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# Atom–wall dispersive forces from the master equation formalism

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## Abstract

Using the general expressions for level shifts obtained from the master equation for a small system interacting with a large one considered as a reservoir, we calculate the dispersive potentials between an atom and a wall in the dipole approximation. We analyse in detail the particular case of a two-level atom in the presence of a perfectly conducting wall. We study the van der Waals as well as the resonant interactions. All distance regimes as well as the high and low temperature regimes are considered. We show that the Casimir–Polder interaction cannot be considered as a direct result of the vacuum fluctuations only. Concerning the interaction between the atom and the wall at high temperatures, we show that a saturation of the potential for all distances occurs. This saturated potential coincides precisely with that obtained in the London–van der Waals limit.

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## 1. Introduction

The explanation for the force between two neutral and non-polar but polarizable molecules, usually called dispersive forces, was possible only after the advent of quantum mechanics. In 1930, F London [1] obtained the interaction potential between two neutral hydrogen atoms in their respective ground states and separated by a distance much larger than the Bohr radius in the static electric dipole limit,  $\lambda_0 \gg r \gg a_0$ , where  $\lambda_0 = 2\pi c/\omega_0$  is the wavelength of the dominant transition and  $a_0$  is the Bohr radius. London's result is  $V(r) \simeq -6.5e^2a_0^5/r^6 \simeq -3\hbar\omega_0\alpha_0^2/4r^6$ .

In 1948, Casimir and Polder [3] considered for the first time the influence of retardation effects on the van der Waals forces between two atoms as well as on the force between an

atom and a perfectly conducting wall. They showed that in the retarded limit the interaction falls as  $1/r^7$  for two atoms (in contrast to London's  $1/r^6$  result) and as  $1/r^4$  for an atom and a perfectly conducting wall, in contrast with the short distance limit (that falls as  $1/r^3$ ) [4].

In 1956, E M Lifshitz developed a general theory of dispersive van der Waals forces between dielectric macroscopic bodies using a non-perturbative approach [5], once the perturbative expansion for many-body interaction breaks down due to the non-additivity of the van der Waals forces. Lifshitz derived a powerful expression for the force at finite temperature between two semi-infinite dispersive media characterized by an electric permittivity and separated by a slab of any other dispersive medium. He also showed that the Casimir–Polder force is a limiting case when one of the media is sufficiently dilute such that the force between the slabs may be obtained by direct pair-wise integration of a single atom–wall interaction [6].

Since then a wide knowledge about the behaviour and nature of dispersive forces has been achieved. In the following decades, many works have appeared, like those made by A D McLachlan [7], in the 60s, where the recently compiled linear response theory developed by R Kubo [8] was applied. In 1970, G Feinberg and J Sucher [9] treated the electric and magnetic contributions to van der Waals interaction in the same foot. In the late 60s and during the 70s some authors analysed the interaction between an excited atom and a wall [10–12]. The first of these works, made by H Morawitz, considered the level and frequency shifts of an excited atom in the presence of a perfectly conducting wall using the image method, which led him to the discovery of the resonant dispersive interaction. In the 80s and 90s the non-additivity character of the van der Waals forces was well exploited [13, 14]; nice works concerning level shifts of atoms and dispersive interactions in cavities [15–19] and thermal contributions to the Casimir–Polder interaction have also been studied [20–22]. For more details and an exhaustive list of references on this and related topics see the recent review by Buhmann and Welsch [23]. In the last few years, the interest for van der Waals and Casimir–Polder forces has increased mainly due to better experimental techniques and the development of nanosciences. The influence of these forces in the stability of Bose–Einstein condensates [24, 25] and on factoring and doping carbon nanotubes are branches of great activity nowadays [26–28].

This paper is a natural sequence of a previous one [29], where we studied the van der Waals interaction between a two-level atom and a perfectly conducting wall using the density matrix formalism [30]. Here, using the same formalism, we study the excited state contributions to the interaction, both in vacuum and thermal states of the electromagnetic field. We give simple interpretations to the ground state contribution (van der Waals interaction) and the excited state contribution (resonant interaction) in terms of the non-resonant and resonant parts of the atomic polarizability. Considering the thermal state of the electromagnetic field, we analyse both high and low temperature limits,  $\hbar\omega_0 \ll k_B T$  and  $\hbar\omega_0 \gg k_B T$  respectively, and show that in the former the interaction between the two-level system and the perfectly conducting wall is temperature independent and behaves exactly as in the London–van der Waals limit at zero temperature for all distances.

## 2. Level shifts and exchange energy rates

In this section, we obtain the level shifts and the exchange energy rates of a multi-level system interacting with the electromagnetic field in the dipole approximation. In the first case, if we consider the boundary conditions imposed to the field by the presence of a given wall, we can extract the position-dependent part, which gives, by derivation, the atom–wall dispersive forces.

### 2.1. General expressions

Our starting point is the master equation for a small system  $\mathcal{S}$  (the atom) which interacts weakly with a large one  $\mathcal{R}$ , that may be considered as a reservoir (quantized electromagnetic field), by the interaction Hamiltonian

$$V = - \sum_j S_j R_j, \quad (1)$$

where  $S_j$  and  $R_j$  are observables associated with  $\mathcal{S}$  and  $\mathcal{R}$ , respectively. In the Schrödinger picture, the master equation may be written as [30–32]

$$\frac{d}{dt} \rho_{ab}^S(t) = -i\omega_{ab} \rho_{ab}^S(t) + \sum_{c,d} \mathcal{J}_{abcd} \rho_{cd}^S(t), \quad (2)$$

$$\begin{aligned} \mathcal{J}_{abcd} = & -\frac{1}{\hbar^2} \sum_{j,k} \int_0^\infty d\tau \left\{ g_{jk}^R(\tau) \left[ \delta_{bd} \sum_n S_{an}^j S_{nc}^k e^{-i\omega_{nc}\tau} - S_{ac}^k S_{db}^j e^{-i\omega_{ac}\tau} \right] \right. \\ & \left. + g_{kj}^R(-\tau) \left[ \delta_{ac} \sum_n S_{dn}^k S_{nb}^j e^{i\omega_{nd}\tau} - S_{ac}^j S_{db}^k e^{i\omega_{bd}\tau} \right] \right\}, \quad (3) \end{aligned}$$

where  $\rho_{ab}^S = \langle a | \rho_S | b \rangle$  is the matrix element of the density operator  $\rho_S$ , associated with the system  $\mathcal{S}$ , between the energy eigenstates  $|a\rangle$  and  $|b\rangle$  with eigenvalues  $E_a$  and  $E_b$  of the unperturbed Hamiltonian operator  $H_S$  of  $\mathcal{S}$  ( $H_S |a\rangle = E_a |a\rangle$ );  $S_{ab}^j = \langle a | S_j | b \rangle$  is the matrix element of the observable  $S_j$  and  $\omega_{ab} = (E_a - E_b)/\hbar$  is the transition frequency between the states  $|a\rangle$  and  $|b\rangle$ . The function  $g_{jk}^R(\tau)$  that appears in equation (3) is defined as

$$g_{jk}^R(\tau) = [g_{kj}^R(-\tau)]^* = \text{Tr}_R[\rho_R R_j(\tau) R_k(0)] = \sum_\mu p_\mu \sum_\nu R_{\mu\nu}^j R_{\nu\mu}^k e^{i\omega_{\mu\nu}\tau}, \quad (4)$$

where  $R_{\mu\nu}^j = \langle \mu | R_j | \nu \rangle$  is the matrix element of the observable  $R_j$  between the energy eigenstates  $|\mu\rangle$  and  $|\nu\rangle$  with energy eigenvalues  $E_\mu$  and  $E_\nu$  of the unperturbed Hamiltonian operator  $H_R$  of  $\mathcal{R}$  ( $H_R |\mu\rangle = E_\mu |\mu\rangle$ );  $\omega_{\mu\nu} = (E_\mu - E_\nu)/\hbar$  is the transition frequency between the states  $|\mu\rangle$  and  $|\nu\rangle$  and  $\rho_R$  is the density matrix associated with  $\mathcal{R}$ , considered constant in time and diagonal in the  $\{|\mu\rangle\}$  base-ket, so that

$$\rho_R = \sum_\mu p_\mu |\mu\rangle \langle \mu|, \quad (5)$$

where  $p_\mu$  is the statistical weight of the state  $|\mu\rangle$  for a given ensemble. For the seek of completeness, let us make a brief resume of the steps for derivation of equations (2) and (3) and, from these, equations (22)–(25). A careful deduction of these equations can be found in [30–32].

