Repulsive lateral van der Waals force

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In the literature, it has been shown that between a neutral polarizable particle and a conducting plane surface arises an attractive dispersive force. A change on this geometry, for instance by the presence of a hole, can be felt by an anisotropic particle as a repulsive force, normal to the surface. In the present paper, we introduce a single slight protuberance, with a certain characteristic width, in the geometry of a perfectly conducting plane, and show that, beyond a correction to the normal attractive force already present in the absence of the protuberance, a neutral anisotropic polarizable particle feels a lateral van der Waals force which, under certain circumstances, repels it towards points that are several widths distant from the center of the protuberance. Moreover, we show that a similar repulsive effect arises in the classical context, involving a neutral particle with a permanent dipole moment.

In 1873, van der Waals proposed an equation of state for real gases, which included a term related to intermolecular attractive forces [1]. For the case of two non-polar molecules, the intermolecular forces, usually called dispersion van der Waals (vdW) forces, are due to the quantum fluctuations in the distributions of charges and currents in these molecules [2, 3]. The influence of retardation effects, related to the speed of light, on these dispersive forces is obtained in the context of the quantum electrodynamics [4–6]. Dispersive forces are also related, for instance, to the attraction between two perfectly conducting parallel plates [7], and between a neutral polarizable particle and a conducting plane surface [7, 8]. In general, dispersive forces depend on the material properties and on the geometry of the material bodies involved [9–16], and the progress in the precision of the experiments has opened possibilities for applications in micro and nanotechnology [17–20].

The repulsive aspect of the dispersive forces has attracted growing interest [6, 21–38]. For example, a conducting spherical shell experiences an outward repulsive dispersive force [22]. Moreover, there can be repulsion between an electrically polarizable atom and a magnetically polarizable one (or between the correspondent macroscopic bodies) [6, 23–26], between two dielectric bodies separated by a fluid [21, 28], and also between two conducting plates separated by a perfect lens [27]. Anisotropic polarizable particles are fundamental in several situations of repulsive dispersive forces [29, 30, 34, 35, 39]. For example, an anisotropic particle can feel a normal repulsive force when put on the symmetry axis of a thin metal plate with a hole [29] [see Fig. 1(a.i)], when it is over a perfectly conducting toroid [35] [see Fig. 1(a.ii)], or over an annular disk [39] [see Fig. 1(a.iii)]. In all these examples, when the repulsion occurs, the interaction energy \( U \) has a shape similar to the one illustrated in Fig. 1(a.iv).

When corrugations are considered, lateral forces appear, which can reveal nontrivial geometric effects in dispersive interactions [34, 40–51]. In the present paper, we consider the geometry of a plane surface \((z = 0)\) with a single slight protuberance [as illustrated in Fig. 1(b.I)], and a neutral anisotropic polarizable particle kept constrained to move on the plane \(z = z_0 > 0\). We show that, for certain particle orientations and characteristic widths of the protuberance, one of the typical dependencies of the vdW interaction energy \(U\) on \(x_0\) is as illustrated in Fig. 1(b.II). Thus, when the particle is over the protuberance, a lateral vdW force repels it to points several widths distant from the protuberance, as illustrated in Fig. 1(b.II). We consider a perfectly conducting surface in the calculations (as done by Casimir and Polder in Ref. [5], and Casimir in Ref. [7]), intending to write simpler formulas, already capable to provide a clear indication of the existence of this repulsive lateral vdW force.

Figure 1. (a) Some examples, from the literature, of configurations \([(a.i) - (a.iii)]\) that produce a normal repulsive dispersive force, and their typical common shape of the interaction energy \(U(z)\) (a.iv). (b) One of the examples, discussed in the present paper, of configuration that produces a repulsive lateral vdW force (b.I). A single slight protuberance, with a certain characteristic width, is added to a plane. A neutral anisotropic polarizable particle, kept constrained to move on the plane \(z = z_0\), feels a repulsive lateral vdW force and is pushed to a point several widths distant from the protuberance (b.I). In (b.II), we illustrate one of the typical dependencies of the vdW interaction energy \(U\) on \(x_0\), found by our calculations.

