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Three-body Casimir-Polder interactions

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Summary. — As part of our program to develop the description of three-body
effects in quantum vacuum phenomena, we study the three-body interaction of two
anisotropically polarizable atoms with a perfect electrically conducting plate, a gen-
eralization of earlier work. Three- and four-scattering effects are important, and
lead to nonmonotonic behavior.

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PACS 11.80.La – Multiple scattering.
PACS 34.35.+a – Interactions of atoms and molecules with surfaces.
PACS 42.50.Lc – Quantum fluctuations, quantum noise, and quantum jumps.

1. – Introduction

Even before the discovery of the Casimir effect [1], Casimir and Polder studied the
retarded dispersion force between two atoms, and between one atom and a perfectly con-
ducting surface [2]. The Casimir-Polder force between an atom and a conducting plate
was, until relatively recently, only observed in one experiment [3], although the temper-
ature dependence of this force has now been confirmed [4]. In contrast, the experimental
observation of the Casimir-Polder force between atoms has remained beyond reach. For
an elementary review of aspects of Casimir-Polder forces see ref. [5].

In this paper we wish to consider three-body Casimir-Polder energies, involving two
polarizable atoms and a perfectly conducting plate. This was considered recently, but
in a somewhat restricted geometry [6]. A scalar analog was also recently examined by
Shajesh and Schaden [7]. (In the nonretarded regime, this was also considered by de
Melo e Souza *et al.*, following earlier work described in ref. [8].) Here we wish to examine
the situation a bit more generally. Our interest is not so much in finding observable
effects, which are probably difficult to detect, but to understand the general features of
three-body interactions; this is a small part of our continuing efforts in this direction.
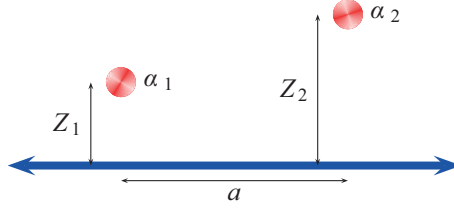
Fig. 1. – Two anisotropically polarizable atoms interacting with a perfectly conducting plate. The atom a, $a = 1, 2$, has polarizability $\boldsymbol{\alpha}_a$, and is a distance Z_a above the plate. The distance between the atoms in the direction parallel to the plate is a. The difference in heights above the plate is $\Delta Z = Z_1 - Z_2$.

2. – Two-body energy

For simplicity, we assume we are in the fully retarded regime, that is, the atoms are sufficiently far from each other or the plate so that we can describe them by their static electric polarizabilities,

$$(1) \qquad \boldsymbol{\alpha}_a = \boldsymbol{\alpha}_a(\omega = 0), \quad a = 1, 2.$$

We also neglect magnetic polarizability, and quadrupole and higher multipole moments of the atoms. We will, however, assume that the atoms are not isotropically polarizable. In the isotropic case, the two-body interaction energy between the atoms, a distance r apart, is given by the famous formula ($\hbar = c = 1$)

$$(2) \qquad E_{12} = -\frac{23}{4\pi} \frac{\alpha_1 \alpha_2}{r^7} \,,$$

but it is considerably more complicated when the atoms are not isotropically polarizable,

$$(3) \qquad E_{12} = -\frac{13 \operatorname{Tr}(\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2) - 56 \, (\hat{\mathbf{r}} \cdot \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 \cdot \hat{\mathbf{r}}) + 63 \, (\hat{\mathbf{r}} \cdot \boldsymbol{\alpha}_1 \cdot \hat{\mathbf{r}})(\hat{\mathbf{r}} \cdot \boldsymbol{\alpha}_2 \cdot \hat{\mathbf{r}})}{8\pi r^7} \,,$$

where $\mathbf{r} = r\hat{\mathbf{r}}$ is the relative position vector of the two atoms. This formula was apparently first given by Craig and Power [9]. In contrast, the interaction energy of a polarizable atom with a perfectly conducting plate a distance Z away is very simple,

$$(4) \qquad E_{\mathrm{CP}} = -\frac{\operatorname{Tr} \boldsymbol{\alpha}}{8\pi Z^4} \,.$$

(One might recall that the dimension of $\boldsymbol{\alpha}$ is (length)^3, and that $\boldsymbol{\alpha}$ is necessarily a symmetric matrix.)

