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Repulsive long-range forces between anisotropic atoms and dielectrics

K. V. Shajesh[*] and M. Schaden[†]

Department of Physics, Rutgers, The State University of New Jersey, 101 Warren Street, Newark, New Jersey 07102, USA

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We investigate long-range forces between atoms with anisotropic electric polarizability interacting with dielectrics having anisotropic permittivity in the weak-coupling approximation. Unstable configurations in which the force between the objects is repulsive are constructed. Such configurations exist for three anisotropic atoms as well as for an anisotropic atom above a dielectric plate with a hole whose permittivity is anisotropic. Apart from the absolute magnitude of the force, the dependence on the configuration is qualitatively the same as for metallic objects for which the anisotropy is a purely geometric effect. In the weak limit, closed analytic expressions for rather complicated configurations are obtained. The nonmonotonic dependence of the interaction energy on separation is related to the fact that the electromagnetic Green's dyadic is not positive definite. The analysis in the weak limit is found to also semiquantitatively explain the dependence of Casimir forces on the orientation of anisotropic dielectrics observed experimentally. Contrary to the scalar case, irreducible electromagnetic three-body energies can change sign. We trace this to the fact that the electromagnetic Green's dyadic is not positive definite.

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I. INTRODUCTION

Fifty-seven years after the postulation of attractive long-range van der Waals forces between neutral atoms [1], London [2–4] described them as a purely quantum mechanical effect. Later, Axilrod and Teller [5] and Muto [6] independently found that the three-body contribution of three atoms to the van der Waals–London interaction energy can change sign and contribute repulsively depending on their configuration. Repulsive long-range forces have so far been established in at least two situations:[1] for two dielectric objects with a suitable dielectric between them [8,9], and for a dielectric object and a magnetic material [10,11]. The latter repulsive effect has not yet been observed. Although it was known that the interaction between anisotropic atoms could have repulsive components [12,13], it came as a surprise that the force on a vertically oriented metallic needle above a hole in a metallic plate can be repulsive as well [14]. The explanation of this effect relied on symmetry arguments and numerical calculations. An analytic solution, in the unretarded regime, for a polarizable particle above a plate with a hole was obtained in Ref. [15] with similar repulsive effects. By summing two-body contributions in the multiple scattering formalism, the effect could also be verified in the retarded regime [16]. The origin of such repulsive effects nevertheless does not seem to have been sufficiently well understood to make reliable predictions for more general situations. For instance, although very interesting repulsive configurations were found in Ref. [17], one of the conclusions was that "there is no repulsion possible in the weak-coupling regime." For anisotropic atoms and dielectrics, this is not the case. This has been acknowledged in Ref. [18], which also obtains most of the results of Sec. II of this paper.

The interaction between anisotropic atoms has been studied extensively (see [19] and references therein). In the following, we identify configurations with repulsive long-range forces between atoms and dielectric materials with anisotropic polarizabilities and permittivities. For weak polarizability and susceptibility, we obtain exact analytic expressions for a wide range of geometries. The force on an atom sufficiently close to a dielectric plate with a hole is found to be repulsive for certain relative orientations of the polarizability and permeability of the atom and the dielectric material. It is always attractive at large separations. The cause for Casimir repulsion is traced to anisotropies in the polarizability of the objects and to the fact that the electromagnetic Green's dyadic is not positive definite. For ideal metals, the anisotropy is geometrical and exact results for dilute dielectrics should qualitatively extend to metals.

We begin by examining long-range forces between anisotropic atoms and dielectrics. As for scalar Casimir energies [20–23], we can show that the two-body contribution to the electromagnetic Casimir interaction is always negative, independent of the relative orientation of polarizability and permittivity tensors. However, contrary to the scalar case, the electromagnetic Casimir interaction energy in general is not a monotonic function of separation and some force components can change sign. Remarkably, torque-free points at which the interaction energy does not depend on the orientation of the atom appear to exist for some configurations of dielectrics. We then examine the three-body correction to the interaction of isotropic atoms [5,24] and find that it never dominates two-body contributions to the Casimir energy. Contrary to the scalar case, irreducible three-body contributions to the electromagnetic Casimir energy can change sign, because the electromagnetic Green's dyadic is not positive definite.

II. ANISOTROPIC POLARIZABLE ATOMS

Long-range interactions of polarizable atoms are described by the van der Waals–London forces [2,3] in the unretarded

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[*] shajesh@andromeda.rutgers.edu; http://andromeda.rutgers.edu/∼shajesh

[†] mschaden@andromeda.rutgers.edu; http://andromeda.rutgers.edu/∼physics/mschaden.htm

[1] We do not include here the repulsive pressure on a sphere found by Boyer [7] because it does not involve two objects.

