Casimir-Polder interatomic potential between two atoms at finite temperature and in the presence of boundary conditions

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Abstract

We evaluate the Casimir-Polder potential between two atoms in the presence of an infinite perfectly conducting plate and at nonzero temperature. In order to calculate the potential, we use a method based on equal-time spatial correlations of the electric field, already used to evaluate the effect of boundary conditions on interatomic potentials. This method gives also a transparent physical picture of the role of a finite temperature and boundary conditions on the Casimir-Polder potential. We obtain an analytical expression of the potential both in the near and far zones, and consider several limiting cases of interest, according to the values of the parameters involved, such as atom-atom distance, atoms-wall distance and temperature.

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I. INTRODUCTION

Casimir-Polder forces are long-range interactions between neutral atoms or molecules due to their common interaction with the electromagnetic radiation field. In the case of two atoms in the vacuum (zero temperature) the Casimir-Polder potential energy behaves as $R^{-6}$ for interatomic distances smaller than typical atomic transition wavelengths from the ground state (near zone) and as $R^{-7}$ for larger distances (far zone) [1]. In the near zone the potential energy coincides with the well-known van der Waals interaction, but in the far zone it decreases more rapidly due to retardation effects. Analogous interactions exist between an atom and a neutral conducting wall and between two conducting or dielectric walls (the so-called Casimir effect) [2]. These interactions are usually considered as a manifestation of the quantum nature of the electromagnetic radiation field and related to the zero-point energy. Although Casimir-Polder and Casimir energies are very small, the Casimir force between macroscopic objects has been measured with remarkable precision (for a review, see [3]). Relevance of Casimir forces to nano- and micro-devices has been also shown [4, 5]. Also the atom-wall Casimir-Polder force has been recently measured with precision, both in the near and in the far zone [6, 7, 8, 9, 10]. The atom-atom van der Waals/Casimir-Polder energy is still weaker, but experimental indirect evidences of them exist since a long time, in agreement with theoretical predictions [11]. Direct measurements of the retarded van der Waals attraction in mesoscopic systems have been also obtained [12, 13]. In order to obtain direct high-precision evidence of the atom-atom force, it can be relevant to evaluate them in realistic situations to be compared with actual laboratory situations, for example by taking into account temperature effects and/or the presence of boundary conditions, as well as to envisage situations where the intensity of these forces could be increased. In a previous paper we have calculated the atom-atom Casimir-Polder interaction energy when the two atoms are placed in the vicinity of a perfectly conducting wall (at zero temperature), obtaining also a transparent physical interpretation of the results in terms of image dipoles [14]. In this paper we generalize this work and consider the Casimir-Polder interaction between two ground-state atoms at finite temperature and with boundary conditions present, such as a conducting wall. We use a method based on spatial correlations of the fields [15], which, beside being well suited as a calculation tool for this kind of problems, also gives a clear physical interpretation of the results obtained. In Section [11] we outline the method used by
reproducing in a simpler and transparent way the result for the Casimir-Polder potential energy between two atoms in a thermal field, well known in the literature (see, for example \[16\]). In Section III we derive and discuss our results for the retarded atom-atom Casimir-Polder interaction when are present both a thermal field and a boundary condition. Several limiting cases involving the relevant parameters of the system (temperature, atom-atom and atoms-wall distances) are explicitly discussed.

II. THE CASIMIR-POLDER POTENTIAL BETWEEN TWO ATOMS AT NONZERO TEMPERATURE IN THE FREE SPACE

We first consider two neutral atoms interacting with the quantum electromagnetic radiation field in a thermal bath at temperature \(T\), and we investigate their Casimir-Polder interaction. Our approach to this problem exploits the idea that field fluctuations induce instantaneous dipole moments in the two atoms, which are correlated because vacuum fluctuations are spatially correlated. The Casimir-Polder potential energy then arises from the classical interaction between the oscillating dipoles of the atoms \[15\]. This method has been used in several different contexts, such as three-body forces \[17\] and time dependent situations \[18, 19\]. It has been recently used also in the case in which boundary conditions are present \[14, 20\]. In this Section we show that this method is valid and computationally useful also for the calculation of Casimir-Polder forces at a nonzero temperature.