We now wish to consider what happens when all three bodies are present, the two atoms and the perfectly conducting plate.

3. – Three-body energy

We wish to consider two polarizable atoms in the neighborhood of a perfectly conducting plate. The geometry is sketched in fig. 1. The two atoms have polarizabilities $\boldsymbol{\alpha}_a$,

and are located at distances from the plate Z_a, $a = 1, 2$. The difference in heights from the plate is $\Delta Z = Z_1 - Z_2$, and the horizontal distance (parallel to the plate) between the two atoms is called a.

To compute the interaction energy, we use the multiple-scattering formalism. For the case at hand, where only a single scattering with each atom need be considered, the two-body terms are (this is just the famous TGTG formula in weak coupling [10,11])

$$(5) \qquad E_{ab} = \frac{i}{2} \int \frac{\mathrm{d}\omega}{2\pi} \operatorname{Tr} \tilde{\mathbf{T}}_a \tilde{\mathbf{T}}_b,$$

where $a, b = 1, 2, 3$, and we denote the two atoms as bodies 1 and 2, while the perfectly conducting plate is body 3. Here the modified scattering operator is

$$(6) \qquad \tilde{\mathbf{T}} = \mathbf{T}\boldsymbol{\Gamma}_0 = \mathbf{V}(\mathbf{1} - \boldsymbol{\Gamma}_0\mathbf{V})^{-1}\boldsymbol{\Gamma}_0.$$

The free propagator $\boldsymbol{\Gamma}_0$ is [12]

$$(7) \qquad \boldsymbol{\Gamma}_0(\mathbf{r}, \mathbf{r}') = -\frac{e^{-|\zeta|R}}{4\pi R^3} \left[\mathbf{1}u(|\zeta|R) - \hat{\mathbf{R}}\hat{\mathbf{R}}v(|\zeta|R) \right], \quad \mathbf{R} = \mathbf{r} - \mathbf{r}',$$

where $\zeta = -i\omega$ is the imaginary frequency, and

$$(8) \qquad u(x) = 1 + x + x^2, \quad v(x) = 3 + 3x + x^2.$$

The scattering matrix for the atom is just the potential,

$$(9) \qquad \mathbf{T}_{1,2} = \mathbf{V}_{1,2} = 4\pi\boldsymbol{\alpha}_{1,2}\delta(\mathbf{r} - \mathbf{r}_{1,2}),$$

where $\mathbf{r}_a$ are the positions of the atoms. The structure in which the scattering matrix for the plate appears is

$$(10) \qquad \boldsymbol{\Gamma}_0\mathbf{T}_3\boldsymbol{\Gamma}_0 = \boldsymbol{\Gamma}_3 - \boldsymbol{\Gamma}_0;$$

$\boldsymbol{\Gamma}_3$ is the Green's dyadic for the plate. In fact, with $\hat{\mathbf{n}}$ denoting the normal to the plate,

$$(11) \qquad (\boldsymbol{\Gamma}_3 - \boldsymbol{\Gamma}_0)(\mathbf{r}, \mathbf{r}') = -\boldsymbol{\Gamma}_0(\mathbf{r}, \mathbf{r}' - 2\hat{\mathbf{n}}\hat{\mathbf{n}} \cdot \mathbf{r}') \cdot (\mathbf{1} - 2\hat{\mathbf{n}}\hat{\mathbf{n}}) \equiv -\overline{\boldsymbol{\Gamma}}(\mathbf{r}, \mathbf{r}').$$

This is just the image construction for a perfect electric mirror [13].