Equations (2), (3) were obtained from the equation of the time evolution of the total density matrix  $\rho(t) \simeq \rho_S(t) \otimes \rho_R$ ,  $-i\hbar\dot{\rho}(t) = [\rho(t), H]$ , where  $H = H_S + H_R + V$  is the Hamiltonian of the total system  $\mathcal{S} + \mathcal{R}$ . Then, one has made implicitly the assumption that there are two very different time scales in the evolution of the total system  $\mathcal{S} + \mathcal{R}$ : the characteristic time  $T_S$  in which the average values of the observables of  $\mathcal{S}$  change significantly and the characteristic time  $\tau_c$ , which is, crudely speaking, the width of  $g_{jk}^R(\tau)$  and measures the time of the fluctuations of the reservoir observables. The approximations used in derivation of the above equations are based on the following conditions,

$$\tau_c \ll \Delta t \ll T_S, \quad (6)$$

where  $\Delta t$  is the time interval that enters in the calculation of the time derivative in equation (2). Last condition tells us that the master equation is a coarse-grained rate, since rapid variations of  $\rho_S$  that occur in times of order of  $\tau_c$  are smoothed in the interval  $\Delta t$ ; since we are interested in times of the order of  $T_S$ , this smoothing remains a good approximation once condition (6) is satisfied. Another supplementary condition for obtaining equation (2), which makes the coefficients  $\mathcal{J}_{abcd}$  independent of  $\Delta t$ , is that frequency differences between the elements of the density matrix should be very small compared to  $1/\Delta t$ , so that  $|\omega_{ac} - \omega_{bd}|\Delta t \ll 1$ . Last condition is called secular condition and the sum in equation (2) is only over secular terms (terms that satisfy the secular condition).

Using more two assumptions, one may conveniently split equation (2) into two other ones: an equation for the diagonal elements  $\rho_{aa}^S$  (populations) and another for the non-diagonal elements  $\rho_{ab}^S$ , with  $a \neq b$  (coherences). For the populations, the assumption is that there is no coherence  $\rho_{cd}^S$  in the sum in equation (2) with too low frequency, so that  $\omega_{cd}T_S \gg 1$ . This implies that all coherences are not secular terms and the master equation for the populations  $\rho_{aa}^S$  may be put into the form

$$\frac{d}{dt}\rho_{aa}^S(t) = \sum_c (\rho_{cc}^S(t) \Gamma_{c \rightarrow a} - \rho_{aa}^S(t) \Gamma_{a \rightarrow c}), \quad (7)$$

$$\Gamma_{c \rightarrow a} = \frac{2\pi}{\hbar} \sum_{\mu} p_{\mu} \sum_v |\langle \mu, c | V | v, a \rangle|^2 \delta(E_{\mu} + E_c - E_v - E_a), \quad (8)$$

where  $V$  is the interaction Hamiltonian given by (1). The quantity  $\Gamma_{c \rightarrow a}$  may be interpreted as the transition rate probability between the states  $|c\rangle$  and  $|a\rangle$  as a result of the interaction of the system with the reservoir.

In order to obtain the equation for coherences we make the second assumption, namely, we consider only the non-degenerate case: the frequency  $\omega_{ab}$  differ from all other frequencies  $\omega_{cd}$  by a quantity of order (or larger than)  $1/\Delta t$ , that is,  $|\omega_{ac} - \omega_{bd}| > 1/\Delta t \gg 1/T_S$ . Then, the only secular term in equation (2) is that one which couples the coherence  $\rho_{ab}^S$  with itself, so that the equation for this coherence may be written as

$$\frac{d}{dt}\rho_{ab}^S(t) = -i(\omega_{ab} + \Delta_{ab})\rho_{ab}^S(t) - \Gamma_{ab}\rho_{ab}^S(t), \quad a \neq b \quad (9)$$

where  $\Delta_{ab} = \Delta_a - \Delta_b$ ,  $\Gamma_{ab} = \Gamma_{ab}^{\text{ad.}} + \Gamma_a^{\text{nad.}} + \Gamma_b^{\text{nad.}}$ ,

$$\Delta_n = \frac{1}{\hbar^2} \sum_{\mu} p_{\mu} \sum_v \sum_j \mathcal{P} \frac{|\langle \mu, n | V | j, v \rangle|^2}{\omega_{\mu v} - \omega_{jn}} \quad (10)$$

$$\Gamma_{ab}^{\text{ad.}} = -\frac{2\pi}{\hbar^2} \sum_{\mu} p_{\mu} \sum_v \langle \mu, b | V | b, v \rangle \langle v, a | V | a, \mu \rangle \delta(\omega_{\mu v}) \quad (11)$$

$$\Gamma_n^{\text{nad.}} = \frac{\pi}{\hbar^2} \sum_{\mu} p_{\mu} \sum_v \sum_j |\langle \mu, n | V | j, v \rangle|^2 \delta(\omega_{\mu v} - \omega_{jn}) = \frac{1}{2} \sum_j \Gamma_{n \rightarrow j} \quad (12)$$

and the symbol  $\mathcal{P}$  in (10) means the Cauchy principal value. From (9) one may conclude that the coherence  $\rho_{ab}^S$ , as a result of its interaction with the reservoir, oscillates with a frequency shifted by  $\Delta_{ab}$  from its free value  $\omega_{ab}$  and decays exponentially with a characteristic time given by  $1/\Gamma_{ab}$ . From equations (7), (8) and (10) one may obtain the exchange energy rates between the system and the reservoir and the energy level shifts of the system, respectively,

since frequency shifts result from level shifts. Recall that  $\delta E_a = \hbar \Delta_a$  is the energy shift of the state  $|a\rangle$  (and equivalently for  $|b\rangle$ ).

For energy rates, considering the time derivative of the average value of the Hamiltonian of the system in Schrödinger and Heisenberg pictures, we find

$$\frac{d\langle H_S \rangle_a}{dt} = \sum_b (E_b - E_a) \Gamma_{a \rightarrow b} = \sum_b \hbar \omega_{ba} \Gamma_{a \rightarrow b}, \quad (13)$$

which may be interpreted as a net rate of changing the average value of the energy of the system  $\mathcal{S}$  when it is in the state  $|a\rangle$  or, in other words, the exchange energy rate between  $\mathcal{S}$  and  $\mathcal{R}$  for the state  $|a\rangle$ . It is possible to put the last result into a more intuitive form that clearly exhibits the roles played by  $\mathcal{S}$  and  $\mathcal{R}$ . Returning to equation (4), one may show that real and imaginary parts of  $g_{jk}^R(\tau)$  are related to the symmetric correlation function  $C_{jk}^R(\tau)$  and the linear susceptibility  $\chi_{jk}^R(\tau)$  [32, 33],

$$C_{jk}^R(\tau) = \text{Re} [g_{jk}^R(\tau)] = \sum_{\mu} p_{\mu} \sum_{\nu} R_{\mu\nu}^j R_{\nu\mu}^k \cos(\omega_{\mu\nu} \tau), \quad (14)$$

$$\chi_{jk}^R(\tau) = \frac{2}{\hbar} \Theta(\tau) \text{Im} [g_{jk}^R(\tau)] = -\frac{2}{\hbar} \sum_{\mu} p_{\mu} \sum_{\nu} R_{\mu\nu}^j R_{\nu\mu}^k \Theta(\tau) \sin(\omega_{\mu\nu} \tau), \quad (15)$$

where  $\Theta(\tau)$  is the Heaviside step function. In the frequency space, we have

$$\hat{C}_{jk}^R(\omega) = \int_{-\infty}^{\infty} d\tau C_{jk}^R(\tau) e^{i\omega\tau} = \pi \sum_{\mu} p_{\mu} \sum_{\nu} R_{\mu\nu}^j R_{\nu\mu}^k [\delta(\omega + \omega_{\mu\nu}) + \delta(\omega - \omega_{\mu\nu})], \quad (16)$$

$$\hat{\chi}_{jk}^R(\omega) = \int_{-\infty}^{\infty} d\tau \chi_{jk}^R(\tau) e^{i\omega\tau} = \hat{\chi}_{jk}^{\prime R}(\omega) + i \hat{\chi}_{jk}^{\prime\prime R}(\omega), \quad (17)$$

$$\hat{\chi}_{jk}^{\prime R}(\omega) = -\frac{1}{\hbar} \sum_{\mu} p_{\mu} \sum_{\nu} R_{\mu\nu}^j R_{\nu\mu}^k \left[ \mathcal{P} \frac{1}{\omega_{\mu\nu} + \omega} + \mathcal{P} \frac{1}{\omega_{\mu\nu} - \omega} \right], \quad (18)$$

$$\hat{\chi}_{jk}^{\prime\prime R}(\omega) = \frac{\pi}{\hbar} \sum_{\mu} p_{\mu} \sum_{\nu} R_{\mu\nu}^j R_{\nu\mu}^k [\delta(\omega_{\mu\nu} + \omega) - \delta(\omega_{\mu\nu} - \omega)]. \quad (19)$$