The relation between the Fourier components of the fluctuating electromagnetic field (zero-point and/or thermal fields) and of the induced dipole moment in the atoms is \[15\]

\[
\mu_l(kj) = \alpha(k) E_l(kj, r) \tag{1}
\]

where

\[
\alpha(k) = \frac{2}{3 \hbar c} \sum_p \frac{k_{p0}}{k_{p0}^2 - k^2} |\mu_{p0}|^2
\]

is the dynamical polarizability of the atoms (assumed isotropic for simplicity), \(\hbar c k_{p0} = E_p - E_0\) is the transition energy from the state \(p\) to the ground state \(0\) of the atom and \(\mu_{p0}\) are matrix elements of the atomic dipole momentum operator. \(E_l(kj, r)\) is the \(l\) component of the electric field operator, that in the multipolar coupling scheme coincides with the
transverse displacement field \[\mathbf{e}(k, r) = i \sqrt{\frac{2\pi \hbar c}{V}} \hat{e}_k e^{ik \cdot r} \] (3)

The Casimir-Polder interaction energy, described as the classical interaction between the induced atomic dipole moments \[15\], is then written as

\[
W_{AB}(R) = \sum_{k,j} \langle \mu_A^k(r) \mu_B^j(r) \rangle V_{lm}(R) = \sum_{k,j} \alpha_A(k) \alpha_B(k) \langle E_l(k, r_A) E_m(k, r_B) \rangle V_{lm}(k, R)
\] (4)

where \( R = |r_B - r_A| \) is the distance between the two atoms and

\[
V_{lm}(k, R) = (\nabla^2 \delta_{lm} - \nabla_l \nabla_m) R \cos kR \frac{R}{R^3} = \frac{1}{R^3} \left\{ \left( \delta_{lm} - 3 \hat{R}_l \hat{R}_m \right) \left( \cos kR + kR \sin kR \right) - \left( \delta_{lm} - \hat{R}_l \hat{R}_m \right) k^2 R^2 \cos kR \right\}
\] (5)

is the classical electromagnetic potential tensor between two oscillating dipoles at frequency \( ck \) \[22\], and the superscript \( R \) indicates the variable with respect the derivatives are taken.

The expectation value of the spatial field correlation \( \langle E_l(k, r_A) E_m(k, r_B) \rangle \) in (4) must be taken on the field state in consideration, in our case the equilibrium thermal state at temperature \( T \) (isotropic and unpolarized). Thus

\[
\langle a_{k,j}^\dagger a_{k,j} \rangle = \frac{1}{e^{\hbar c k/k_B T} - 1}
\] (6)

where \( k_B \) is the Boltzmann constant. We assume that the temperature is such that the atomic excitation probability due to the thermal field is negligible (that is, \( k_B T \ll \hbar \omega_0 \), \( \omega_0 \) being a typical transition frequency of the atom).

In the continuum limit, we can easily perform the polarization sum and the angular integration

\[
\sum_j \int d\Omega_k \langle E_l(k, r_A) E_m(k, r_B) \rangle = \frac{8\pi^2 \hbar c k}{V} \coth \left( \frac{\hbar c k}{2k_B T} \right) \tau_{lm}(k, R)
\] (7)

where we have used (6) and defined the tensor

\[
\tau_{lm}(k, R) = \frac{1}{4\pi} \int d\Omega_k \left( \delta_{lm} - \hat{R}_l \hat{R}_m \right) e^{\pm i k \cdot R} = -(\nabla^2 \delta_{lm} - \nabla_l \nabla_m) R \sin kR \frac{R}{k^3 R^3} + \left( \delta_{lm} - 3 \hat{R}_l \hat{R}_m \right) \left( \frac{\cos kR}{k^2 R^2} - \frac{\sin kR}{k^3 R^3} \right)
\] (8)
The final expression for Casimir-Polder energy, valid at any distance $R$ between the atoms outside regions of wavefunctions overlapping, is
\[
W_{AB}(R) = \frac{\hbar c}{\pi} \int_0^\infty k^3 \alpha_A(k)\alpha_B(k) \coth \left( \frac{\hbar c k}{2k_B T} \right) V_{lm}(k, R)\tau_{lm}(k, R)
\]
\[
= -\frac{\hbar c}{\pi} \int dk \alpha_A(k)\alpha_B(k) \coth \left( \frac{\hbar c k}{2k_B T} \right) \times \left( \left( \nabla^2 \delta_{lm} - \nabla_i \nabla_m \right) R \cos kR \right) \left( \left( \nabla^2 \delta_{lm} - \nabla_i \nabla_m \right) R \sin kR \right)
\]
\[
= -\frac{\hbar c}{\pi R^3} \int_0^\infty dk k^3 \alpha_A(k)\alpha_B(k) \coth \left( \frac{\hbar c k}{2k_B T} \right) \left( kR \sin 2kR \cos 2kR - 5 \frac{\sin 2kR}{kR} - 6 \frac{\cos 2kR}{k^2 R^2} + 3 \frac{\sin 2kR}{k^3 R^3} \right).
\]