Using these constructions, the results in the previous section are easily derived. Our concern here is with the three-body terms. These are of three, related, types [14], where the subscripts on the right-hand side refer to the ordering of the scattering between the bodies,

$$(12) \qquad \Delta E_3 = E_{123} + E_{213} + E_{1323}.$$

The three-scattering energy is

$$(13) \qquad E_{123} = \frac{i}{2} \int \frac{\mathrm{d}\omega}{2\pi} \operatorname{Tr} \tilde{\mathbf{T}}_1 \tilde{\mathbf{T}}_2 \tilde{\mathbf{T}}_3 = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\mathrm{d}\zeta}{2\pi} \operatorname{Tr} \mathbf{V}_1\boldsymbol{\Gamma}_0\mathbf{V}_2\overline{\boldsymbol{\Gamma}},$$

while E_{213} is obtained by interchanging 1 and 2. The four-scattering contribution is

$$(14) \qquad E_{1323} = \frac{i}{2} \int \frac{d\omega}{2\pi} \operatorname{Tr} \tilde{\mathbf{T}}_1 \tilde{\mathbf{T}}_3 \tilde{\mathbf{T}}_2 \tilde{\mathbf{T}}_3 = -\frac{1}{2} \int_{-\infty}^{\infty} \frac{d\zeta}{2\pi} \operatorname{Tr} \mathbf{V}_1 \overline{\boldsymbol{\Gamma}} \mathbf{V}_2 \overline{\boldsymbol{\Gamma}}.$$

It is very straightforward to work out these contributions in the static approximation (1), where we ignore the frequency dependence of the polarizability. Let us now choose the plate to lie in the x-y plane. Because of the operator appearing in $\overline{\boldsymbol{\Gamma}}$, it is convenient to define $\boldsymbol{\beta}_a = (\mathbf{1}_\perp - \hat{\mathbf{z}}\hat{\mathbf{z}}) \cdot \boldsymbol{\alpha}_a$, $\mathbf{1}_\perp = \hat{\mathbf{x}}\hat{\mathbf{x}} + \hat{\mathbf{y}}\hat{\mathbf{y}}$. We can write all the energy contributions, including the two-atom ones, as follows:

$$(15a) \qquad\qquad E_{12}(\mathbf{r}_{12}) = -F(\mathbf{r}_{12}, \mathbf{r}_{21}; \boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2),$$

$$(15b) \qquad\qquad E_{123}(\mathbf{r}_{12}, \mathbf{r}_{2\bar{1}}) = F(\mathbf{r}_{12}, \mathbf{r}_{2\bar{1}}; \boldsymbol{\alpha}_2, \boldsymbol{\beta}_1),$$

$$(15c) \qquad\qquad E_{213}(\mathbf{r}_{21}, \mathbf{r}_{1\bar{2}}) = F(\mathbf{r}_{21}, \mathbf{r}_{1\bar{2}}; \boldsymbol{\alpha}_1, \boldsymbol{\beta}_2),$$

$$(15d) \qquad\qquad E_{1323}(\mathbf{r}_{2\bar{1}}, \mathbf{r}_{1\bar{2}}) = -F(\mathbf{r}_{2\bar{1}}, \mathbf{r}_{1\bar{2}}; \boldsymbol{\beta}_1, \boldsymbol{\beta}_2).$$

Here $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$, and the positions of the images of the atoms are denoted by $\mathbf{r}_{\bar{a}}$. These relative position vectors satisfy

$$(16a) \qquad\qquad \mathbf{r}_{21} + \mathbf{r}_{1\bar{2}} + \mathbf{r}_{2\bar{1}} + \mathbf{r}_{\bar{1}2} = \mathbf{0},$$

$$(16b) \qquad\qquad (\mathbf{r}_{21} + \mathbf{r}_{1\bar{2}}) \cdot (\mathbf{r}_{1\bar{2}} + \mathbf{r}_{\bar{1}2}) = 0.$$

The function appearing in the energies is

$$(17) \qquad F(\mathbf{x}, \mathbf{y}; \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{4\pi x^3 y^3 (x+y)} [A(x,y) \operatorname{Tr}(\boldsymbol{\alpha} \cdot \boldsymbol{\beta}) - B(x,y)(\hat{\mathbf{y}} \cdot \boldsymbol{\beta} \cdot \boldsymbol{\alpha} \cdot \hat{\mathbf{y}})$$
$$- B(y,x)(\hat{\mathbf{x}} \cdot \boldsymbol{\alpha} \cdot \boldsymbol{\beta} \cdot \hat{\mathbf{x}}) + C(x,y)(\hat{\mathbf{x}} \cdot \boldsymbol{\alpha} \cdot \hat{\mathbf{y}})(\hat{\mathbf{y}} \cdot \boldsymbol{\beta} \cdot \hat{\mathbf{x}})],$$