The symmetric correlation function given by (16) may be interpreted as a dispersion of the observables  $R_j$  and  $R_k$  around a frequency  $\omega$ . It is a measure of the fluctuations of the reservoir dynamical variables. The real part of the susceptibility defined in equation (18) is called the dispersive or reactive part and is related to the polarization of a system by an external perturbation. On the other hand, the imaginary part is directly responsible for the absorption and dissipation of energy by the system and, for this reason it is called dissipative part of susceptibility [34].

Now, let us come back to equations (10) and (13). Using the quantities defined in equations (16)–(19), the energy level shifts and the exchange energy rates may be cast into the form

$$\delta E_a = \delta E_a^{fr} + \delta E_a^{rr}, \quad (20)$$

$$\frac{d\langle H_S \rangle_a}{dt} = \dot{Q}_a = \dot{Q}_a^{fr} + \dot{Q}_a^{rr}, \quad (21)$$

$$\delta E_a^{fr} = -\frac{1}{2} \sum_{j,k} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \hat{\chi}_{jk}^{\prime S,a}(\omega) \hat{C}_{kj}^R(\omega), \quad (22)$$

$$\delta E_a^{rr} = -\frac{1}{2} \sum_{j,k} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \hat{\chi}_{jk}^{\prime R}(\omega) \hat{C}_{kj}^{S,a}(\omega), \quad (23)$$

$$\hat{Q}_a^{fr} = \sum_{j,k} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega \hat{\chi}_{jk}^{\prime S,a}(\omega) \hat{C}_{kj}^R(\omega), \quad (24)$$

$$\hat{Q}_a^{rr} = -\sum_{j,k} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega \hat{\chi}_{jk}^{\prime R}(\omega) \hat{C}_{kj}^{S,a}(\omega), \quad (25)$$

where

$$\hat{C}_{jk}^{S,a}(\omega) = \pi \sum_n S_{an}^j S_{na}^k [\delta(\omega + \omega_{an}) + \delta(\omega - \omega_{an})], \quad (26)$$

$$\hat{\chi}_{jk}^{\prime S,a}(\omega) = -\frac{1}{\hbar} \sum_n S_{an}^j S_{na}^k \left[ \mathcal{P} \frac{1}{\omega_{an} + \omega} + \mathcal{P} \frac{1}{\omega_{an} - \omega} \right], \quad (27)$$

$$\hat{\chi}_{jk}^{\prime R}(\omega) = \frac{\pi}{\hbar} \sum_n S_{an}^j S_{na}^k [\delta(\omega_{an} + \omega) - \delta(\omega_{an} - \omega)] \quad (28)$$

are the symmetric correlation functions and the dispersive and dissipative parts of the susceptibility of the system  $\mathcal{S}$  in the state  $|a\rangle$ , respectively. Equations (22)–(25) are the general expressions for the level shifts and the exchange energy rates of a small system interacting with a reservoir.

The physical interpretation of equations (22) and (23) is simple. The former gives the contribution to the level shift due to the polarization of the system  $\mathcal{S}$  by the fluctuations of the reservoir ( $fr$ ) and the latter gives the contribution of the polarization of the reservoir by the fluctuations of the system, or the reservoir reaction ( $rr$ ) contribution.

A similar interpretation may be done for equations (24) and (25). The first of them may be understood as the power absorbed by the system  $\mathcal{S}$  from the reservoir fluctuations and the second represents the power dissipated by the system or, equivalently, the power lost to the reservoir.

## 2.2. Dipole interacting with the radiation field

Let us consider a small neutral but polarizable system which interacts weakly with the radiation field. Assuming the dipole approximation and considering the total quantized electric field operator at the position  $\mathbf{x}$  of the centre of mass of the system as a sum over all possible modes, the interacting Hamiltonian takes the form

$$V = -\mathbf{d} \cdot \mathbf{E}(\mathbf{x}, t) = e \sum_{\mathbf{k}\lambda} \sum_j (x_j f_{\mathbf{k}\lambda}^j(\mathbf{x}) e^{i\omega_{\mathbf{k}}t} a_{\mathbf{k}\lambda}^\dagger + \text{h.c.}), \quad (29)$$

where  $\mathbf{d} = -e\mathbf{r}$  is the dipole moment operator of the system,  $-e$  its electric charge,  $\mathbf{r} = (x_1, x_2, x_3)$  is the position operator of the charge and functions  $\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{x}) = \hat{x}_j f_{\mathbf{k}\lambda}^j(\mathbf{x})$  (Einstein's convention is assumed), where  $\hat{x}_j$  is the unitary vector in the direction of component  $x_j$  of  $\mathbf{r}$ , carry the information about the boundary conditions and possible source contributions. The index  $j$  runs over Cartesian components ( $j = 1, 2, 3$ ) and the index  $\mathbf{k}\lambda$  specifies a field mode, where  $\mathbf{k}$  is its wave-vector and  $\lambda$  its corresponding polarization. Operators  $a_{\mathbf{k}\lambda}$  and  $a_{\mathbf{k}\lambda}^\dagger$  are the annihilation and creation operators, respectively, of one photon in the mode  $\mathbf{k}\lambda$  and satisfy the usual commutation relations

$$[a_{\mathbf{k}\lambda}, a_{\mathbf{k}'\lambda'}^\dagger] = [a_{\mathbf{k}\lambda}^\dagger, a_{\mathbf{k}'\lambda'}] = 0, \quad [a_{\mathbf{k}\lambda}, a_{\mathbf{k}'\lambda'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'}. \quad (30)$$

Choosing the coordinate axis in a manner such that the susceptibility and the correlation function of the system are diagonal we have

$$\hat{C}_{jk}^{S,a}(\omega) = \hat{C}_{aj}(\omega)\delta_{jk}, \quad (31)$$

$$\hat{\chi}_{jk}^{\prime S,a}(\omega) = \alpha'_{aj}(\omega)\delta_{jk}, \quad (32)$$

$$\hat{\chi}_{jk}^{\prime\prime S,a}(\omega) = \alpha''_{aj}(\omega)\delta_{jk}, \quad (33)$$

where

$$\hat{C}_{aj}(\omega) = \pi\hbar \sum_b \frac{\alpha_{ab}^j \omega_{ba}}{2} [\delta(\omega_{ba} + \omega) + \delta(\omega_{ba} - \omega)], \quad (34)$$

$$\alpha'_{aj}(\omega) = \sum_b \frac{\alpha_{ab}^j \omega_{ba}}{2} \left[ \mathcal{P} \frac{1}{\omega_{ba} + \omega} + \mathcal{P} \frac{1}{\omega_{ba} - \omega} \right], \quad (35)$$

$$\alpha''_{aj}(\omega) = \pi \sum_b \frac{\alpha_{ab}^j \omega_{ba}}{2} [\delta(\omega_{ba} - \omega) - \delta(\omega_{ba} + \omega)], \quad (36)$$

and  $\alpha_{ab}^j = -2e^2 | \langle a | x_j | b \rangle |^2 / \hbar \omega_{ab}$  is the static polarizability of the system in the direction  $\hat{x}_j$  between the states  $|a\rangle$  and  $|b\rangle$ . Using last equations in (22)–(25), making  $|\mu\rangle = |n_{\mathbf{k}\lambda}\rangle$  in equation (5) (which means a Fock state with  $n_{\mathbf{k}\lambda}$  photons in the mode  $\mathbf{k}\lambda$ ) and performing the integration on  $\omega$ , we obtain, after some calculations,