regime and by Casimir-Polder forces [25] in the retarded regime. In the multiple scattering formalism, the interaction energy for two polarizable atoms is

$$E_{12} = \frac{1}{2}\int_{-\infty}^{\infty}\frac{d\zeta}{2\pi}\,\mathrm{Tr}\,\ln[\mathbf{1} - \boldsymbol{\Gamma}_0\cdot\mathbf{T}_1\cdot\boldsymbol{\Gamma}_0\cdot\mathbf{T}_2], \tag{1}$$

an expression already obtained for atoms in Ref. [26]. The free Green's dyadic $\boldsymbol{\Gamma}_0$ in Eq. (1) is

$$\boldsymbol{\Gamma}_0(\mathbf{r};i\zeta) = \frac{e^{-|\zeta|r}}{4\pi r^3}[-u(|\zeta|r)\mathbf{1} + v(|\zeta|r)\hat{\mathbf{r}}\,\hat{\mathbf{r}}], \tag{2}$$

with $u(x) = 1 + x + x^2$ and $v(x) = 3 + 3x + x^2$. Neglecting quadruple and higher moments, the scattering matrix $\mathbf{T}_i$ for the ith atom with atomic dipole polarizability $\boldsymbol{\alpha}_i(i\zeta)$ is

$$\mathbf{T}_i(\mathbf{x},\mathbf{x}';i\zeta) = 4\pi\boldsymbol{\alpha}_i(i\zeta)\delta^{(3)}(\mathbf{x}-\mathbf{x}_i)\delta^{(3)}(\mathbf{x}'-\mathbf{x}_i), \tag{3}$$

where $\mathbf{x}_i$ specifies the position of the atom. The δ functions in Eq. (3) permit a trivial evaluation of the spatial integrals of the trace in Eq. (1). For separations r_{ij} satisfying $r_{ij}^6 \gg |\boldsymbol{\alpha}_i(0)\boldsymbol{\alpha}_j(0)|$, the logarithm in Eq. (1) may be expanded.[2] The weak approximation consists of retaining only the leading term of this expansion and we have

$$\begin{aligned} E_{12}^W = -\frac{1}{2\pi r^6}\int_0^\infty d\zeta\, e^{-2\zeta r}[&u^2(\zeta r)\mathrm{Tr}\{\boldsymbol{\alpha}_1(i\zeta)\cdot\boldsymbol{\alpha}_2(i\zeta)\}\\ &-2u(\zeta r)v(\zeta r)\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_1(i\zeta)\cdot\boldsymbol{\alpha}_2(i\zeta)\cdot\hat{\mathbf{r}}\}\\ &+v^2(\zeta r)\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_1(i\zeta)\cdot\hat{\mathbf{r}}\}\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_2(i\zeta)\cdot\hat{\mathbf{r}}\}], \end{aligned} \tag{4}$$

which is the interaction obtained in Refs. [12,13]. We used the property that polarizability is a symmetric tensor, of the form $\boldsymbol{\alpha}_i = \sum_n \alpha_i^n \hat{\mathbf{e}}_i^n\hat{\mathbf{e}}_i^n$, where the $\hat{\mathbf{e}}_i^n$, $n = 1,2,3$, are the orthogonal principal axes satisfying $\hat{\mathbf{e}}_i^m\cdot\hat{\mathbf{e}}_i^n = \delta^{mn}$ and $\hat{\mathbf{e}}_i^m\times\hat{\mathbf{e}}_i^n = \varepsilon^{mnl}\hat{\mathbf{e}}_i^l$. For stable atoms, the corresponding principal polarizabilities α_i^n necessarily are non-negative. A simple model for the frequency dependence of the atomic polarizability is

$$\boldsymbol{\alpha}_i(i\zeta) = \boldsymbol{\alpha}_i(0)\frac{\omega_i^2}{\omega_i^2+\zeta^2}, \tag{5}$$

where ω_i is the excitation energy of the (two-level) atom and $\boldsymbol{\alpha}_i(0)$ is its static polarizability. One of the ways to calculate atomic polarizability is by Dalgarno's method [27].

The exponential dependence on the separation distance in Eq. (2) implies that the frequency dependence of the polarizability $\boldsymbol{\alpha}_i(i\zeta)$ in Eq. (5) is negligible for $\alpha^{\frac{1}{3}} < c/\omega_i \ll r$. In this asymptotic retarded (Casimir-Polder) regime, the polarizabilities can be approximated by their static values and the ζ integration in Eq. (4) performed to yield [12,13]

$$\begin{aligned} E_{12}^{\mathrm{CP}}(\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2;\mathbf{r}) = -\frac{1}{8\pi r^7}[&13\,\mathrm{Tr}\{\boldsymbol{\alpha}_1(0)\cdot\boldsymbol{\alpha}_2(0)\}\\ &-56\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_1(0)\cdot\boldsymbol{\alpha}_2(0)\cdot\hat{\mathbf{r}}\}\\ &+63\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_1(0)\cdot\hat{\mathbf{r}}\}\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_2(0)\cdot\hat{\mathbf{r}}\}]. \end{aligned} \tag{6}$$

For atoms with isotropic polarizabilities, $\boldsymbol{\alpha}_1 = \alpha_1\mathbf{1}$ and $\boldsymbol{\alpha}_2 = \alpha_2\mathbf{1}$, Eq. (6) reproduces the Casimir-Polder interaction [25]:

$$E_{12}^{\mathrm{CP}}(\alpha_1\mathbf{1},\alpha_2\mathbf{1};r) = -\frac{\alpha_1(0)\alpha_2(0)}{r^7}\frac{23}{4\pi}. \tag{7}$$