I. MODEL AND APPROACH

Let us start considering an anisotropic polarizable particle characterized by a frequency dependent polarizability...
tensor $\alpha$ given by (see, for instance, Ref. [52]) $\alpha(\omega) = \alpha_1(\omega)\hat{e}_1'\hat{e}_1' + \alpha_2(\omega)\hat{e}_2'\hat{e}_2' + \alpha_3(\omega)\hat{e}_3'\hat{e}_3'$, where $\hat{e}_1'$, $\hat{e}_2'$ and $\hat{e}_3'$ are unit vectors pointing in the directions of the principal axes of the particle (see Fig. 2). Denoting the Euler angles by $(\phi, \theta, \psi)$, according to the convention usually adopted in quantum mechanics [53, 54], we have $\hat{e}_i' = \sum_j R_{ij}\hat{e}_j$, where $R_{ij}$ are the elements of the Euler rotation matrix $R(\phi, \theta, \psi)$, $\hat{e}_1 = \hat{x}$, $\hat{e}_2 = \hat{y}$, and $\hat{e}_3 = \hat{z}$ are unit vectors related to the laboratory coordinate system $xyz$, and $R_{11} = \cos(\theta) \cos(\psi) \cos(\phi) - \sin(\psi) \sin(\phi)$, $R_{12} = - \cos(\theta) \sin(\psi) \cos(\phi) - \cos(\psi) \sin(\phi)$, $R_{13} = \sin(\phi)$, $R_{21} = \cos(\theta) \cos(\psi) \sin(\phi) + \sin(\psi) \cos(\phi)$, $R_{22} = \cos(\theta) \sin(\phi)$, $R_{31} = - \sin(\phi) \cos(\psi)$, $R_{32} = \sin(\phi) \sin(\psi)$, $R_{33} = \cos(\phi)$.

The particle is located at $r_0 = r_{0||} + z_0\hat{z}$ (with $z_0 > 0$ and $r_{0||} = x_0\hat{x} + y_0\hat{y}$), above a grounded conducting corrugated surface described by $z = h(r_0)$, with $h(r_0)$ describing a general subtle modification $\max(h(r_0)) = a \ll z'$ to a grounded planar conducting surface at $z = 0$ (see Fig. 2).

![Figure 2. Illustration of a neutral polarizable anisotropic particle, arbitrarily oriented in space, located at $r_0 = r_{0||} + z_0\hat{z}$ (with $z_0 > 0$), interacting with a general grounded conducting corrugated surface, whose corrugation profile is described by $z = h(r_0)$. The unit vectors $\hat{e}_1'$, $\hat{e}_2'$ and $\hat{e}_3'$ are those pointing to the directions of the principal axes of the particle, in whose directions the particle presents the polarizabilities $\alpha_1(\omega)$, $\alpha_2(\omega)$, and $\alpha_3(\omega)$, respectively.](image)

To investigate the vdW interaction energy $U_{vdW}$ between the particle and the corrugated surface, we take as basis the analytical perturbative approach presented by us in Ref. [51], according to which $U_{vdW} \approx U_{vdW}^{(0)} + U_{vdW}^{(1)}$, where $U_{vdW}^{(0)}$ is the vdW potential for the case of a grounded conducting plane [8], and $U_{vdW}^{(1)}$ (the first-order correction of $U_{vdW}^{(0)}$ due to the surface corrugation) is given by $U_{vdW}^{(1)}(r_0) = - \frac{\pi}{a^3} \sum_{j=1}^{3} K_{ij}(r_0, h) \int_{0}^{\infty} d\xi \alpha_{ij}(\xi) h(4\pi^2 \varepsilon_0 \omega \xi^2) e^{i K_{ij}(z_0 q)}$ where $\alpha_{ij}$ are the components of the polarizability tensor in the laboratory system, $K_{ij}(r_0, h) = \frac{1}{a} \int_{(2\pi)^3} d^3q h(q) e^{i q \cdot r_0} J_{ij}(\omega) q$ are dimensionless functions, and the functions $J_{ij} = J_{ji}$ are written as

$$J_{xx}(u) = \frac{3}{8} |u|^3 K_3(|u|) - \frac{3}{8} u_x^2 |u|^2 K_2(|u|),$$

$$J_{yy}(u) = \frac{3}{8} |u|^3 K_3(|u|) - \frac{3}{8} u_y^2 |u|^2 K_2(|u|),$$

$$J_{zz}(u) = \left(2 + \frac{3}{8} |u|^2\right) |u|^2 K_2(|u|) + \frac{1}{4} |u|^3 K_3(|u|),$$