$$\delta E_a^{rr} = -\frac{1}{2} \sum_j \sum_{\mathbf{k}\lambda} \alpha_{aj}^{\prime(-)}(k) |f_{\mathbf{k}\lambda}^j(\mathbf{x})|^2, \quad (37)$$

$$\dot{Q}_a^{rr} = -\sum_j \sum_{\mathbf{k}\lambda} ck \alpha_{aj}^{\prime\prime(-)}(k) |f_{\mathbf{k}\lambda}^j(\mathbf{x})|^2, \quad (38)$$

$$\delta E_a^{fr} = -\sum_j \sum_{\mathbf{k}\lambda} \alpha_{aj}^{\prime(+)}(k) |f_{\mathbf{k}\lambda}^j(\mathbf{x})|^2 \left( \langle n_{\mathbf{k}\lambda} \rangle + \frac{1}{2} \right), \quad (39)$$

$$\dot{Q}_a^{fr} = \sum_j \sum_{\mathbf{k}\lambda} ck \alpha_{aj}^{\prime\prime(+)}(k) |f_{\mathbf{k}\lambda}^j(\mathbf{x})|^2 (2\langle n_{\mathbf{k}\lambda} \rangle + 1), \quad (40)$$

$$\alpha_{aj}^{\prime(\mp)}(k) = \sum_b \frac{\alpha_{ab}^j k_{ba}}{2} \left[ \mathcal{P} \frac{1}{k + k_{ba}} \pm \mathcal{P} \frac{1}{k - k_{ba}} \right], \quad (41)$$

$$\alpha_{aj}^{\prime\prime(\mp)}(k) = \pi \sum_b \frac{\alpha_{ab}^j k_{ba}}{2} [\delta(k - k_{ba}) \pm \delta(k + k_{ba})], \quad (42)$$

where  $k = \omega_k/c$ ,  $k_{ab} = \omega_{ab}/c$  and  $\langle n_{\mathbf{k}\lambda} \rangle$  is the average number of photons in the mode  $\mathbf{k}\lambda$ . Equations (37)–(40) are nothing but equations (22)–(25) applied to a neutral but polarizable system interacting with the electromagnetic field. The validity of these equations, once assumed the dipole approximation, is determined by the validity of condition (6). This implies that the field correlation function in time  $C_{ij}^R(\tau)$ , obtained from equation (14), must have all its characteristic frequencies much larger than any characteristic frequency of the system, so that the correlation time  $\tau_c$  obeys the condition:  $\tau_c \ll 1/\omega_0$ , where  $\omega_0$  is the largest characteristic frequency of the system.



Equations (37) and (38) give the ( $rr$ ) contributions to level shifts and energy rates of the system and equations (39) and (40) give the corresponding ( $fr$ ) contributions. We see that ( $rr$ ) contributions do not depend on  $\langle n_{\mathbf{k}\lambda} \rangle$ , which carries all information about the field state. This information is concentrated on ( $fr$ ) contributions. Of course, for  $\langle n_{\mathbf{k}\lambda} \rangle = 0$ , there is still a residual term which can be associated with the contribution of the vacuum fluctuations of the field.

Functions  $\alpha_{aj}^{(+)}(k)$  and  $\alpha_{aj}^{\prime(+)}(k)$  appearing in the ( $fr$ ) terms are nothing but the dispersive and dissipative parts of the susceptibility of the system. In the ( $rr$ ) contributions, however, we have the functions  $\alpha_{aj}^{(-)}(k)$  and  $\alpha_{aj}^{\prime(-)}(k)$ , which do not have a direct interpretation like their corresponding 'plus' functions. The difference is only in the sign of the  $k - k_{ba}$  terms for the first and  $k + k_{ba}$  for the second. But this fact will be crucial to determine the behaviour of the dispersive interactions: it is precisely this difference of sign which makes possible the existence of the dispersive van der Waals interaction. This fact will become clear when we discuss the two-level system.

### 3. Calculation of the dispersive forces

In this section, we shall apply the expressions deduced in the previous section for level shifts and energy rates of a polarizable system interacting with the electromagnetic field. We shall discuss a two-level atom, considered as an isotropic system, in the presence of a perfectly conducting wall.

Let us consider two parallel square plates with sides  $L$  fixed at  $z = 0$  and at  $z = \ell$ , where  $L \gg \ell$ , and a small polarizable system on the  $OZ$  axes at position  $z$  that satisfies the condition  $0 < z \ll \ell$ . Hence, for a given wave vector  $\mathbf{k}$ , the quantized electric field (without sources) in the region  $0 < z < \ell$  is given by [35]

$$\begin{aligned} \mathbf{E}_{\mathbf{k}_\parallel n}(\mathbf{r}_\parallel, z, t) = & \iota \left( \frac{4\pi\hbar kc}{\ell L^2} \right)^{1/2} \left\{ a_{\mathbf{k}_\parallel n}^{(1)} \left( \frac{\mathbf{k}_\parallel}{k_\parallel} \times \hat{\mathbf{z}} \right) \sin \left( \frac{n\pi}{\ell} z \right) \right. \\ & \left. + a_{\mathbf{k}_\parallel n}^{(2)} \left[ \iota \frac{n\pi}{k\ell} \frac{\mathbf{k}_\parallel}{k_\parallel} \sin \left( \frac{n\pi}{\ell} z \right) - \hat{\mathbf{z}} \frac{k_\parallel}{k} \cos \left( \frac{n\pi}{\ell} z \right) \right] \right\} e^{i(\mathbf{k}_\parallel \cdot \mathbf{r}_\parallel - \omega_k t)} + \text{h.c.}, \end{aligned} \quad (43)$$

where

$$[a_{\mathbf{k}_\parallel n}^\lambda, a_{\mathbf{k}'_\parallel n'}^{\lambda'}] = [a_{\mathbf{k}_\parallel n}^{\dagger\lambda}, a_{\mathbf{k}'_\parallel n'}^{\dagger\lambda'}] = 0, \quad (44)$$

$$[a_{\mathbf{k}_\parallel n}^\lambda, a_{\mathbf{k}'_\parallel n'}^{\dagger\lambda'}] = \delta_{\lambda\lambda'} \delta_{nn'} \delta_{\mathbf{k}_\parallel \mathbf{k}'_\parallel}, \quad (45)$$

$$\frac{\omega_k^2}{c^2} = k^2 = k_\parallel^2 + (n\pi/\ell)^2, \quad (46)$$

$$\mathbf{k}_\parallel = k_x \hat{x} + k_y \hat{y}, \quad \mathbf{r}_\parallel = x \hat{x} + y \hat{y}, \quad (47)$$

with  $n$  being a non-negative integer number. The mode with  $n = 0$  has an additional factor  $1/\sqrt{2}$  not shown. Using this expression for the field in the limit  $\ell \rightarrow \infty$ , we shall be able to calculate the desired dispersive potentials between the atom and the single wall at  $z = 0$ .

### 3.1. Two-level system

First of all, let us assume isotropy, so that the polarizability defined previously in the text is independent of the space direction, namely,

$$\alpha_{ge}^j = \alpha_{ge} = -\alpha_{eg} = \frac{2e^2}{3\hbar\omega_0} |\langle g|\mathbf{r}|e\rangle|^2 = \alpha_0, \quad (48)$$

where  $|g\rangle$  and  $|e\rangle$  are the ground and excited states of the two-level system under consideration with energies  $E_g$  and  $E_e$ , and  $\omega_0$  is the transition frequency, given by  $\omega_0 = k_0c = (E_e - E_g)/\hbar$ . Hence, equations (37) and (39) for level shifts take the form

$$\delta E_g^{rr} = \delta E_e^{rr} = -\frac{1}{2} \sum_{\mathbf{k}\lambda} \alpha'_-(k) |\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{x})|^2, \quad (49)$$

$$\delta E_g^{fr} = -\delta E_e^{fr} = -\sum_{\mathbf{k}\lambda} \alpha'_+(k) |\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{x})|^2 \left( \langle n_{\mathbf{k}\lambda} \rangle + \frac{1}{2} \right), \quad (50)$$

$$\alpha'_{\mp}(k) = \frac{\alpha_0 k_0}{2} \left( \mathcal{P} \frac{1}{k+k_0} \pm \mathcal{P} \frac{1}{k-k_0} \right). \quad (51)$$