In the unretarded (London) regime ($\alpha^{\frac{1}{3}} < r \ll c/\omega_i$), the frequency dependence in Eq. (2) may be neglected and the free dyadic in Eq. (4) approximated by the static dipole-dipole interaction $\boldsymbol{\Gamma}_0(\boldsymbol{r};0)$ to yield [12,13]

$$\begin{aligned} E_{12}^{\mathrm{Lon}}(\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2;\mathbf{r}) = -\frac{1}{2\pi r^6}\int_0^\infty d\zeta\,[&\mathrm{Tr}\{\boldsymbol{\alpha}_1(i\zeta)\cdot\boldsymbol{\alpha}_2(i\zeta)\}\\ &-6\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_1(i\zeta)\cdot\boldsymbol{\alpha}_2(i\zeta)\cdot\hat{\mathbf{r}}\}\\ &+9\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_1(i\zeta)\cdot\hat{\mathbf{r}}\}\{\hat{\mathbf{r}}\cdot\boldsymbol{\alpha}_2(i\zeta)\cdot\hat{\mathbf{r}}\}]. \end{aligned} \tag{8}$$

For atoms with isotropic polarizabilities, this reproduces London's expression for the van der Waals interaction,

$$E_{12}^{\mathrm{Lon}}(\alpha_1\mathbf{1},\alpha_2\mathbf{1};r) = -\frac{3}{\pi r^6}\int_0^\infty d\zeta\,\alpha_1(i\zeta)\alpha_2(i\zeta), \tag{9}$$

which is inversely proportional to the sixth power in the separation r. To evaluate the coefficient, the frequency dependence of the polarizabilities has to be known or modeled. For the simple model in Eq. (5) (letting $\omega_1 = \omega_2 = \omega_0$), one has

$$E_{12}^{\mathrm{Lon}}(\alpha_1\mathbf{1},\alpha_2\mathbf{1};r) = -\frac{\alpha_1(0)\alpha_2(0)}{r^6}\frac{3\omega_0}{4}. \tag{10}$$

With modern computing power it is only slightly more complicated to perform the complete frequency integral in Eq. (4) numerically.

To illustrate the orientation dependence of the Casimir-Polder interaction, consider the special case where one of the atoms is isotropic and the other a linear molecule that essentially can only be polarized along its axis with a polarizability given by $\boldsymbol{\alpha}_1 = \alpha_1\,\hat{\mathbf{e}}\,\hat{\mathbf{e}}$. With $\hat{\mathbf{e}}\cdot\hat{\mathbf{r}} = \cos\theta$, Eq. (6) then becomes

$$E_{12}^{\mathrm{CP}}(\boldsymbol{\alpha}_1,\alpha_2\mathbf{1};\mathbf{r}) = -\frac{\alpha_1(0)\alpha_2(0)}{8\pi r^7}[13 + 7\cos^2\theta]. \tag{11}$$

The minimum energy configuration is at $\theta = 0$ or $\theta = \pi$, corresponding to the alignment of the axis $\hat{\mathbf{e}}$ of the molecule with $\boldsymbol{r}$. Note that the interaction energy of Eq. (11) is negative for any orientation.

Consider next two atoms with general static anisotropic polarizability tensors $\boldsymbol{\alpha}_i = \sum_n \alpha_i^n\hat{\mathbf{e}}_i^n\hat{\mathbf{e}}_i^n$ (see Fig. 1). Inserting these in Eq. (6), the interaction energy in the retarded regime is of the form

$$E_{12}^{\mathrm{CP}}(\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2;\mathbf{r}) = -\frac{1}{8\pi r^7}\sum_{m,n=1}^{3}\alpha_1^m(0)\alpha_2^n(0)C_{12}^{mn}, \tag{12}$$

with

$$C_{12}^{mn} = \tfrac{1}{13}\left|13\big(\hat{\mathbf{e}}_1^m\cdot\hat{\mathbf{e}}_2^n\big) - (28 + i\sqrt{35})\big(\hat{\mathbf{e}}_1^m\cdot\hat{\mathbf{r}}\big)\big(\hat{\mathbf{e}}_2^n\cdot\hat{\mathbf{r}}\big)\right|^2. \tag{13}$$

The potential energy surface of the interaction given in Eq. (12) is rich, with (local) extrema of individual C_{12}^{mn} at $C_{12}^{mn} = 20,13,5/9$, and 0. These extremums are summarized

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[2] Approximating atoms as pointlike objects in Eq. (3) is not justified for $r_{ij}^6 \lesssim |\boldsymbol{\alpha}_i(0)\boldsymbol{\alpha}_j(0)|$.