where

$$(18a) \qquad A(x,y) = \frac{8}{(x+y)^4} \left[x^4 + 5x^3 y + 14x^2 y^2 + 5xy^3 + y^4 \right] \xrightarrow{x=y} 13,$$

$$(18b) \qquad B(x,y) = \frac{8}{(x+y)^4} \left[3x^4 + 15x^3 y + 26x^2 y^2 + 10xy^3 + 2y^4 \right] \xrightarrow{x=y} 28,$$

$$(18c) \qquad C(x,y) = \frac{48}{(x+y)^4} \left[x^4 + 5x^3 y + 9x^2 y^2 + 5xy^3 + y^4 \right] \xrightarrow{x=y} 63.$$

4. – Special cases

4`1. *Isotropically polarizable atoms, equidistant from the plate*. – Let us first consider isotropic atoms equidistant from the plate, so $\Delta Z = 0$ and $Z_1 = Z_2 = Z$. Defining

$$(19) \qquad\qquad \gamma = \sqrt{1 + \frac{4Z^2}{a^2}},$$

we express the three-body interaction in terms of the two-atom Casimir-Polder energy,

$$(20) \qquad\qquad \Delta E_3 = E_{123} + E_{213} + E_{1323} = g(\gamma) E_{12},$$
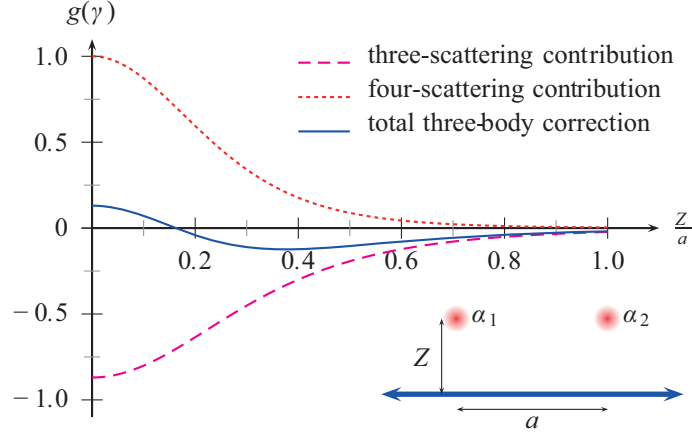
Fig. 2. – The three-body correction to the Casimir-Polder force between two atoms in the presence of a perfectly conducting plate. Here it is assumed that the atoms are isotropically polarizable, and are equidistant from the plate. What is plotted is the ratio of the three-body correction relative to the two-atom energy, plotted as a function of Z/a. The variable γ is defined in eq. (19).

where in this case E_{12} is given by eq. (2). Here

$$(21) \qquad\qquad g(\gamma) = -\frac{64(1+4\gamma)}{23\gamma^3(1+\gamma)^4} + \frac{1}{\gamma^7} \,,$$

where the last term is the four-scattering contribution. This function vanishes as $\gamma \to \infty$, that is, at large distances from the plate, and has a maximum negative deviation of about 12%, and has the value on the plate, at $Z = 0$, of $g(1) = 3/23 \approx 0.13$, as shown in fig. 2. (In the scalar analog considered in ref. [7], the correction on the plate is $g(1) = -1$, so the three-body energy cancels the two-atom energy when the atoms touch the plate([1]).) Note that the three-scattering terms, which are always negative, dominate for $Z/a > 0.16$, but very close to the plate the four-scattering term, which is always positive, causes the sign of the correction to reverse. However, close to the plate, these corrections are negligible compared to the two-body atom-wall energy (4), because

$$(22) \qquad\qquad \frac{E_{12}}{E_{\mathrm{CP}}} = \frac{\alpha_2}{r^3}\frac{46}{3}\left(\frac{Z}{r}\right)^4 \ll 1,$$

since typical values of $\alpha \sim (10^{-8}\,\mathrm{cm})^3$, while the separation consistent with our macroscopic approximation is not going to be smaller than $r \sim 10^{-6}\,\mathrm{cm}$. We might note that if the atoms and the plate are all equidistant, $Z = a$, the three-body effect is small, and the four-scattering contribution is totally negligible.