Note that, while  $(rr)$  contribution for level shifts of  $|g\rangle$  and  $|e\rangle$  states are exactly the same,  $(fr)$  contribution have the same magnitude but opposite signs. Using the expression (43) in equations (49) and (50), taking the limit  $\ell \rightarrow \infty$  and considering a continuous spectra for the field, we are faced with integrals of the form

$$\frac{\alpha_0 k_0}{2} \mathcal{A}_{\lambda}^{(\pm)}(k_0, f) = \int_0^{\infty} dk f(k) \alpha'_{\pm}(k) e^{ik\lambda}, \quad (52)$$

where  $\lambda > 0$  is a real parameter. For an analytical function  $f$  satisfying the condition

$$\lim_{|\text{Im}[k]| \rightarrow \infty} |f(k)| e^{-\lambda|\text{Im}[k]|} = 0$$

in the whole complex plane, it is possible to write

$$\mathcal{A}_{\lambda}^{(\pm)}(k_0, f) = \mp i\pi f(k_0) e^{ik_0\lambda} + \int_0^{\infty} \frac{dk}{k+k_0} [f(k) e^{ik\lambda} \mp f(-k) e^{-ik\lambda}]. \quad (53)$$

Hence, with the aid of the last result, the  $z$ -dependent parts of equations (49) and (50), which give the dispersive potentials between the atom and the wall, when the average number of photons per mode is independent of the polarization,  $\langle n_{\mathbf{k}\lambda} \rangle = \langle n_k \rangle$ , take the form

$$V_g(z, \langle n \rangle) = V_0^{rr}(z) + V_0^{fr}(z) + V_{\langle n \rangle}^{fr}(z), \quad (54)$$

$$V_e(z, \langle n \rangle) = V_0^{rr}(z) - V_0^{fr}(z) - V_{\langle n \rangle}^{fr}(z), \quad (55)$$

$$V_0^{rr}(z) = \frac{\hbar\omega_0}{8\pi} \frac{\alpha_0}{z^3} \mathcal{H}_0^{rr}(2k_0z), \quad (56)$$

$$V_0^{fr}(z) = \frac{\hbar\omega_0}{8\pi} \frac{\alpha_0}{z^3} [\mathcal{H}_0(2k_0z) - \mathcal{H}_0^{rr}(2k_0z)], \quad (57)$$

$$V_{\langle n \rangle}^{fr}(z) = \frac{2\hbar c}{\pi} \int_0^{\infty} k^3 \alpha'_+(k) \langle n_k \rangle G(2kz) dk, \quad (58)$$

$$G(x) = \frac{\sin x}{x} + 2 \frac{\cos x}{x^2} - 2 \frac{\sin x}{x^3}, \quad (59)$$

$$\mathcal{H}_0^{rr}(x) = -\pi \left( \cos x + x \sin x - \frac{1}{2}x^2 \cos x \right), \quad (60)$$

$$\mathcal{H}_0(x) = (x^2 - 2)\mathcal{F}(x) + 2x\mathcal{G}(x) - x, \quad (61)$$

$$\mathcal{F}(x) = Ci(x) \sin x - si(x) \cos x, \quad \mathcal{G}(x) = \frac{d}{dx}\mathcal{F}(x), \quad (62)$$

$$si(x) = -\frac{\pi}{2} + \int_0^x dt \frac{\sin t}{t}, \quad Ci(x) = \gamma + \ln x + \int_0^x dt \frac{\cos t - 1}{t}, \quad (63)$$

where  $V_0^{rr}(z)$  and  $V_0^{fr}(z)$  are the ( $rr$ ) and ( $fr$ ) terms of the vacuum contribution to the interaction and  $\gamma$  is the Euler–Mascheronni constant. The term  $V_{(n)}^{fr}(z)$  carries the information about field state (thermal state, for example) and does not contribute when there is no real photons in any mode of the field. For this last case,  $\langle n_k \rangle = 0$ , which means that the field is in its vacuum state, we have

$$V_g(z, 0) = V_0^{rr}(z) + V_0^{fr}(z) =: V_0(z), \quad (64)$$

$$V_e(z, 0) = V_0^{rr}(z) - V_0^{fr}(z) = 2V_0^{rr}(z) - V_0(z), \quad (65)$$

for the ground state and excited state vacuum contributions to dispersive potentials, respectively. Analysing the small and large distance limits, one may show that

- For  $k_0z \ll 1$  (short distance limit):

$$V_e(z, 0) \simeq V_g(z, 0) = -\frac{\hbar\omega_0 \alpha_0}{8 z^3} + \mathcal{O}(z^{-2}). \quad (66)$$

- For  $k_0z \gg 1$  (large distance limit):

$$V_g(z, 0) = -\frac{3\hbar c \alpha_0}{8\pi z^4} + \mathcal{O}(z^{-6}), \quad (67)$$

$$V_e(z, 0) \simeq \frac{3\hbar c \alpha_0}{8\pi z^4} + \hbar c \alpha_0 k_0^4 \frac{\cos(2k_0z)}{2k_0z}. \quad (68)$$

Equation (66) can be recognized as the interaction between the atom and the wall in the London–van der Waals limit [4]. In this limit, both excited and ground state potentials coincide and are mainly given by the ( $rr$ ) contribution (only radiation reaction is important) as one can easily verify from equation (56) when  $k_0z \ll 1$ .

Equation (67), which gives the ground state potential at large distances, is the well-known Casimir–Polder potential [3]. However, by equation (68), we see that in this limit the excited state potential does not coincide with the ground state potential anymore. Apart from a Casimir–Polder term with opposite sign, there is an oscillating one that falls as  $1/z$  [16, 35] and since the Casimir–Polder term falls as  $1/z^4$ , the oscillatory term dominates over all large distance limits and the interaction presents an infinite number of potential wells.

In order to get a better understanding about last results, let us come back to equations (49) and (50). Making  $\langle n_{\mathbf{k}\lambda} \rangle = 0$ , the ground and excited state level shifts of the atom take the form

$$\delta E_g = \delta E_g^{fr} + \delta E_g^{rr} = -\frac{\alpha_0 k_0}{2} \sum_{\mathbf{k}\lambda} \frac{|\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{x})|^2}{k + k_0}, \quad (69)$$

$$\delta E_e = \delta E_e^{fr} + \delta E_e^{rr} = -\frac{\alpha_0 k_0}{2} \mathcal{P} \sum_{\mathbf{k}\lambda} \frac{|\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{x})|^2}{k - k_0}. \quad (70)$$

From last equations we clearly see that the potential associated with the ground state depends only on the non-resonant part of the atomic polarizability, while the potential associated with the excited state depends only on the resonant part. Since van der Waals force is related to level shift of the ground state of the atom [36], it may be called the dispersive non-resonant interaction. On the other hand, for obvious reasons, the excited state potential may be called as the dispersive resonant interaction. Last equations permit us also to understand why the resonant interaction is very much stronger than van der Waals interaction at large distances and practically equals to it at short distances. The position-dependent part of the modulus square of the amplitude of a field mode (subject to boundary conditions) which appears in the sums of equations (69) and (70), is usually an oscillating function of products of characteristic distances and the frequency associated with the mode. In our case the characteristic distance is  $z$ , which means that for high frequencies such that  $k > 2\pi/z$ , the oscillatory behaviour of the summands leads to a small contribution to the total sum compared to the contribution coming from the low frequencies ( $k < 2\pi/z$ ).

Taking into account that the number of modes per frequency is proportional to  $k^2$ , at short distances virtual photons with high frequencies ( $k \sim 2\pi/z \gg k_0$ ) are much more important to the interaction than those with low frequencies ( $k \ll k_0$ ), so that  $k_0$  may be neglected in denominators of the sums in equations (69) and (70) and the level shifts will be approximately the same. However, as the distance between the atom and wall becomes large, smaller and smaller frequencies become important to the interaction. For the ground state contribution, this leads to a monotonic variation of the interaction with the position. However, for the excited state contribution, when the distance becomes of the order  $2\pi/k_0$ , there is a strong increasing of the interaction, so the summand becomes singular at the frequency  $\omega_0$ . At very large distances, small frequencies become more important and both ground and excited state potentials become weak, but the excited state potential still remains very much stronger than the ground state potential.