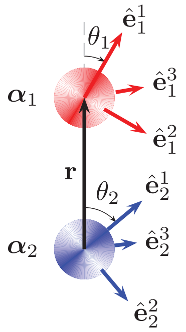


FIG. 1. (Color online) Two atoms with anisotropic polarizabilities.

in Table I. The C_{12}^{mn}'s are non-negative and vanish only if $\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{e}}_1^n = 0$ and $(\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{r}})(\hat{\mathbf{e}}_2^n \cdot \hat{\mathbf{r}}) = 0$. Since the eigenvalues of the polarization tensor are non-negative, the two-body interaction between two anisotropic atoms therefore is always negative. The maximum value of $C_{12}^{mn} = 20$ corresponds to the energetically most favorable orientation, $\hat{\mathbf{e}}_1^m = \pm\hat{\mathbf{r}}$, $\hat{\mathbf{e}}_2^n = \pm\hat{\mathbf{r}}$, where both atoms are aligned with $\mathbf{r}$. The potential energy surface has a saddle point when $(\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{r}})(\hat{\mathbf{e}}_2^n \cdot \hat{\mathbf{r}}) = 0$ and $\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{e}}_1^n = \pm 1$ that corresponds to $C_{12}^{mn} = 13$. Interesting extremum for $(\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{r}}) = \pm 2/3 = (\hat{\mathbf{e}}_2^n \cdot \hat{\mathbf{r}})$ and $\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{e}}_1^n = \pm 1$ correspond to $C_{12}^{mn} = 5/9$. Note that $(\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{r}}) = \pm 2/3$ represents an angle of about 48.2° between the polarizabilities and $\hat{\mathbf{r}}$. The interaction energy in Eq. (12) gives rise to a noncentral force between anisotropic atoms,

$$\mathbf{F} = -\frac{1}{2\pi r^8}\sum_{m,n=1}^{3}\alpha_1^m(0)\alpha_2^n(0)\big[7\hat{\mathbf{r}}C_{12}^{mn} - r\nabla C_{12}^{mn}\big]. \qquad (14)$$

The second term in Eq. (14) is a torque that vanishes for the extremal configurations of Table I.

III. CASIMIR REPULSION

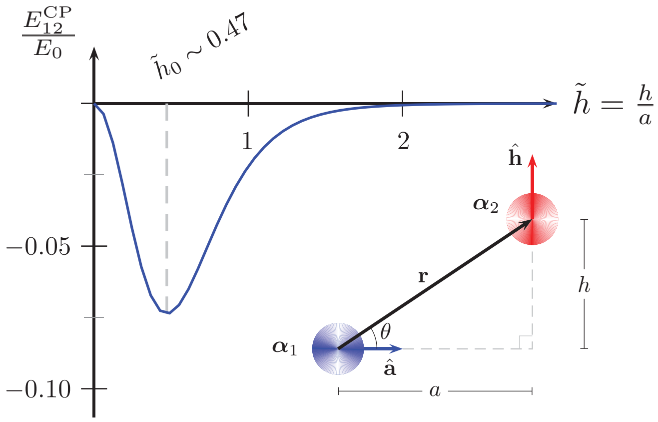


FIG. 2. (Color online) Dimensionless energy, with $E_0 = 63\alpha_1(0)\alpha_2(0)/8\pi\, a^7$, for two atoms with orthogonal polarizabilities in Eq. (15), sketched in the inset, plotted with respect to h/a.

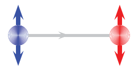
Since the Casimir-Polder energy can vanish for particular orientations of anisotropic atoms and is always negative, it is clear from the foregoing discussion that, in general, it is not a monotonic function of the distance between the atoms and that for fixed orientation of the atoms components of the force between them can be repulsive. To see this more explicitly, consider two linear atoms with polarizabilities that are orthogonal to each other: $\boldsymbol{\alpha}_1 = \alpha_1\hat{\mathbf{a}}\,\hat{\mathbf{a}}$, $\boldsymbol{\alpha}_2 = \alpha_2\hat{\mathbf{h}}\,\hat{\mathbf{h}}$, with $\hat{\mathbf{a}} \cdot \hat{\mathbf{h}} = 0$. Let $\hat{\mathbf{a}} \cdot \hat{\mathbf{r}} = \cos\theta$, $\hat{\mathbf{h}} \cdot \hat{\mathbf{r}} = \sin\theta$, and $r^2 = a^2 + h^2$. (See inset in Fig. 2.) Equation (6) gives the interaction energy for this configuration as

$$E_{12}^{\rm CP}(\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2;\mathbf{r}) = -\frac{\alpha_1(0)\alpha_2(0)}{a^7}\,\frac{63}{8\pi}\,\frac{\tilde{h}^2}{(1+\tilde{h}^2)^{\frac{11}{2}}}. \qquad (15)$$

For fixed horizontal separation a, the dimensionless interaction energy of Eq. (15) is shown in Fig. 2. It vanishes for $h = 0$ and $h \to \infty$ and is negative otherwise. The minimum at $\tilde{h} = h/a = \sqrt{2}/3 \sim 0.47$ implies that the vertical component of the force on atom 2 along $\mathbf{h}$ changes sign when $3h = \sqrt{2}a$. Regimes with repulsive components of the noncentral force between anisotropic atoms exist for all values of $\hat{\mathbf{a}} \cdot \hat{\mathbf{h}}$. For $|\hat{\mathbf{a}} \cdot \hat{\mathbf{h}}|$ sufficiently close to unity, the repulsive regime splits into two or more disjoint regions in $\tilde{h}$. In particular, for $|\hat{\mathbf{a}} \cdot \hat{\mathbf{h}}| = 1$, the two repulsive regimes are disjoint, symmetrical, and above and below the plate.