4$^{\cdot}$2. *Anisotropically polarizable atoms, equidistant from the plate*. – As a second example, we show the result considered in ref. [6], when the atoms are at equal heights,

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([1]) $g(\gamma)$ for the scalar analog reported in ref. [7] has an error of a factor of 2 in its first term.
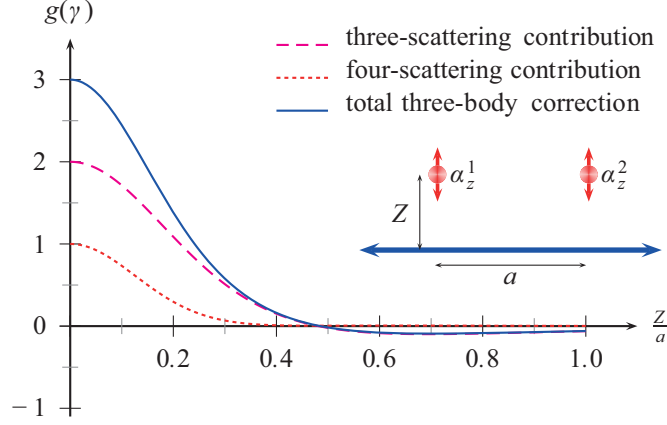
Fig. 3. – The three-body correction to the Casimir-Polder force between two atoms in the presence of a perfectly conducting plate. Here it is assumed that the atoms are completely anisotropic, being polarizable only in the direction perpendicular to the plate, and are the same distance from the plate. What is plotted is the ratio of the three-body correction relative to the two-atom energy, plotted as a function Z/a. The variable γ is again defined in eq. (19).

$\Delta Z = 0$, with a simple anisotropic polarizability,

$$\boldsymbol{\alpha}_a = \mathrm{diag}(\alpha_\perp^a, \alpha_\perp^a, \alpha_z^a), \quad a = 1, 2. \tag{23}$$

Then

$$\begin{aligned} E_{123} = \frac{2}{\pi a^7} \frac{1}{\gamma^5} \frac{1}{(1+\gamma)^5} & \left[\alpha_z^1 \alpha_z^2 (-3 - 15\gamma - 24\gamma^2 + 10\gamma^4 + 5\gamma^5 + \gamma^6) \right. \\ & \left. + \alpha_\perp^1 \alpha_\perp^2 (3 + 15\gamma + 28\gamma^2 + 20\gamma^3 + 6\gamma^4 - 5\gamma^5 - \gamma^6) \right]. \end{aligned} \tag{24}$$

This agrees with the result given in ref. [6], when the identical contribution of E_{213} is included.

The four-scattering term may be given in a similar form

$$\begin{aligned} E_{1323} = -\frac{1}{8\pi a^7 \gamma^{11}} [& \alpha_z^1 \alpha_z^2 (63 - 70\gamma^2 + 20\gamma^4) \\ & + \alpha_\perp^1 \alpha_\perp^2 (63 - 56\gamma^2 + 26\gamma^4) + (\alpha_\perp^1 \alpha_z^2 + \alpha_z^1 \alpha_\perp^2) 63(\gamma^2 - 1)]. \end{aligned} \tag{25}$$

This is identical to the corresponding term in ref. [6]. These energies, of course, agree with the result (21) in the isotropic case $\alpha_\perp^a = \alpha_z^a$.

We plot the contributions for the $\alpha_z^1 \alpha_z^2$ terms in fig. 3. That is, suppose the atoms are only polarizable in the z direction. Then the two-body Casimir-Polder interaction between the atoms is

$$E_{12} = -\frac{13}{8\pi a^7} \alpha_z^1 \alpha_z^2, \tag{26}$$

and we normalize the three- and four-scattering contributions relative to this value

$$(27) \qquad \frac{2E_{123}}{E_{12}} = g_3(\gamma), \qquad \frac{E_{1323}}{E_{12}} = g_4(\gamma), \qquad g(\gamma) = g_3(\gamma) + g_4(\gamma).$$

Again it is seen that the four-scattering contribution is significant only very close to the plate. Now the sign of the correction is negative only for $Z/a > 0.485$.

