T_b, T_c \to \infty \). This is to be expected, as our delayed re-radiation accounts implicitly for the interaction with a thermal bath which has infinite degrees of freedom. Our dissipative system together with the thermal bath forms an extended closed system whose modes are actually real [19] and form a quasi-continuum. Our approach above is an alternative to the introduction of ancillary systems to account for dissipation [16, 20].

The actual number of modes \( \Delta N \) within a small frequency range \( \Delta \Omega \) may be obtained using Cauchy's argument principle
\[ \Delta N = \frac{1}{2\pi i} \oint_{\gamma} \frac{d}{d\omega} \log f(\omega), \]
where \( \gamma \) is a contour that encircles counterclockwise the interval \( \Delta \Omega \) and \( f(\omega) \) is an analytical function that has the same zeroes as \( D \) (equation (4)) and no poles within \( \gamma \). We choose a contour \( \gamma \) that moves toward the right a distance \( \eta \) below the real axis, then crosses the axis, moves back a distance \( \eta \) above the real axis and finally crosses the axis to closes upon itself [19] (figure 2). Choosing as \( f(\omega) \) the analytical continuation from the real axis unto the complex plane of
\[ f(\omega) = (1 + s_b^* e^{i\delta_b} e^{i\omega T_b})(1 + s_c^* e^{i\delta_c} e^{i\omega T_c}) - (s_b + e^{i\delta_b} e^{i\omega T_b})(s_c + e^{i\delta_c} e^{i\omega T_c}), \]
we obtain
\[ \Delta N = \frac{1}{2\pi i} \Delta f(\omega) \bigg|_{\omega \to i\eta} - \frac{1}{2\pi i} \Delta \log \left[ \frac{1 - s_b s_c^*}{1 - s_b s_c} \right] i(\delta_b + \delta_c) + i\omega (T_b + T_c) + \eta (T_b + T_c) \]
in the limit \( T_x \to \infty, \eta \to 0, \eta T_x \to \infty \). Subtracting the number \( \Delta N_0 \) of modes corresponding to vacuum and the thermal reservoir only, obtained from equation (14) by replacing \( s_b \to 0, s_c \to 1 \), we obtain
\[ \Delta N - \Delta N_0 = -\frac{1}{\pi} \Delta \text{Im} \log(1 - s_b s_c) \equiv \rho(\omega) \Delta \Omega, \]
where we identify the contribution of the scatterers to the density of states,
\[ \rho(\omega) = -\frac{1}{\pi} \frac{d}{d\omega} \log(1 - s_b s_c), \]
for each value of \( l, m \) and \( \zeta \).
Figure 2. Integration contour γ employed to obtain the density of states. We indicate the normal modes (crosses) separated approximately by Δω0.

From the density of states, one can proceed to calculate all the thermodynamic quantities. For example, multiplying \( \rho(\omega) \) by the ground state energy \( \hbar \omega/2 \) of an oscillator of frequency \( \omega \), integrating over all frequencies and adding over all angular momenta and polarizations we obtain the contribution of the scatterers to the ground state energy,

\[
U_0 = \frac{\hbar}{2\pi} \sum_{l,m,\zeta} \int_0^\infty du \log \left| 1 - s_{b,lm}^\zeta(iu)s_{c,lm}^\zeta(iu) \right|, \tag{16}
\]

where we have already rotated the integration trajectory unto the imaginary axis.

Equation (16) and similar equations easily derived for other thermodynamic quantities are the main results of the present paper. In order to evaluate them the only requirement is knowledge of the scattering amplitudes corresponding to the surface of the cavity and to the scatterer at the center.

3. Empty cavity within a uniform medium

For an empty cavity \( s_{c,lm}^\zeta = 1 \), as the incoming field becomes an outgoing field after crossing the origin. If the cavity is surrounded by a uniform medium with a dielectric function \( \epsilon(\omega) \), then \( s_{b,lm}^\zeta \) may easily be found by writing the field within the cavity as a linear combination of outgoing and ingoing fields (equation (1)), writing the field within the medium as an outgoing field and matching both solutions through the usual boundary conditions, i.e., the continuity of the projections of both the electric and magnetic fields along the surface. The result [21] is simply given by

\[
s_{TE,b,lm}(\omega) = -\frac{Q_{MV,0}^{V0M0} - Q_{V0M0}^{V0M0}}{Q_{V0M0}^{V0M0} - Q_{V0M0}^{V0M0}}, \tag{17}
\]

where

\[
Q_{i}^{AAD',d,d'} \equiv k_A h^d_A(k_A R) \hat{D} h^{d'}_{A'}(k_A R), \quad A, A' = V, M, \quad d, d' = i, o, \tag{18}
\]

\( k_A \) is the wavenumber within vacuum \( (A = V, k_V = k = \omega/c) \) or within the medium \( (A = M, k_M = k/\sqrt{\epsilon}) \), \( h^d_A \) are the ingoing \( (d = i) \) or outgoing \( (d = o) \) spherical Hankel functions and \( \hat{D} \) is the operator

\[
\hat{D}g(x) \equiv g'(x) + g/x. \tag{19}
\]

Similarly, for TM polarization we have

\[
s_{TM,b,lm}(\omega) = -\frac{Q_{MO,0}^{MO0} - Q_{MO0}^{MO0}}{Q_{MO0}^{MO0} - Q_{MO0}^{MO0}/\epsilon}. \tag{20}
\]

As \( s_{c,lm}^\zeta \) is independent of \( m \), we may replace the sum over \( m \) in equation (16) by a factor of \( 2l + 1 \).