In the previous example, the horizontal component of the force between the two atoms was always attractive. However, this component of the force on atom 2 may be compensated by placing a third atom with polarization tensor $\boldsymbol{\alpha}_3 = \pm\alpha_1\hat{\mathbf{a}}\,\hat{\mathbf{a}}$ in the symmetric point with the three atoms forming an isosceles triangle. Of course, real atoms would not maintain these orientations and positions unless they are part of a

TABLE I. (Color online) Configurations with extremal energies for two linearly polarizable molecules. In the rows corresponding to $C_{12}^{mn} = 20$, and 5/9, the signs in the first two columns should concur.

$(\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{e}}_1^n)$	$(\hat{\mathbf{e}}_1^m \cdot \hat{\mathbf{r}})(\hat{\mathbf{e}}_2^n \cdot \hat{\mathbf{r}})$	$-C_{12}^{mn}$	Comments	Example
± 1	± 1	-20	Minima	
± 1	0	-13	Saddle	
± 1	$\pm\frac{4}{9}$	$-\frac{5}{9}$	Saddle	
0	0	0	Maxima	

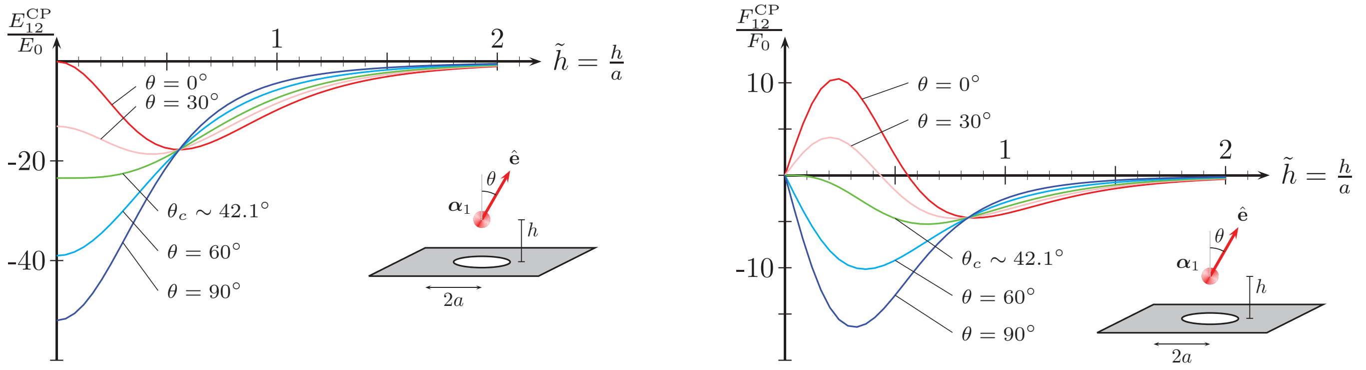


FIG. 3. (Color online) The energy of Eq. (18) in units of $E_0 = \alpha\lambda/320\pi a^5$ (left) and the force of Eq. (19) in units of $F_0 = \alpha\lambda/64\pi a^5$ (right) as functions of h/a for an anisotropic atom at a height h above the center of a dielectric plate with a hole of radius a as sketched in the insets. The curves correspond to different orientation θ of the atomic polarizability.

material. These considerations bring us to the analog of the geometry of a metallic needle above a metallic plate [14]. We therefore consider an atom with anisotropic polarizability centered above a dilute dielectric material with a hole as sketched in the insets of Fig. 3. In the weak limit, the scattering matrix of dilute dielectric objects can be approximated by their dielectric permittivity with $\mathbf{T}_i(\mathbf{x},\mathbf{y}) \sim \boldsymbol{V}_i(\mathbf{x})\delta^{(3)}(\mathbf{x}-\mathbf{y})$ and $\boldsymbol{V}_i(\mathbf{x}) = [\boldsymbol{\varepsilon}(\mathbf{x}) - \mathbf{1}] \sim 4\pi\boldsymbol{\alpha}_i n_i(\mathbf{x})$, where $n_i(\mathbf{x})$ is the number density of the atoms the dielectric is composed of and $\boldsymbol{\alpha}_i$ is their polarizability. In this weak limit, Eq. (1) in the retarded regime takes the form

$$\begin{aligned} E_{12}^{\rm CP} = &-\frac{1}{128\pi^3}\int d^3x \int d^3x' \frac{1}{|\mathbf{x}-\mathbf{x}'|^7}[13\,\mathrm{Tr}\{\mathbf{V}_1(\mathbf{x})\cdot\mathbf{V}_2(\mathbf{x}')\} \\ &- 56\hat{\mathbf{r}}\cdot\mathbf{V}_1(\mathbf{x})\cdot\mathbf{V}_2(\mathbf{x}')\cdot\hat{\mathbf{r}} \\ &+ 63\{\hat{\mathbf{r}}\cdot\mathbf{V}_1(\mathbf{x})\cdot\hat{\mathbf{r}}\}\{\hat{\mathbf{r}}\cdot\mathbf{V}_2(\mathbf{x}')\cdot\hat{\mathbf{r}}\}]. \end{aligned} \tag{16}$$

Equation (16) generalizes the corresponding expression for isotropic dielectric functions in Ref. [28] to the anisotropic case.