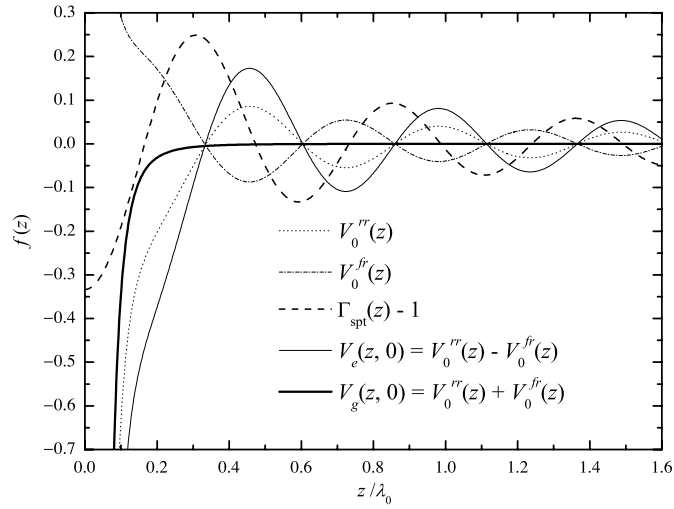
One can get a simple interpretation of this fact. Looking at equation (68) more carefully we easily see that a maximum and a minimum of the potential occur, respectively, at

$$z \simeq n \frac{\lambda_0}{2} \quad (\text{maximum}), \quad z \simeq \left(n - \frac{1}{2}\right) \frac{\lambda_0}{2} \quad (\text{minimum}), \quad (71)$$

where  $\lambda_0 = 2\pi c/\omega_0$  is the transition wavelength and  $n \geq 1$  is an integer (of course, these approximations will be better for higher values of  $n$ ). Equations (71) are nothing but the conditions for the existence of stationary waves with wavelength  $\lambda_0$  in the ‘cavity’ defined by the atom and the wall: the former is the resonant condition for a one-dimensional cavity with the ‘closed ends’ and the latter is the resonant condition for a cavity with one ‘closed end’ and one ‘opened end’. Then, it is intuitive why the interacting potentials have the maximum magnitude, or, in other words, a maximum response at that distances, and not at others.

In figure 1 we show the exact potentials given by equations (64) and (65) and the ( $rr$ ) and ( $fr$ ) contributions given by equations (56) and (57). As we pointed out previously, the ground and excited state potentials are approximately the same as the London–van der Waals potential (66) at short distances. At large distances, the excited state potential has an oscillatory behaviour while the ground state potential is given by the Casimir–Polder potential (67).

We saw that at short distances the radiation reaction on the polarizable system is the dominant contribution to the interaction, a well-established result in the literature [10, 15, 16]. However, the Casimir–Polder potential is usually interpreted as a Stark shift due to the field



**Figure 1.** Dispersive potentials associated with the ground (van der Waals interaction) and excited (resonant interaction) states with corresponding (*fr*) and (*rr*) contributions. The total spontaneous emission rate as a function of  $z$ ,  $\Gamma_{\text{spt}}(z)$ , is also shown. The potentials are in units of  $\hbar c \alpha_0 k_0^4$  and the spontaneous rate is in units of  $2c \alpha_0 k_0^4$ , which is the value for the spontaneous rate in the free space.

fluctuations mainly [16]. It is usual to adopt expressions similar to equation (50), for  $\langle n_{\mathbf{k}\lambda} \rangle = 0$ , in order to calculate the Casimir–Polder potential only replacing the atomic polarizability  $\alpha'_+(k)$  by its static value  $\alpha'_+(0) = \alpha_0$  in the summation [37]. This procedure can be justified if we invoke the argument that frequencies smaller than  $k \sim 2\pi/z \ll k_0$  give the main contribution to the interaction, so that the substitution of  $\alpha'_+(k)$  by  $\alpha_0$  causes a little error but gives the correct leading term of the potential (see papers by Ford [38], which make a careful discussion about this point).

Now, despite the success of this procedure, this seems to hide the true physical content behind it. As one can see from figure 1, both (*rr*) and (*fr*) contributions are of the same order of magnitude for distances  $z > 0.2\lambda_0$ , but have opposite signs. For this reason, the excited state interaction given by equation (65) is about two times (*rr*) contribution in the above-mentioned interval.

However, for the ground state potential given by (64), the (*rr*) and (*fr*) contributions almost cancel each other, leading to a small potential value which is precisely the van der Waals interaction, which reduces to the Casimir–Polder potential for  $z > \lambda_0$ . Then, both vacuum field fluctuations and radiation reaction play a crucial role for the interaction at large distances and the interpretation of the Casimir–Polder interaction as a shift due only to field fluctuations is not complete.

In order to conclude this section, let us make a comment about the exchange energy rates for the two-level system. From equations (38) and (40), one may easily show that  $\dot{Q}_g = 0$  and

$$\dot{Q}_e = -\pi \alpha_0 k_0^2 c \sum_{\mathbf{k}\lambda} |\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{x})|^2 \delta(k - k_0), \quad (72)$$

where we considered the field in its vacuum state. For the geometry treated here, namely, with a two-level atom at a distance  $z$  from an infinite perfectly conducting wall, the last equation

leads to [37]

$$\dot{Q}_e = -\hbar\omega_0\Gamma_{\text{spt}}(z), \quad \Gamma_{\text{spt}}(z) = \Gamma_{e \rightarrow g}^{\text{spt}}[1 - G(2k_0z)], \quad (73)$$

where  $\Gamma_{\text{spt}}(z)$  is the total spontaneous emission rate of the atom in the presence of the wall and  $\Gamma_{e \rightarrow g}^{\text{spt}} = 2c\alpha_0k_0^4 = 4\alpha|\langle e|\mathbf{r}|g\rangle|^2\omega_0^3/3c^2$  is the spontaneous emission for the atom in the empty space,  $\alpha = e^2/\hbar c \simeq 1/137$  being the fine structure constant. Then, the life time of the excited state of the atom is of the order  $1/\Gamma_{\text{spt}}(z)$ , so that the resonant interaction is unstable and at a finite time (generally about  $10^{-7}$ s in the visible region [39]) the van der Waals interaction takes place.

Equation (73) for  $\Gamma_{\text{spt}}(z)$  is also plotted in figure 1. The behaviour of the spontaneous emission is similar to the behaviour of the resonant potential. However, we should note that there is a difference of phase between the potential and the spontaneous emission of approximately  $\pi/2$ . Corresponding to a maximum or a minimum of the potential, the spontaneous emission is exactly the same as if the atom was in the empty space. Somehow this could have been anticipated once for these cases, from conditions (71), there is a node on the wall. One may also note that the fact that the potential is in quadrature with the spontaneous emission rate may be understood if we remember that these quantities are related to real and imaginary parts, respectively, of the susceptibilities (of the atom and the field) and these quantities are, of course, in quadrature.

### 3.2. Thermal corrections to the interaction

Let us now turn our attention to the thermal corrections of dispersive interactions by considering both ground and excited states of the atom. There are many works in the literature treating thermal corrections to dispersive van der Waals forces, see for instance [5, 9, 21] to mention just a few. However, we have not found works that have analysed also thermal corrections to the resonant interaction or the high temperature limit for dispersive interaction between the two-level system and the perfectly conducting wall. This is our aim in this section.

From equations (54) and (55), one may see that the only term that accounts for corrections to the interaction due to non-trivial states of the field is  $V_{(n)}^{fr}(z)$ , which is given by equation (58). For a thermal state of the field at temperature  $T$ , we write

$$V_{(n)}^{fr}(z) = V_T(z) = \frac{2\hbar c}{\pi} \int_0^\infty \frac{k^3 \alpha'_+(k)}{e^{k\lambda_T} - 1} G(2kz) dk, \quad (74)$$

where  $\lambda_T = \hbar c/k_B T$  is the thermal length, which defines the length scale beyond which thermal contributions pass to dominate over vacuum contribution of the van der Waals interaction. At room temperature,  $\lambda_T \simeq 7.63 \mu\text{m}$ .