In figure 3 we show the TM contribution to the integrand of equation (16) as a function of the imaginary part of the frequency \( u = \omega/i \) calculated for a dielectric cavity with a
Lorentzian response $\epsilon = 1 + \omega_p^2 / (\omega_0^2 - \omega^2 - i \gamma \omega)$. The figure shows integrable singularities at $u = 0$. A second singularity is seen for even values of $l$. Nevertheless, it is clearly seen that the contributions to the energy grow with $l$ and that equation (16) does not converge.

Our calculation above includes a realistic dielectric response for the medium surrounding the cavity and in our calculation the electromagnetic field permeates all space. Thus, the singularities above are of a different physical nature than the singularities arising in naive calculations for flat surfaces. For example, the singularities in the Casimir force among perfect conducting slabs may be removed by introducing a high-frequency cutoff which accounts for the high-frequency transparency of real metals and by considering the mechanical properties of the field beyond the slabs. Those recipes would not cure the present divergence.

Note that large $l$s correspond to spatial oscillations around the sphere with a small lengthscale $d = 2 \pi R / l$. As we may assume a smallest lengthscale $d_{at}$ of atomic dimensions, it seems reasonable to impose a corresponding cutoff at $l_{\text{max}} = 2 \pi R / d_{at}$. A careful analysis [21] shows that in this case equation (16) converges, but that the leading terms are of the order $(R / d_{at})^3$ and $(R / d_{at})^2$, i.e., of the order of the number of atoms within the volume and the surface of a sphere of radius $R$. Mathematically, these terms arise from the leading terms in an expansion of the integrand of equation (16) for large $l$, which, after summing over $m$ are of the orders $l^2$ and $l$ (with logarithmic corrections). Physically, the reason is that equation (16) includes the electromagnetic interaction between nearest neighbor atoms, which in a continuum description are infinitely small and infinitely close to each other. Similar divergent terms were found in a pairwise perturbative calculation [22] for cavities surrounded by a very diluted dielectric. As argued in [22], these short-range contributions should be taken into account before conclusions about the sign of the Casimir force can be drawn.

A finite Casimir energy may be obtained by subtracting from our result above those terms that contribute to the divergence before we take the limit $d_{at} \rightarrow 0$. Nevertheless, the resulting energy would be an experimentally inaccessible quantity for a spherical cavity, as changing the cavity radius would require adding or removing atoms or else introducing strains that would
produce an elastic stress [23]. Furthermore, a full calculation of the interatomic interactions would be required in order to compare experimental results to theoretical calculations, and our equation (16) would be insufficient. One way out of these difficulties is to study other geometries where motion introduces no elastic stresses. For example, it has been found [23] that for a piston sliding along a cylinder, the contribution of its position to the Casimir energy is free of cutoff-dependent singularities and is attractive.

4. Atom within a cavity

On the other hand, equation (16) would still be useful in situations where the geometry of the cavity is left unchanged. For example, it may be used to calculate the change

$$
\Delta U = \frac{\hbar}{2\pi} \sum_{l,m,\zeta} \int_0^\infty du \log \left| \frac{1 - s_{b,lm}(iu)s_{c,lm}(iu)}{1 - s_{b,lm}(iu)} \right|
$$

(21)

in the energy of the system when an atom is introduced at the center of the cavity. Using the usual selection rules, we obtain that the dispersion amplitude for an atom, $s_{c,lm} = 1$, would be the same as for empty space, unless $l = 1$ and the polarization $\zeta = TM$, in which case,

$$
s_{TM}^{c,lm} = \frac{1 + \frac{3}{2}i k^3 \alpha}{1 - \frac{3}{2}i k^3 \alpha},
$$

(22)

where $\alpha$ is the electric-dipole polarizability of the atom. Therefore, there is only one finite term in equation (21).

In figure 4 we show the contribution to the energy of a cavity from an atom lying at its center. The atomic polarizability is taken as a Lorentzian

$$
\alpha(\omega) = \frac{e^2}{m} \frac{1}{\omega_0^2 - \omega^2}
$$

(23)

with a single resonance frequency $\omega_0$. The energy is negative and proportional to $R^{-3}$ and is of the order of tens of meVs for radii of a few nanometers.
5. Conclusions

Based on a scattering approach we have derived an expression for the Casimir energy of a spherical cavity with dispersive and absorptive dielectric properties. It turns out that the expression is divergent due to the summation over angular momenta, independent of the dielectric behavior of the cavity walls. This may be regularized by imposing a cutoff associated with the finite separation of atomic scatterers forming the boundary of the cavity, leading to contributions proportional to the number of atoms in the volume and surface of the cavity. On the other hand, the energy shift for an atom placed at the center of the cavity is finite, since its introduction does not modify the geometry of the cavity.

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