Using Eq. (16), we now can study the analog of the configuration proposed in Ref. [14] for dilute anisotropic dielectrics and atoms. In a Cartesian coordinate system with axes in the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ directions, we consider a dielectric plate in the xy plane with a hole of radius a centered at the origin and an anisotropic (linear) atom at the height h on the z axis. The scattering potential of the anisotropic atom is modeled by $\mathbf{V}_1(\mathbf{x}) = 4\pi\boldsymbol{\alpha}\delta(x)\delta(y)\delta(z-h)$ with the anisotropic static polarizability $\boldsymbol{\alpha} = \alpha\,\hat{\mathbf{e}}\hat{\mathbf{e}}$ and $\hat{\mathbf{e}}\cdot\hat{\mathbf{z}} = \cos\theta$. The scattering potential of the dielectric plate of thickness d with a hole of radius a is described by

$$\mathbf{V}_2(\mathbf{x}) = (\boldsymbol{\varepsilon} - \mathbf{1})\theta(\rho - a)[\theta(z+d) - \theta(z)] \sim \boldsymbol{\lambda}\theta(\rho - a)\delta(z), \tag{17}$$

with $\rho^2 = x^2 + y^2$. To simplify the calculation, we consider a thin plate and define $\boldsymbol{\lambda} \sim (\boldsymbol{\varepsilon} - \mathbf{1})d \sim 4\pi\boldsymbol{\alpha}\sigma$, with $\sigma = nd$ the planar density of atoms. We furthermore assume that the dielectric material is polarizable in the plane of the dielectric only and therefore demand that $\boldsymbol{\lambda}\cdot\hat{\mathbf{z}} = 0$. If $\boldsymbol{\lambda}$ is isotropic in the xy plane, we can insert $\boldsymbol{\lambda} = \lambda(\hat{\mathbf{x}}\hat{\mathbf{x}} + \hat{\mathbf{y}}\hat{\mathbf{y}})$ in Eq. (16) to obtain

$$\begin{aligned} E_{12}^{\rm CP}(a,h,\theta) = &-\frac{\alpha\lambda}{320\pi a^5}\frac{1}{(1+\tilde{h}^2)^{\frac{9}{2}}}[(36\tilde{h}^4 + 97\tilde{h}^2 + 26) \\ &+ (4\tilde{h}^4 + 83\tilde{h}^2 - 26)\cos 2\theta] \end{aligned} \tag{18}$$

for the interaction energy in the retarded regime. Figure 3 shows the dependence of Eq. (18) on the dimensionless height $\tilde{h} = h/a$ for different orientations θ of the anisotropic atom. At the intersection of all the curves in Fig. 3, the interaction energy does not depend on the orientation θ of the atom and the anisotropic atom is torsion free. This is the case when the coefficient of $\cos 2\theta$ in Eq. (18) vanishes, that is for $4\tilde{h}^4 + 83\tilde{h}^2 - 26 = 0$, giving $\tilde{h} \sim 0.56$. The torsion-free point coincides with the highest (unstable) equilibrium point, attained for $\theta = 0$. For heights above the torsion-free point, the energy is minimized for vertical orientation of the polarizability and below it the energy is minimized for horizontal orientations. The transition from vertical to horizontal orientation is sudden and happens at the torsion-free point without expense in energy. The net force on the atom in z direction is

$$\begin{aligned} F_{12}^{\rm CP}(a,h,\theta) = &-\frac{\alpha\lambda}{64\pi a^5}\frac{\tilde{h}}{(1+\tilde{h}^2)^{\frac{11}{2}}}[(36\tilde{h}^4 + 107\tilde{h}^2 + 8) \\ &+ (4\tilde{h}^4 + 113\tilde{h}^2 - 80)\cos 2\theta], \end{aligned} \tag{19}$$

and is shown in Fig. 3 as a function of $\tilde{h}$ for several orientations θ of the atom. The orientation-independent value for the vertical force occurs when $4\tilde{h}^4 + 113\tilde{h}^2 - 80 = 0$ and corresponds to $\tilde{h} \sim 0.83$. The force on the atom given by Eq. (19) is repulsive when

$$\tilde{h}^2 = \frac{h^2}{a^2} < \frac{-(107 + 113\,\cos 2\theta) + \sqrt{(107 + 113\,\cos 2\theta)^2 - 128(9 + \cos 2\theta)(1 - 10\,\cos 2\theta)}}{8(9 + \cos 2\theta)}, \tag{20}$$

which has real solutions for

$$0 < \theta < \tfrac{1}{2}\cos^{-1}\left(\tfrac{1}{10}\right) \quad \text{and} \quad \pi - \tfrac{1}{2}\cos^{-1}\left(\tfrac{1}{10}\right) < \theta < \pi. \tag{21}$$

The critical value for the orientation angle, $\theta_c = 0.5\cos^{-1}(0.1) \sim 42.1^\circ$, is the angle beyond which no repulsive regime exists.