In the so-called near zone, that is for interatomic distances smaller than typical atomic transition wavelengths from the ground state, we can approximate $kR \ll 1$, and this expression reduces to
\[
W_{AB}(R) \simeq -\frac{3\hbar c}{\pi R^6} \int dk \alpha_A(k)\alpha_B(k) \coth \left( \frac{\hbar c k}{2k_B T} \right) \sin 2kR
\]
which coincides with the result obtained in [23] with different methods. For larger distances, in the so-called far zone, we can replace the dynamical polarizabilities $\alpha_{A,B}(k)$ with their static values $\alpha_{A,B} = \alpha_{A,B}(0)$. After integration over $k$, we obtain
\[
W_{AB}(R) = \alpha_A\alpha_B k_B T Q^R \coth \left( \frac{2\pi k_B T R}{\hbar c} \right)
\]
where the differential operator
\[
Q^R = \left( -\frac{1}{16r^2} \frac{\partial^4}{\partial r^4} + \frac{1}{4r^3} \frac{\partial^3}{\partial r^3} - \frac{5}{4r^4} \frac{\partial^2}{\partial r^2} + \frac{3}{r^5} \frac{\partial}{\partial r} - \frac{3}{r^6} \right)
\]
has been defined. The result (11) was already obtained by Boyer in the framework of stochastic electrodynamics [24]. Our method has allowed us to reproduce known results in a simpler way, also obtaining a transparent physical interpretation of Casimir-Polder forces at finite temperature in terms of the atomic dipole moments induced by both vacuum and thermal field fluctuations.

We can consider two limiting cases of (11) (far zone), given by $2\pi k_B TR/\hbar c \ll 1$ and $2\pi k_B TR/\hbar c \gg 1$; they can be considered as a low- and high-temperature limit of the Casimir-Polder energy, respectively. Alternatively, for a given value of the temperature, as it is known, there is a new distance scale inside the far zone given by $\hbar c/2\pi k_B T$: for distances smaller than this scale, equation (11) gives a potential energy as $R^{-7}$, while for larger distances the potential behaves as $R^{-6}$, as in the near zone [16, 23, 26].
III. THE CASIMIR-POLDER INTERACTION BETWEEN TWO ATOMS AT NONZERO TEMPERATURE IN THE PRESENCE OF A CONDUCTING WALL

We now consider how the presence of a boundary condition such as a perfectly conducting wall modifies the Casimir-Polder interaction between the two atoms at finite temperature. We use the same method discussed in Section II. The electric field operator is now

\[ E(r) = \sum_{kj} E(k_j, r) = i \sum_{kj} \sqrt{\frac{2\pi \hbar c k}{V}} f(k_j, r) \left( a_{kj} - a_{kj}^\dagger \right), \]  

where \( f(k_j, r) \) are appropriate mode functions given by the boundary conditions for the field operators (\( j \) is a polarization index). As shown in [14], the presence of the wall requires also a modification of the classical interaction between the induced atomic dipoles to be used in our method, because the image dipoles (reflected on the wall) must be taken into account. We assume the wall located at \( z = 0 \), and that \( r_A, r_B \) are respectively the positions of atoms A and B.

Thus we write the atom-atom Casimir-Polder interaction energy as

\[ W_{AB}(R, \bar{R}) = \sum_{kj} \mu^A_l(k_j) \mu^B_m(k_j) V_{lm}(k, R, \bar{R}) \]

\[ = \sum_{kj} \alpha_A(k) \alpha_B(k) \langle E_l(k_j, r_A) E_m(k_j, r_B) \rangle V_{lm}(k, R, \bar{R}) \]  

where the quantum average of the field operators is taken on a thermal state of the radiation field at temperature \( T \). As already mentioned, the potential tensor \( V_{lm}(k, R, \bar{R}) \) should now take into account not only the interaction between the two induced atomic dipoles, but also the interaction between the induced dipole of one atom and the image reflected on the wall of the induced dipole of the other atom. So we take the following expression for the potential tensor