$$J_{xy}(u) = - \frac{3}{8} u_x u_y |u|^2 K_2(|u|),$$

$$J_{xz}(u) = i u_x |u|^2 K_2(|u|) - \frac{3i}{8} u_y |u|^3 K_3(|u|),$$

$$J_{yz}(u) = u_y |u|^2 K_2(|u|) - \frac{3i}{8} u_x |u|^3 K_3(|u|),$$

where $K_2$ and $K_3$ are modified Bessel functions of the second kind. Note that, $a/z_0 \ll 1$ is our perturbative parameter, $K_{ij}$ are dimensionless functions storing information on the corrugation, and the remaining terms have dimension of energy.

Since we are interested in a particle arbitrarily oriented in space, using the Euler angles we write $\int_{0}^{\infty} d\xi \alpha_{ij}(\xi) = R(\phi, \theta, \psi) A^{-1}(\phi, \theta, \psi)$, where $A = \int_{0}^{\infty} d\xi \text{diag}[\alpha_1(\xi), \alpha_2(\xi), \alpha_3(\xi)]$. Motivated by the discussion in Ref. [55], we write $A = \gamma_{iso} \Pi(\gamma_s, \gamma_a)$ where $\Pi(\gamma_s, \gamma_a) = I + \gamma_s M_s + \gamma_a M_a$. $I$ is the $3 \times 3$ identity matrix, $M_s = \text{diag}(-1, -1, 2)$, $M_a = \text{diag}(-3, 3, 0)$, and we introduced the parameters $\gamma_{iso}$, $\gamma_s$, and $\gamma_a$, which characterize, in a convenient manner, the particle anisotropy, and are given by $\gamma_{iso} = \frac{1}{3} \text{Tr}(A)$, $\gamma_s = \frac{1}{3\text{Tr}(A)} [A_{33} - \frac{1}{2} (A_{22} + A_{11})]$, $\gamma_a = \frac{1}{3\text{Tr}(A)} [A_{22} - A_{11}]$ (assuming the principal axes of the particle have been enumerated in such a way that $A_{11} \leq A_{22} \leq A_{33}$). The $\gamma_s$ parameters are such that $0 \leq \gamma_s < 1$, $0 \leq \gamma_a \leq \min(\gamma_s, 1 - \gamma_s)$. Note that $\gamma_s = \gamma_a = 0$ if, and only if, the particle is isotropic. When $\gamma_s > 0$ and $\gamma_a = 0$, one has a class of cylindrically symmetric polarizable particles, of which belongs, for example, a CO$_2$ molecule. As $\gamma_s \rightarrow 1$, one has $\gamma_a \rightarrow 0$, and the polarizability becomes predominant in one of the principal axes of the particle. Taking all this into account, we write

$$U_{vdW}(r_0; \phi, \theta, \psi)/U(z_0) =$$

$$- \text{Tr}[K(r_0, h) R(\phi, \theta, \psi) \Pi(\gamma_s, \gamma_a) R^{-1}(\phi, \theta, \psi)],$$

where $U(z_0) = h\gamma_{iso}/(64\pi^2 \varepsilon_0 \omega^2 z_0^3)$. The dimensionless ratio $U_{vdW}(z_0)/U(z_0)$ in Eq. (1) is useful to investigate the behavior of the lateral vdW force for a general anisotropic particle, arbitrarily oriented in space, interacting with a perfectly conducting corrugated surface.

### II. APPLICATIONS

We first apply Eq. (1) to investigate the vdW interaction for the situation of a perfectly conducting plane surface with a single slightly protruding strip, as illustrated in Fig. 1(b). Specifically, we consider a strip of height $a$ and width $d$, given by $h(r_1) = a \{ \Theta(x + \frac{d}{2}) - \Theta(x - \frac{d}{2}) \}$, where $\Theta$ is
the Heaviside step function. For this case, we obtain
\[ K_{ij} = \frac{3}{16} \left[ f_{ij} \left( \frac{x_0}{z_0} + \frac{d}{2 z_0} \right) - f_{ij} \left( \frac{x_0}{z_0} - \frac{d}{2 z_0} \right) \right], \tag{2} \]
with
\[
\begin{align*}
    f_{xx}(u) &= \frac{u^3(8u^4 + 28u^2 + 35)}{(u^2 + 1)^{7/2}}, \\
    f_{yy}(u) &= \frac{u(8u^4 + 20u^2 + 15)}{(u^2 + 1)^{5/2}}, \\
    f_{zz}(u) &= \frac{u(16u^6 + 56u^4 + 66u^2 + 41)}{(u^2 + 1)^{7/2}}, \\
    f_{xz}(u) &= \frac{8u^2 - 7}{(u^2 + 1)^{7/2}}, \\
    f_{xy}(u) &= f_{yz}(u) = 0.
\end{align*}
\]