To emphasize how weakly interacting configurations could lead to a semiquantitative understanding of their strongly interacting counterparts, we next consider the configuration in Ref. [29], where the Casimir force between gold and the anisotropic cuprate superconductor $\mathrm{Bi_2Sr_2CaCu_2O_{8+\delta}}$ (BSCCO) was found to decrease in magnitude by as much as 10%–20% when the BSCCO planes were oriented parallel to the gold plate rather than perpendicular to it. Let us replace the gold plate by a semi-infinite dielectric slab with isotropic permittivity described by $\mathbf{V}_1(\mathbf{x}) = [\boldsymbol{\varepsilon}_1 - \mathbf{1}]\theta(-z)$ with $(\boldsymbol{\varepsilon}_1 - \mathbf{1}) = (\varepsilon_1 - 1)\mathbf{1}$, and replace the BSCCO by a semi-infinite dielectric slab with $\mathbf{V}_2(\mathbf{x}) = [\boldsymbol{\varepsilon}_2 - \mathbf{1}]\theta(z-a)$ and $(\boldsymbol{\varepsilon}_2 - \mathbf{1}) = (\varepsilon_2 - 1)_\perp(\hat{\mathbf{x}}\hat{\mathbf{x}} + \hat{\mathbf{y}}\hat{\mathbf{y}}) + (\varepsilon_2 - 1)_{||}\hat{\mathbf{z}}\hat{\mathbf{z}}$ when the BSCCO planes are parallel to the xy plane (perpendicular cleave in Ref. [29]) and $(\boldsymbol{\varepsilon}_2 - \mathbf{1}) = (\varepsilon_2 - 1)_{||}\hat{\mathbf{x}}\hat{\mathbf{x}} + (\varepsilon_2 - 1)_\perp(\hat{\mathbf{y}}\hat{\mathbf{y}} + \hat{\mathbf{z}}\hat{\mathbf{z}})$ if they are oriented parallel to the xz plane (parallel cleave in Ref. [29]). Using Eq. (16), one obtains for the ratio of the Casimir force in the two orientations

$$\frac{F_{||\,\mathrm{cleave}}}{F_{\perp\,\mathrm{cleave}}} = 1 + \frac{2[(\varepsilon_2 - 1)_\perp - (\varepsilon_2 - 1)_{||}]}{[14(\varepsilon_2 - 1)_\perp + 9(\varepsilon_2 - 1)_{||}]}. \tag{22}$$

If we assume $(\varepsilon_2 - 1)_{||} \ll (\varepsilon_2 - 1)_\perp$, which is a good approximation for BSCCO, the magnitude of the Casimir force in the retarded regime changes by $1/7 \sim 14\%$, in semiquantitative agreement with [29].

IV. THREE-ATOM CASIMIR ENERGIES

Irreducible many-body Casimir energies were proven to remain finite in Refs. [20,23] when some, but not all, objects overlap. For a massless scalar quantum field with local potential interactions, the sign of the N-body Casimir energy was found to be simply $(-1)^{N+1}$. These theorems were verified in all examples studied in Refs. [20–23], where closed expressions for irreducible many-body Casimir energies were derived in the framework of the multiple scattering expansion. The proof of the sign of irreducible many-body contributions in the scalar case relied on the positivity of the free scalar Green's function. The electromagnetic free Green's dyadic of Eq. (2) is not a positive definite operator. The eigenvalues of this matrix, corresponding to eigenvectors parallel to $\mathbf{r}$ and orthogonal to it, are proportional to $(u(x) - v(x), u(x), u(x))$, where $u(x)$ and $v(x)$ were defined after Eq. (2). Here we investigate consequences of this for the sign of the irreducible three-body contribution to the Casimir energy between three isotropic atoms [5,24].

Inserting the free Green's dyadic of Eq. (2) into the expression for the irreducible three-body contribution to the Casimir energy in Ref. [21], and using scattering matrices for isotropic atoms given by Eq. (3) with $\boldsymbol{\alpha}_i = \alpha_i(i\zeta)\mathbf{1}$, one obtains

$$E^W_{123} = \frac{1}{\pi}\frac{1}{r^3_{12}r^3_{23}r^3_{31}}\int_0^\infty d\zeta\, e^{-\zeta(r_{12}+r_{23}+r_{31})}\alpha_1(i\zeta)\alpha_2(i\zeta)\alpha_3(i\zeta) \times Q_{123}(\mathbf{r}_{12},\mathbf{r}_{23}), \tag{23}$$

where the displacements $\mathbf{r}_{ij}$ are the sides of the triangle formed by the three atoms and satisfy $\mathbf{r}_{12} + \mathbf{r}_{23} + \mathbf{r}_{31} = 0$. The function Q_{123} in Eq. (23) is

$$\begin{aligned} Q_{123}(\mathbf{r}_{12},\mathbf{r}_{23}) = {} & 3u_{12}u_{23}u_{31} - u_{12}u_{23}v_{31} - u_{12}v_{23}u_{31} \\ & - v_{12}u_{23}u_{31} + u_{12}v_{23}v_{31}\cos^2\theta_3 \\ & + v_{12}u_{23}v_{31}\cos^2\theta_1 + v_{12}v_{23}u_{31}\cos^2\theta_2 \\ & + v_{12}v_{23}v_{31}\cos\theta_1\cos\theta_2\cos\theta_3, \end{aligned} \tag{24}$$

with $u_{ij} = u(|\zeta|r_{ij})$, $v_{ij} = v(|\zeta|r_{ij})$; the θ_i's $(i = 1,2,3)$ denote the internal angles of the triangle. In the unretarded limit, Eq. (23) simplifies to the expression obtained in Ref. [5],

$$E^{\mathrm{Lon}}_{123} = \frac{(1 + 3\cos\theta_1\cos\theta_2\cos\theta_3)}{r^3_{12}r^3_{23}r^3_{31}} \times \frac{3}{\pi}\int_0^\infty d\zeta\,\alpha_1(i\zeta)\alpha_2(i\zeta)\alpha_3(i\zeta). \tag{25}$$