\[ V_{lm}(k, R, \bar{R}) = V_{lm}(k, R) - \sigma_{lp} V_{pm}(k, \bar{R}) \]

\[ = (\nabla^2 \delta_{lm} - \nabla_l \nabla_m) R \frac{\cos kR}{R} - \sigma_{lp} (\nabla^2 \delta_{pm} - \nabla_p \nabla_m) \bar{R} \frac{\cos k\bar{R}}{\bar{R}} \]  

where the matrix

\[ \sigma = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \]
gives a reflection on the conducting plate, supposed orthogonal to the z axis, and \( R = |r_B - \sigma r_A| \) is the distance between one atom and the image of the other atom reflected on the plate. The atom-atom Casimir-Polder potential energy \([14]\) adds to the well-known atom-wall Casimir-Polder interaction energy, of course.

The equal-time spatial correlation of the electric field at points \( r_A \) and \( r_B \) in \([14]\), in the presence of the conducting plate and evaluated on the thermal state of the field, is

\[
\langle E_i(k, r_A) E_m(k, r_B) \rangle = \frac{2 \pi \hbar c k}{V} f_i(k; r_A) f_m(k; r_B) \left( 2 \langle a_{kj}^\dagger a_{kj} \rangle + 1 \right)
\]

\[= \frac{2 \pi \hbar c k}{V} f_i(k, r_A) f_m(k, r_B) \coth \left( \frac{\hbar c k}{2 k_B T} \right) \tag{17}\]

In the continuum limit, performing the sum over polarizations and the angular integration over the directions of \( k \) and using the appropriate mode functions \([27]\), we obtain

\[
\frac{1}{4 \pi} \int d\Omega_k \sum_j f_i(k; r_A) f_m(k; r_B) = \tau_{lm}(k, R) - \sigma_{ln} \tau_{nm}(k, \bar{R}) \tag{18}\]

Substitution of \([15], [17], [18]\) into \([14]\) yields

\[
W_{AB}(R, \bar{R}) = \frac{\hbar c}{\pi} \int dk k^3 \alpha_A(k) \alpha_B(k) \coth \left( \frac{\hbar c k}{2 k_B T} \right) \times (V_{lm}(k, R) - \sigma_{lp} V_{pm}(k, \bar{R})) (\tau_{lm}(k, R) - \sigma_{ln} \tau_{nm}(k, \bar{R})) \tag{19}\]

Using \([5]\) and \([8]\), this expression can be written in the following form

\[
W_{AB}(R, \bar{R}) = -\frac{\hbar c}{\pi} \int dk \alpha_A(k) \alpha_B(k) \coth \left( \frac{\hbar c k}{2 k_B T} \right) \times \left( \frac{\nabla^2 \delta_{lm} - \nabla_l \nabla_m}{R} \right) \left( \frac{\nabla^2 \delta_{lm} - \nabla_l \nabla_m}{R} \right) \right)
\]

\[
+ \frac{\hbar c}{\pi} \sigma_{ln} \left( \frac{\nabla^2 \delta_{lm} - \nabla_l \nabla_m}{R} \right) \left( \frac{\nabla^2 \delta_{nm} - \nabla_n \nabla_m}{R} \right) \frac{1}{R}
\]

\[
\times \int dk \alpha_A(k) \alpha_B(k) \sin k(R + \bar{R}) \coth \left( \frac{\hbar c k}{2 k_B T} \right) \tag{20}\]

Comparing \([20]\) with \([9]\), it is evident that, in the presence of the conducting plate, the atom-atom Casimir-Polder potential energy at nonzero temperature is the sum of three contributions: i) the “direct” interaction between the two atoms, as in absence of the wall:
this is the first term in (20), which depends only on $R$; ii) the interaction between an atom and the image of the other atom, which has the same formal expression of the previous contribution, but in terms of $\bar{R}$; iii) a term depending from both distances $R$ and $\bar{R}$. In the limit of zero temperature, equation (20) reduces to previous results at zero temperature in reference [14, 27].