4·3. *Anisotropically polarizable atoms, unequal distances from the plate*. – As a final example, let us assume that the atoms are only polarizable in the z direction, $\alpha_z^a \neq 0$, $\alpha_\perp^a = 0$, but that the atoms are at different distances from the plate, $\Delta Z \neq 0$. Then, with the distances between the atoms being r, and the distance between one atom and the image of the other being $R \equiv \Gamma r$, that is

$$(28) \qquad R^2 = a^2 + (Z_1 + Z_2)^2, \qquad r^2 = a^2 + (Z_1 - Z_2)^2,$$

we easily find

$$(29a) \qquad E_{12} = -\frac{\alpha_z^1 \alpha_z^2}{8\pi r^7} \left(20 - 70\frac{a^2}{r^2} + 63\frac{a^4}{r^4} \right),$$

$$(29b) \qquad E_{123} = E_{213} = -\frac{2\alpha_z^1 \alpha_z^2}{\pi r^7 \Gamma^5 (1+\Gamma)^5} \left[2\Gamma^2 (1+\Gamma)^2 (1+3\Gamma+\Gamma^2) \right.$$

$$- \frac{a^2}{r^2}(1+\Gamma)^2 (3+9\Gamma+11\Gamma^2+9\Gamma^3+3\Gamma^4)$$

$$\left. +6\frac{a^4}{r^4}(1+5\Gamma+9\Gamma^2+5\Gamma^3+\Gamma^4) \right],$$

$$(29c) \qquad E_{1323} = -\frac{\alpha_z^1 \alpha_z^2}{8\pi r^7 \Gamma^7} \left(20 - 70\frac{a^2}{\Gamma^2 r^2} + 63\frac{a^4}{\Gamma^4 r^4} \right).$$

We plot these functions *versus* Γ in fig. 4.

The figure shows that although the four-scattering term is generally negligible compared to the three-scattering term, it is significant near the plate. In fact, for $\Gamma = 1$, which corresponds to one atom touching the plate, the following relation holds:

$$(30) \qquad E_{123} = E_{1323} = E_{12}, \quad r = R,$$

so the total energy is (again, we exclude the infinite two-body atom-wall energy)

$$(31) \qquad E = E_{12} + 2E_{123} + E_{1323} = 4E_{12}$$

at that unphysical point. Nonmonotonic effects can be seen when a/r is sufficiently near 1, or $\Delta Z/a$ sufficiently small.
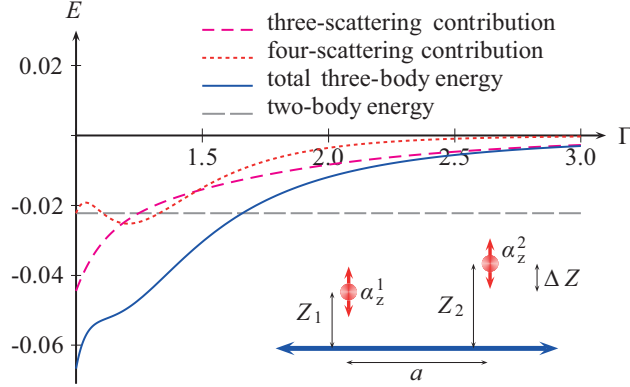
Fig. 4. – The three-body correction to the Casimir-Polder energy (in units of $\alpha_z^1 \alpha_z^2 / r^7$) between two atoms in the presence of a perfectly conducting plate. Here, it is assumed that the atoms are polarizable only in the direction perpendicular to the plate, and are at different distances from the plate. Note that although for large distances, that is, for large values of Γ, the three-scattering contribution dominates, for values close to $\Gamma = 1$ the four-scattering contribution is significant, and leads to nonmonotonicity in the slope. The energies plotted are for $a/r = 0.75$, or $\Delta Z/a \approx 0.88$, where the effect of the four-scattering term is most significant.