Using the simple model in Eq. (5) for three identical isotropic atoms with $\omega_1 = \omega_2 = \omega_3 = \omega_0$, the integral in Eq. (25) is readily performed to yield [30]

$$E^{\mathrm{Lon}}_{123} = \frac{\alpha_1(0)\alpha_2(0)\alpha_3(0)}{a^{10}}\omega_0 a C^{\mathrm{Lon}}_{123}(\theta_1,\theta_2), \tag{26}$$

where the angular dependence is given by [24]

$$C^{\mathrm{Lon}}_{123}(\theta_1,\theta_2) = \frac{9}{16}\frac{\sin^6\theta_3(1 + 3\cos\theta_1\cos\theta_2\cos\theta_3)}{\sin^3\theta_1\sin^3\theta_2}, \tag{27}$$

with the three sides and angles of the triangle related by the law of sines. It was noted in Ref. [5] that the three-body contribution in the unretarded regime is negative when the atoms form an acute triangle and positive when it is (very) obtuse. For isosceles triangles, this behavior is seen in Fig. 4. References [30–32] attempted to explain the crystal structures of rare gases by three-body contributions to the total energy. Although this turned out not to be possible, three-body effects typically contribute between 10% and 20% to the total energy.

The ζ integral in Eq. (23) can be performed analytically in the retarded limit, but the result is not very illuminating and too lengthy to be presented here. In the special case when the atoms are arranged to form an isosceles triangle with side lengths $r_{12} = a$, $r_{23} = r_{31} = r$, and $\theta_1 = \theta_2 = \theta$ (see inset in Fig. 4), the retarded interaction is [24]

$$E^{\mathrm{CP}}_{123}(a,\theta) = \frac{\alpha_1(0)\alpha_2(0)\alpha_3(0)}{a^{10}}C^{\mathrm{CP}}_{123}(\cos\theta), \tag{28}$$

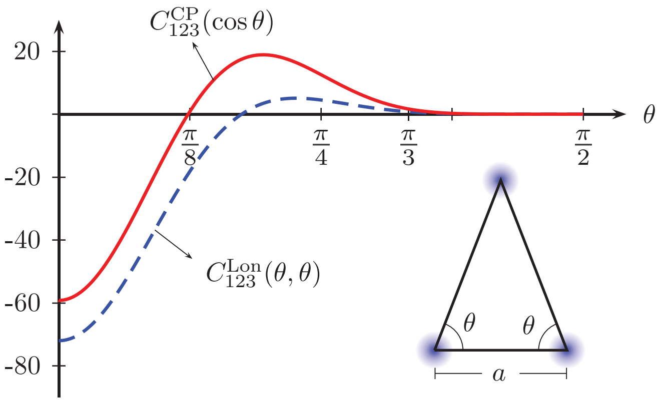


FIG. 4. (Color online) Angular dependence of three-body contributions to the long-range forces in the retarded (CP) and unretarded (Lon) regime for three atoms forming an isosceles triangle.

with

$$C^{\rm CP}_{123}(x) = \frac{1}{4\pi}\left[\frac{2x}{1+x}\right]^7 [7 + 49x + 611x^2 + 1533x^3 + 868x^4 - 1372x^5 - 1672x^6 - 672x^7 - 96x^8]. \tag{29}$$

For an equilateral triangle, it yields $E^{\rm CP}_{123}(a,\pi/3) = \alpha_1(0)\alpha_2(0)\alpha_3(0)1264/243\pi a^{10}$ in agreement with [24]. As in the unretarded limit, the angular dependence in the retarded limit also leads to configurations in which the three-body force contributes repulsively. Figure 4, in fact, shows that the irreducible three-body contribution to the potential is less attractive in the retarded regime. However, for isotropic atoms, the three-body contribution never dominates over two-body contributions in the regime $\alpha < r^3$, where a pointlike description of the atoms is justified. Evidently, the analysis of atomic many-body interaction is only a little more involved for anisotropic atoms and molecules.

V. CONCLUSION

We have shown that the force between atoms with anisotropic polarizabilities and dilute dielectrics with anisotropic permeabilities can have repulsive components. The weakly interacting configurations we considered give a semiquantitative understanding of the analogous strongly interacting case. That the two-body Casimir energy is not always monotonic in the separation is associated with the tensorial structure of the polarizabilities and the electromagnetic Green's dyadic. The analysis of an anisotropic atom above a dilute dielectric plate with a hole provides considerable insight into the analogous configuration involving perfect metals considered in Ref. [14]. A closed analytic solution for this configuration reveals torque-free points at which the interaction energy is independent of the orientation of the atomic polarizability. Although a single hole in a dielectric plate does not lead to stable points, multiple holes are expected to introduce stable points in the potential energy surface of an oriented atom.

Unlike the scalar case, for which the irreducible three-body contribution to Casimir energy is always positive [20–23], we find the electromagnetic three-body Casimir energy can change sign. The three-body contributions to the energy are found to never dominate the two-body contributions for isotropic atoms.

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