In the far zone, the expression (20) of the potential energy can be written in a more compact form using the operator defined in equation (12)

$$W_{AB}(R, \bar{R}) = \alpha_A \alpha_B k_B T \left\{ Q^R \coth \left( \frac{R}{\lambda_T} \right) + Q^{\bar{R}} \coth \left( \frac{\bar{R}}{\lambda_T} \right) + \sigma_{ln} \left( \nabla^2 \delta_{lm} - \nabla_l \nabla_m \right) \frac{1}{R} \left( \nabla^2 \delta_{nm} - \nabla_n \nabla_m \right) \frac{1}{\bar{R}} \coth \left( \frac{R + \bar{R}}{2 \lambda_T} \right) \right\}$$

(21)

where $\alpha_{A,B}$ are the static polarizabilities of the atoms and we have introduced the thermal length $\lambda_T = \hbar c/2\pi k_B T$.

It is worth to consider different limiting cases of (21) according to the values of $R$, $\bar{R}$ and $\lambda_T$.

If $R, \bar{R} \ll \lambda_T$, we obtain

$$W_{AB}(R, \bar{R}) = -\alpha_A \alpha_B \left( \frac{23 \hbar c}{4\pi R^7} + \frac{3 \hbar c}{4\pi \bar{R}^7} \right) - \frac{\hbar c}{\pi} \sigma_{ln} \left( \nabla^2 \delta_{lm} - \nabla_l \nabla_m \right) \frac{1}{R} \left( \nabla^2 \delta_{nm} - \nabla_n \nabla_m \right) \frac{1}{\bar{R}} \left( \frac{R + \bar{R}}{\lambda_T} \right)$$

(22)

which shows that the potential in this case scales as the inverse of the seventh power of the distance. Equation (22) indeed reproduces the zero-temperature result [14, 27].

If $R \ll \lambda_T$ and $\bar{R} \gg \lambda_T$, equation (21) yields

$$W_{AB}(R, \bar{R}) = -\alpha_A \alpha_B \left( \frac{23 \hbar c}{4\pi R^7} + \frac{3 k_B T}{R^6} - \frac{k_B T}{R^3 \bar{R}^3} \left( 3 \sin^2 \theta + 3 \sin^2 \bar{\theta} - 2 \right) \right)$$

(23)

where $\theta$ and $\bar{\theta}$ are respectively the angles that $R$ and $\bar{R}$ make with the axis perpendicular to the wall. Being $R \ll \bar{R}$ and $R \ll \lambda_T$, the last two terms inside the brackets are negligible compared to the first one, and thus the Casimir-Polder potential between the two atoms is essentially the same as for atoms in the free space at zero temperature.

If $R, \bar{R} \gg \lambda_T$, equation (21) yields

$$W_{AB}(R, \bar{R}) = -\alpha_A \alpha_B k_B T \left( \frac{3}{R^6} + \frac{3}{\bar{R}^6} - \frac{1}{R^3 \bar{R}^3} \left( 3 \sin^2 \theta + 3 \sin^2 \bar{\theta} - 2 \right) \right)$$

(24)
Equation (24) shows that in this case the potential scales as the inverse of distance to the sixth power. We also notice from (24) that the last term, containing both distances $R$ and $\bar{R}$, gives a contribution to the potential opposite to the other two terms; however, by taking into account that $\bar{R} > R$, it is easy to show that the potential is attractive for any spatial configuration of the atoms with respect to the wall. However, in this case both the presence of the wall and the finite temperature of the field significantly affect the Casimir-Polder potential energy between the two atoms.

IV. CONCLUSION

In this paper we have considered the Casimir-Polder potential energy between two atoms near a perfectly conducting plate and at nonzero temperature, both in the near and far zone. We have investigated the effect of the boundary condition and of the finite temperature on the potential, in order to consider situations close to realistic experimental setups. We have used a method based on spatial field correlations, which has proved quite convenient and physically transparent in dealing with this kind of problems. Using this method we have first reproduced in a more transparent way the known results for the atom-atom Casimir-Polder potential in the free space at finite temperature. Then we have applied the same method, with appropriate modifications, to derive the expression of the atom-atom potential at nonzero temperature, when a conducting plate is also present. We have obtained an analytical expression of the potential both in the near and the far zone. We have then analyzed limiting cases of interest, according to the relation between atom-atom and atoms-wall distances with the thermal length, which is proportional to $T^{-1}$. In the future, we plan to extend this work to the case in which one or both atoms are in their excited state and/or when they are in the space between two parallel walls, where resonance effects could yield relevant modifications of the Casimir-Polder interatomic potential.
Acknowledgments

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