To close this section, we consider the same geometry, but atoms that are only polarizable transversely, $\alpha_z^a = 0$, $\alpha_\perp^a \neq 0$. Then we immediately find

$$(32a) \qquad E_{12} = -\frac{\alpha_\perp^1 \alpha_\perp^2}{8\pi r^7} \left(26 - 56\frac{a^2}{r^2} + 63\frac{a^4}{r^4} \right),$$

$$(32b) \qquad E_{123} = E_{213} = \frac{2}{\pi r^7 \Gamma^5 (1+\Gamma)^5} \Big[2\Gamma^2 (1 + 5\Gamma + 14\Gamma^2 + 5\Gamma^3 + \Gamma^4)$$

$$-\frac{a^2}{r^2}(3 + 15\Gamma + 28\Gamma^2 + 20\Gamma^3 + 28\Gamma^4 + 15\Gamma^5 + 3\Gamma^6)$$

$$+6\frac{a^4}{r^4}(1 + 5\Gamma + 9\Gamma^2 + 5\Gamma^3 + \Gamma^4)\Big],$$

$$(32c) \qquad E_{1323} = -\frac{\alpha_\perp^1 \alpha_\perp^2}{8\pi r^7 \Gamma^7} \left[26 - 56\frac{a^2}{\Gamma^2 r^2} + 63\frac{a^4}{\Gamma^4 r^4} \right].$$

Now the effects of the four-scattering terms are always much less dramatic. For example, for $a/r = 0.5$, in fig. 5 we plot the contributions to the correction to the Casimir-Polder energy between the atoms. The three-scattering contribution always dominates, although the four-scattering term can be important near the plate. Now, at the unphysical point $\Gamma = 1$ we have

$$(33) \qquad E_{123} = -E_{1323} = -E_{12},$$

so the total energy is zero there. Thus, $g(1) = -1$ for this case, similar to the scalar analog considered in ref. [7], where the three-body energy cancels the two-body energy when the atoms touch the plate. Of course, this result does not include the infinite Casimir-Polder energy (4) corresponding to the atom touching the plate.
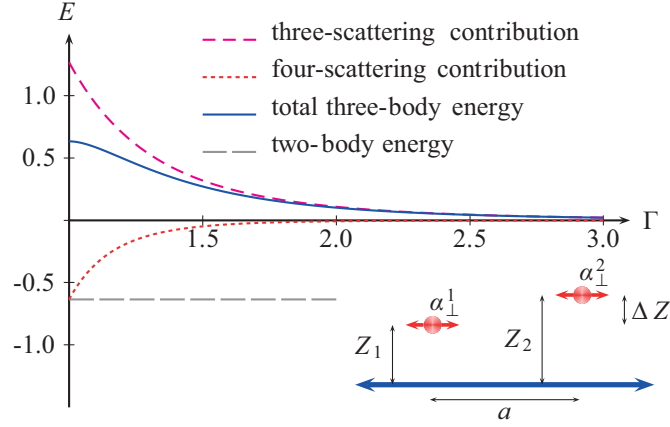
Fig. 5. – Here we plot the three-body correction (in units of $\alpha_\perp^1 \alpha_\perp^2 / r^7$) to the Casimir-Polder energy E_{12} for $a/r = 0.5$, for atoms polarizable only in directions parallel to the plate. Now there are no nonmonotonic effects, and the three-scattering contribution is dominant, although the four-scattering term can be significant near the plate.

5. – Conclusions

We have illustrated, in the simple context of two polarizable atoms interacting with each other and a nearby perfectly conducting plate, the three-body interactions beyond the two-body Casimir-Polder forces. These three-body energies break up into three- and four-scattering terms in this context, where the atom interactions are regarded as weak. This work generalizes that of ref. [6], which considered atoms equidistant from the plate, and that of ref. [7], which considered a scalar analog of the Casimir-Polder interaction. We observe regions of nonmonotonicity in the energy, which is reminiscent of results found earlier, numerically, in the context of rectangular objects near conducting surfaces [15, 16].

These effects are of conceptual interest only, because they generally represent small corrections to the Casimir-Polder interaction between atoms, which itself has never been directly observed, due to lack of sufficiently refined experimental technique. Where the three-body interactions are comparable to the two-body atom-atom energy, they are dwarfed by the two-body atom-wall interaction (4). The importance of this work lies in its contribution to our developing understanding of three-body effects in Casimir or quantum vacuum energy calculations. Further examples of these effects, in more nontrivial contexts, will appear elsewhere.

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