As a first case, we consider a particle characterized by \( \gamma_a = 0 \) and \( \gamma_s = 0.6, \) kept constrained to move on the plane \( z = z_0, \) and oriented with \( \phi = 0, \theta = \pi/2, \psi = 0, \) which means that \( \hat{e}^3_3 \) coincides with \( \hat{x}. \) For \( d/z_0 = 0.1, \) the ratio \( U_{vdw}^{(1)} / U \) versus \( x_0/z_0 \) is shown in Fig. 3. The behavior of \( U_{vdw}^{(1)} / U \) reveals the existence of two minimum points at \( x_0/z_0 \approx \pm 0.4, \) and an unstable equilibrium point at \( x_0 = 0. \) Thus, when the particle is slightly dislocated from the position \( x_0 = 0, \) it feels a repulsive lateral vDW force pushing it to distances four times the strip width.

![Figure 3](image-url)

Figure 3. Behavior of the ratio \( U_{vdw}^{(1)} / U \) versus \( x_0/z_0, \) for a particle fixed at \( z = z_0, \) and oriented with \( \phi = 0, \theta = \pi/2, \psi = 0. \) The solid line represents the profile of the surface. For \( d/z_0 = 0.1, \) the ratio \( U_{vdw}^{(1)} / U \) shows the existence of two minimum points at \( x_0/z_0 \approx \pm 0.4, \) and an unstable equilibrium point at \( x_0 = 0. \) Thus, when the particle is slightly dislocated from the position \( x_0 = 0, \) it feels a repulsive lateral vDW force pushing it to distances four times the strip width.

The behavior of \( U_{vdw}^{(1)} / U, \) and consequently the existence of a repulsive lateral vDW force, is strongly affected by the particle orientation. For instance, we consider the same particle characterized by \( \gamma_a = 0 \) and \( \gamma_s = 0.6, \) oriented with \( \phi = 0, \psi = 0, \) but now considering different values of \( \theta, \) which is shown in Fig. 4. The behavior of \( U_{vdw}^{(1)} / U \) for the case \( \theta = 0 (\hat{e}^3_3 \) coincides with \( \hat{z}), \) represented by the dotted line in Fig. 4, presents a minimum point at \( x_0 = 0. \) Thus, when the particle is over the strip \( (d/2 \leq x_0 \leq d/2) \) and dislocated from the position \( x_0 = 0, \) it feels an attractive lateral vDW force pulling it back to \( x_0 = 0. \) When \( \theta = \pi/4 \) (dot-dashed line), the minimum point, \( x_0 = x_{min} \) of \( U_{vdw}^{(1)} / U \) is such that \( x_{min} > d/2. \) This means that when the particle is over the strip it feels a repulsive lateral vDW force, pushing it towards a point distant from the strip. When \( \theta = \pi/2, \) the dashed line shows the same repulsive case already illustrated in Fig. 3. Note that, in this case, \( |x_{min}| \) is greater than that found for \( \theta = \pi/4. \) Since \( |x_{min}| \) becomes greater when \( \hat{e}^3_3 \) coincides with \( \hat{x}, \) hereafter we focus on this orientation.