In the low temperature limit,  $k_0\lambda_T \gg 1$ , we have already calculated the last integral in both small and large distance limits in a previous work [29], which for thermal corrections are defined by conditions  $z \ll \lambda_T$  and  $z > \lambda_T$ , respectively.

For  $z \ll \lambda_T$ , we have

$$V_T(z) \simeq C(T) - \frac{(2\pi)^5 \hbar c \alpha_0}{315 \lambda_T^6} z^2, \quad (75)$$

where  $C(T) = 2\pi^3 \hbar c \alpha_0 / 45 \lambda_T^4$  is independent of  $z$  and does not contribute to the force. The above result, that represents a small correction for the vacuum contribution, fits well the exact potential given by (74) within an error smaller than 3% for  $z < 0.10\lambda_T$  and, since it does not depend explicitly on  $\lambda_0$ , it is valid for both London–van der Waals and Casimir–Polder limits<sup>3</sup>.

<sup>3</sup> For the Casimir–Polder limit, the condition  $\lambda_0 < z \ll \lambda_T$  must be valid.

For  $z \sim \lambda_T$  or larger, we have

$$V_g(z) + V_T(z) \simeq V_{\text{Lif}}(z, T) = -\frac{k_B T}{4} \frac{\alpha_0}{z^3}, \quad (76)$$

which is exactly the Lifshitz asymptotic result [5], which we hereafter call only Lifshitz's potential for simplicity. If we consider only the ground state interaction, last equation fits the exact potential within an error smaller than 0.1% for  $z > \lambda_T$ .

The ground and excited state potentials with the corresponding thermal contributions are

$$V_g(z, T) = V_0^{rr}(z) + V_0^{fr}(z) + V_T(z) =: V(z, T), \quad (77)$$

$$V_e(z, T) = V_0^{rr}(z) - V_0^{fr}(z) - V_T(z) = 2V_0^{rr}(z) - V(z, T). \quad (78)$$

Considering the atom in thermal equilibrium with the field, we must consider the thermal average value of last potentials, since this average is the observed potential. If  $p$  is the probability of the atom to be found in its ground state,  $1 - p$  is the probability of finding it in its excited state. In a thermal equilibrium at a temperature  $T$ , we have  $p = (1 + e^{-k_0 \lambda_T})^{-1}$ , so that the average potential takes the form

$$\bar{V}(z, T) = \tanh\left(\frac{1}{2}k_0 \lambda_T\right) V(z, T) + \frac{2V_0^{rr}(z)}{e^{k_0 \lambda_T} + 1}. \quad (79)$$

At low temperatures,  $k_0 \lambda_T \gg 1$ , one has

$$\bar{V}_{\text{low}}(z, T) \simeq V(z, T) - 2e^{-k_0 \lambda_T} [V_0^{fr}(z) + V_T(z)].$$

The average potential is given by the ground state potential minus twice the ( $fr$ ) contribution weighted by the exponential factor  $e^{-k_0 \lambda_T} \ll 1$ , so that the average potential is practically due to the ground state potential only, as expected: the thermal photons do not have enough energy to excite the transition and populate the excited state, which makes negligible its contribution to the interaction. For example, at room temperature and for a transition frequency in the visible region,  $k_0 \simeq 10 \mu\text{m}^{-1}$ , the factor multiplying the ( $fr$ ) term is about  $7.1 \times 10^{-34}$ .

For the high temperature limit, however, things are different. In this limit, the excited state gives an important contribution to the interaction. In order to account the excited state influence on the interaction at high temperatures,  $k_0 \lambda_T < 1$ , it is necessary to recalculate the integral in (74) with the help of Bernoulli's numbers, defined by the expansion [40]

$$\frac{\xi}{e^\xi - 1} = 1 - \frac{1}{2}\xi + \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} \xi^{2n}.$$

Substituting the last expression into equation (74), we obtain  $V_T(z) = \hbar \Delta_T^{(1)} + \hbar \Delta_T^{(2)} + \hbar \Delta_T^{(3)}$ ,

$$\hbar \Delta_T^{(1)} = \frac{k_B T}{4\pi z^3} \int_0^\infty x^2 \alpha'_+(x) G(x) dx, \quad (80)$$

$$\hbar \Delta_T^{(2)} = -\frac{\hbar c}{16\pi z^4} \int_0^\infty x^3 \alpha'_+(x) G(x) dx = -V_0^{fr}(z), \quad (81)$$

$$\hbar \Delta_T^{(3)} = \frac{k_B T}{4\pi z^3} \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} \eta^{2n} \int_0^\infty x^{2n+2} \alpha'_+(x) G(x) dx, \quad (82)$$

where  $\eta = \lambda_T/2z$  and  $x = 2kz$ . Integrals in equation (82) may be easily calculated with the help of equation (53), which leads to

$$\hbar \Delta_T^{(3)} = V_0^{rr}(z) \left[ \frac{2}{k_0 \lambda_T} - \coth\left(\frac{1}{2}k_0 \lambda_T\right) \right]. \quad (83)$$

The integral in equation (80) may be also calculated in a simple manner from equation (53), but note that the function  $f(x) = x^2 G(x)$  is not analytical at  $x = 0$  and a direct application of (53) depends on the analyticity of  $f(x)$  over all complex planes. This problem may be avoided by splitting the integral in (80) as follows:

$$\int_0^\infty x^2 \alpha'_+(x) G(x) dx = \pi \alpha_0 \left( x_0 \sin x_0 - \frac{1}{2} x_0^2 \cos x_0 \right) - 2 \int_0^\infty \alpha'_+(x) \frac{\sin x}{x} dx, \quad (84)$$

where  $x_0 = 2k_0 z$ . The last term in the previous equation can be calculated as

$$\int_0^\infty \alpha'_+(x) \frac{\sin x}{x} dx = \alpha_0 \int_0^\infty \frac{\sin x}{x} dx - \frac{1}{x_0} \int_0^\infty \alpha'_-(x) \sin x dx = \frac{\pi \alpha_0}{2} (1 - \cos x_0). \quad (85)$$

Combining equations (85) and (84), equation (80) may be written as

$$\hbar \Delta_T^{(1)} = -\frac{k_B T}{4} \frac{\alpha_0}{z^3} - \frac{2}{k_0 \lambda_T} V_0^{rr}(z) \quad (86)$$

and the ground state potential (77) takes the form

$$V(z, T) = -\frac{k_B T}{4} \frac{\alpha_0}{z^3} - \frac{2V_0^{rr}(z)}{e^{k_0 \lambda_T} - 1}. \quad (87)$$

Inserting the last result into equation (79), the average potential may finally be written as

$$\bar{V}(z, \theta) = -\frac{\hbar \omega_0}{8} \frac{\alpha_0}{z^3} \theta \tanh(1/\theta), \quad (88)$$

where we defined the normalized temperature  $\theta = 2k_B T / \hbar \omega_0 = 2/k_0 \lambda_T$ . We derived equation (88) by assuming the high temperature limit, which means  $\theta \sim 1$  or higher. However, if we consider the opposite limit,  $\theta \ll 1$ , we easily see that equation (88) reduces to equation (76),

$$\bar{V}(z, T) = -\frac{k_B T}{4} \frac{\alpha_0}{z^3} (1 - 2e^{-k_0 \lambda_T} + 2e^{-2k_0 \lambda_T} + \dots) \simeq -\frac{k_B T}{4} \frac{\alpha_0}{z^3},$$

which is valid for all distances larger than the thermal length, that is, for  $z > \lambda_T$ . Hence, equation (88), which takes into account the excited state contribution, is also valid for all distances larger than the thermal length.

In figure 2 we plot the potentials (88) and (76) normalized by the potential (66). At low temperatures, as we have already anticipated, the excited state plays no role in the interaction and the ground state potential, which is given by Lifshitz's potential (76), coincides with the average potential. However, at high temperatures, the difference between Lifshitz's and the average potentials is evident, as can be checked in figure 2 for values of  $\theta$  greater than  $\theta \simeq 0.4$  approximately, which is equivalent to a temperature about  $2800\text{K} \times 1\mu\text{m}/\lambda_0$ ; at this point the relative error between the two potentials, defined as  $|\Delta V|/V_{\text{Lif}}$ , is about 1.3% (for  $\theta = 1.0$  the error is already  $\simeq 24\%$ ).