Now, let us investigate how the condition \( |x_{min}| > d/2 \) (which effectively indicates the possibility of existence of a repulsive lateral vDW force) depends on the ratio \( d/z_0. \) Let us use, again, the particle characterized by \( \gamma_a = 0 \) and \( \gamma_s = 0.6, \) and oriented with \( \phi = 0, \theta = \pi/2, \psi = 0. \) In Fig. 5, we plot \( x_{min}/z_0 \) as a function of \( d/z_0, \) for \( \gamma_s = 0.6, \) in the dashed line. We highlight the critical value of \( d/z_0, \) called \( (d/z_0)_{crit}, \) which, in this case, is \( (d/z_0)_{crit} \approx 0.68. \) One can see that when \( d/z_0 \gtrsim (d/z_0)_{crit}, \) one has the \( x_{min} \) less than \( d/2, \) so that the particle is bounded over the strip (attractive lateral vDW force). When \( d/z_0 \lesssim (d/z_0)_{crit}, \) \( |x_{min}| > d/2, \) and we have the particle repelled in relation to the strip (repulsive lateral vDW force). In Fig. 5 it is also shown the behavior of \( x_{min}/z_0 \) versus \( d/z_0 \) for other values of \( \gamma_s. \) Note that, as the value of \( \gamma_s \) decreases, \( (d/z_0)_{crit} \) decreases too, so that the repulsive effect in the lateral vDW force tends to cease.

Since Eq. (1) can be applied to any surface profile, we apply it to other surface geometries to investigate the generality of the repulsive effects discussed so far. For instance, the behavior of the ratio \( U_{vdw}^{(1)} / U \) for the case of a Gaussian protuberance, described by \( h(r) = ae^{-(r/d)^2}, \) is shown in Fig. 6(a). As another example, we consider a trapezoidal protuberance, described by \( h(r) = a[\Theta(d/2 - |x|) + 2(1 - |x|/d)\Theta(|x| - d/2) - \Theta(|x| - d)] \)
whose results are shown in Fig. 6(b). Note that in both cases the repulsive lateral vdW force occurs

III. CLASSICAL CASE

To investigate the existence of lateral repulsive forces in a classical context, involving a neutral particle with a permanent dipole moment $\mathbf{p}$, we again take as basis the perturbative approach showed in Ref. [51], according to which the interaction energy $U_{\text{cl}}(z)$ between a dipolar particle and a corrugated surface, is given by $U_{\text{cl}} \approx U_{\text{cl}}^{(0)} + U_{\text{cl}}^{(1)}$, where $U_{\text{cl}}^{(0)}$ is the interaction energy for the case of a grounded conducting plane [56], and $U_{\text{cl}}^{(1)}$ is given by $U_{\text{cl}}^{(1)}(\mathbf{r}_0) = -\frac{d}{dz} \sum_{ij} K_{ij}(\mathbf{r}_0, h)p_ip_j/(64\pi\epsilon_0 z_0^3)$. After manipulation of this formula, we obtain

$$U_{\text{cl}}^{(1)}(\mathbf{r}_0; \phi, \theta, \psi)/U_{\text{cl}}(z_0) = -\frac{d}{dz} \sum_{ij} K_{ij}(\mathbf{r}_0, h)p_ip_j/(64\pi\epsilon_0 z_0^3),$$

where $U_{\text{cl}}(z_0) = a|\mathbf{p}|^2/(192\pi\epsilon_0 z_0^4)$. Note that the behavior of the classical ratio $U_{\text{cl}}^{(1)}(\mathbf{r}_0; \phi, \theta, \psi)/U_{\text{cl}}(z_0)$ is the same of the quantum ratio $U_{\text{vdW}}^{(1)}(\mathbf{r}_0; \phi, \theta, \psi)/U(\mathbf{r}_0)$ for $\gamma_s = 1$, and $\gamma_a = 0$. Therefore, similar repulsive effects also arise in the classical context.

IV. FINAL REMARKS

From the literature it is known that the particle anisotropy plays a decisive role in the emergency of normal repulsive dispersive forces, as those illustrated in Figs. 1(a.i), (a.ii) and (a.iii). Here, considering an anisotropic particle, we predict the existence of repulsive lateral vdW forces, as illustrated in Fig. 1(b.i). This repulsive effect is strongly affected by the particle orientation and by the characteristic width of the protuberance introduced on a plane surface. For certain values of these parameters, the particle is pushed towards points that are several widths distant from the center of the protuberance. Moreover, we show that a similar repulsive effect arises in the classical context, involving a neutral particle with a permanent dipole moment. The comprehension of this subtle repulsive aspect in the lateral forces may be relevant to achieve a higher degree of control of the interaction between anisotropic particles near corrugated surfaces, in both quantum and classical domains.

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