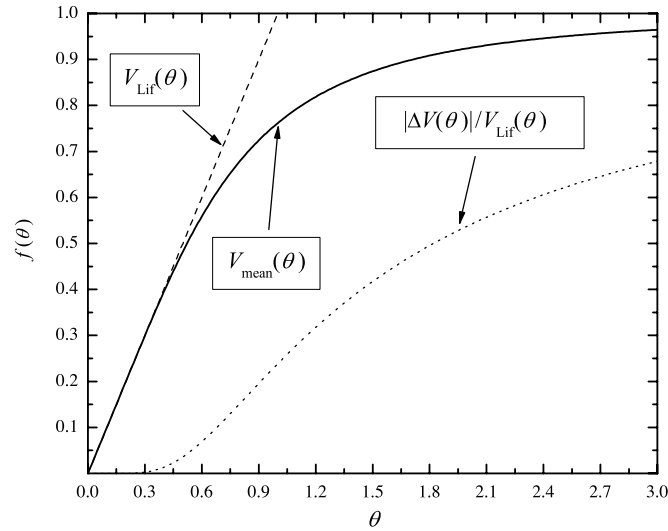
Nevertheless, the most interesting thing that happens as the temperature becomes higher is that the average potential saturates at a value independent of the temperature. In this case, the potential can be approximated by

$$\bar{V}(z, \theta) = -\frac{\hbar \omega_0}{8} \frac{\alpha_0}{z^3} \left( 1 - \frac{1}{3\theta^2} + \frac{2}{15\theta^4} - \dots \right), \quad (89)$$

which coincides exactly with the potential (66) in the limit of very high temperatures,  $\theta \rightarrow \infty$ .

As mentioned before, expression (66) gives the vacuum term of the dispersive potential between the atom and the wall, for both ground and excited states of the atom, in the small distance limit ( $0 < z \ll \lambda_0$ ). Further, when the system interacts with the field in a thermal state, thermal corrections to the potential become important only for distances larger than the





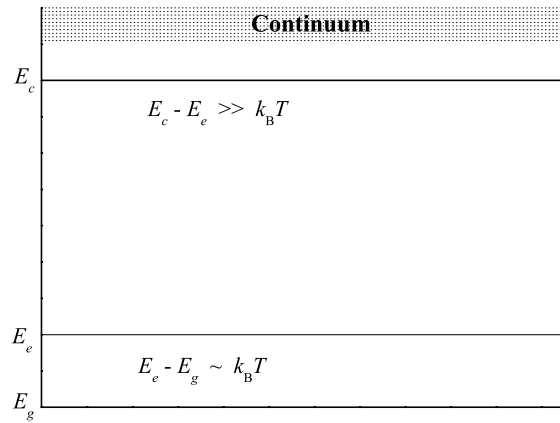
**Figure 2.** Dispersive potentials between a two-level atom and a perfectly conducting wall in a thermal bath at temperature  $T$ . We plot the temperature dependence of the thermal-averaged potential  $\bar{V}(z, T)$ , as well as the potential associated with the ground state only  $V_{\text{Lif}}(z, T)$ , normalized by  $-\hbar\omega_0\alpha_0/8z^3$  ( $V_{\text{mean}}(\theta)$  and  $V_{\text{Lif}}(\theta)$  respectively). The relative error  $|\Delta V(\theta)|/V_{\text{Lif}}(\theta)$  is also plotted. In the above figure it is assumed that  $z > \lambda_T$  and  $\theta = 2k_B T/\hbar\omega_0$ .

thermal length  $\lambda_T$ . Equation (89) is approximately valid for  $z > \lambda_T$  at very high temperatures,  $\theta \gg 1$ . This condition necessarily implies  $\lambda_T \ll \lambda_0$ . Hence, combining the last condition with the two just mentioned conditions for the separation  $z$  in which potentials (66) and (89) may be applied, one can see that the London–van der Waals potential describes the interaction at very high temperatures in the interval  $0 < z < \infty$ . In other words, for very high temperatures, the London–van der Waals potential is valid for all distance regimes. This is a quite curious result.

However, though expression (66) and the leading term of (89) are the same, there are some important differences in the physics behind them. The former is interpreted as the interaction between the instantaneous dipole and its mirror image so that retardation does not play any role at all on interaction and, as already mentioned, the main contribution is due to the radiation reaction only. The second one is the net result of the competition of the fluctuations of the field acting on the ground and excited states of the atom simultaneously.

From equations (77) and (78), one can see that thermal corrections have opposite signs and since at high temperatures the probability of finding the system in its ground or excited states is practically the same,  $p \simeq 1 - p \simeq 0.5$ , the  $(fr)$  terms cancel each other and the temperature dependence tends to disappear in the average potential, as it occurs in (89). We also see that in equations (77) and (78) the  $(rr)$  terms are the same, which leads to a net average potential different of zero. Hence, both equations (66) and (89) come from the radiation reaction, though from different ways. The fact that retardation does not seem to have any effect on the average potential is a feature of thermal fluctuations which, for distances larger than  $\lambda_T$ , destroy the influence of the finiteness of the velocity of light on the interaction, as one can see also in (76).

As a final comment, one may argue that equation (89) is an unrealistic one because there are not systems in the real world which can be treated as a two-level system at very high



**Figure 3.** System which simulates a two-level one and that can be used to check our result (88). Levels  $E_e$  and  $E_g$  are sufficiently close to each other so that thermal fluctuations can populate significantly both of them:  $E_e - E_g \sim k_B T \simeq 1/40$  eV at room temperature. Level  $E_c$  is so far from  $E_e$  and  $E_g$  ( $E_c - E_e \gg k_B T$ ) that, in practice, it cannot be populated by thermal fluctuations.

temperatures. Actually, all known systems usually have an infinite number of energy levels and the coupling between them at high temperatures should not be neglected, so that a different behaviour of that preconized for the two-level system is expected [12]. Even though, the two-level system model showed to be a very useful one in the study of the dispersive interactions and, particularly, in the comprehension of the roles played by ( $rr$ ) and ( $fr$ ) contributions.

Though equation (89) is, in some sense, unrealistic, the same cannot be said about equation (88). It is plausible to consider a system where the two lowest levels  $|g\rangle$  and  $|e\rangle$  are far enough to a third level  $|c\rangle$ , as sketched in figure 3. If the largest dimension  $D_0$  of this system is much smaller than the transition wavelength,  $D_0 \ll 2\pi\hbar c/(E_e - E_g)$ , and the temperature satisfies the condition  $E_e - E_g \sim k_B T \ll E_c - E_e$ , then equation (88) will be valid for a relatively wide range of temperature and a deviation of the behaviour predicted by equation (76), like that shown in figure 2, should be observed for not too high values of temperature.

#### 4. Conclusions

In this work, we applied the master equation formalism, widely used in quantum optics, in order to obtain the general expressions for the level shifts and the exchange energy rates of a multi-level system interacting with the radiation field in the dipole approximation. We then particularized our discussion to a two-level atom in the presence of a perfectly conducting wall. We studied the dispersive potentials, between the atom and the wall, for the ground and excited states of the atom, which can be associated with the van der Waals and the resonant interactions, respectively. All distance regimes as well as the low and high temperature limits were treated. Considering the ground state potentials in the short distance limit, we reobtained the London–van der Waals potential given by (66), showing that it may be explained mainly by the reservoir reaction (radiation reaction) contribution to the level shift, as it is well accept. For large distances, we rederived the Casimir–Polder interaction and showed that it cannot be considered as a direct result of the vacuum fluctuations only, as usually interpreted. Otherwise, we showed that the field fluctuations and the radiation-reaction contributions are of the same

order and too much stronger than the Casimir–Polder potential, but these effects ‘cancel each other’ leaving a small observed interaction.

For the case of the excited state potential, we emphasized that the maximum magnitudes of the potential occur approximately at the positions of resonant condition for stationary waves with wavelength  $\lambda_0$  in the ‘cavity’ defined by the atom and the wall. Taking into account the thermal corrections to the interaction, we rederived the short and large distance potentials at low temperatures, where the excited state contribution can be disregarded. However, for high temperatures, since the excited state contribution should not be neglected anymore, we showed that its inclusion may cause considerable deviations from the Lifshitz asymptotic potential. A curious result that we found is that at very high temperatures the potential saturate in a temperature-independent value which is exactly equal to the London–van der Waals potential but, now, valid for all distance regimes.

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