Sign inversion in the lateral van der Waals force between an anisotropic particle and a plane with a hemispherical protuberance: an exact calculation

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Received 1 September 2022; revised 23 November 2022
Accepted for publication 19 January 2023
Published 22 February 2023

Abstract
We investigate the lateral van der Waals (vdW) force between an anisotropic polarizable particle and a perfectly conducting plane with a hemispherical protuberance with radius $R$. We predict, via an exact calculation, a sign inversion in the lateral vdW force, in the sense that, instead of pointing to the protuberance, in certain situations this force points to the opposite direction. In the literature, predictions of sign inversions in the lateral vdW force were based on perturbative solutions, valid when the height of the protuberance is very small when compared to the distance $z_0$ between the particle and the plane. Here, taking into account exact formulas, we investigate how such nontrivial geometric effect depends on the ratio $R/z_0$, and how the particle orientation and anisotropy affect this sign inversion.

Keywords: lateral van der Waals force, sign inversion, exact calculation

(Some figures may appear in colour only in the online journal)

1. Introduction
Investigations of the Casimir–Polder–van der Waals (CP-vdW) [1] interaction considering anisotropic particles generally involves nontrivial behaviors. Among them is the prediction of a repulsive CP-vdW force [2–7] and a torque on a particle [8–10]. Beyond this, when considering
the lateral CP-vdW force that acts on a particle interacting with a corrugated surface, nontrivial behaviors of this force are predicted when calculations are made beyond the proximity force approximation (PFA). As an example, it was predicted the presence of regimes in the behavior of the lateral vdW force when an anisotropic polarizable particle interacts with a periodic corrugated surface [11, 12]. In addition, recently it was predicted that, for an anisotropic particle interacting with a conducting plane with a protuberance, a sign inversion in the lateral vdW force can occur, in the sense that, instead of pointing to the protuberance, in certain situations the force points to the opposite direction [13].

The prediction discussed in [13] was based on the application of a formula proposed by Eberlein and Zietal in [14] to compute the vdW interaction between a neutral polarizable particle and a perfectly conducting surface of arbitrary shape. This formula is written in terms of the homogeneous part of the Green’s function of the Laplacian operator, where it is stored the information about the geometry of the surface. In [13], it was considered a perturbative analytical solution for the Green’s function for the case of a perfectly conducting plane with a protuberance and, using it in the Eberlein–Zietal formula, it was predicted the mentioned sign inversion in the lateral vdW force up to first perturbative order in the ratio $a/z_0 \ll 1$ ($z_0$ is the distance from the particle to the plane, and $a$ is the height of the protuberance).

In [15], the Eberlein–Zietal formula was combined with the well known solution for the Green’s function for the problem of a perfectly conducting plane with a hemispherical protuberance with radius $R$ [16], and it was investigated the curvature effects of the hemisphere on the vdW force normal to the plane. In the present paper, we use the same calculation technique but focus our attention specifically on the lateral vdW force. This enables us to confirm, now via an exact calculation, the sign inversion predicted in [13] in the context of a perturbative approach. Moreover, while such perturbative approach consider that the height of the protuberance is very small when compared to the distance between the particle and the plane, the exact calculation discussed here enables us to study the lateral vdW force with no restriction on the particle position and on the size of the hemisphere. In this way, we compare these two calculations and show situations in which the perturbative one predicts results in considerable disagreement in comparison with the exact results. In addition, we show how such nontrivial geometric effects are regulated by the ratio $R/z_0$, and how the existence of these effects depend on the particle orientation and its anisotropy.

The paper is organized as follows. In section 2, we make a brief review of the perturbative predictions made in [13]. In section 3, we present the exact calculation made to write the formulas for interaction between a neutral polarizable particle and a conducting plane with a hemisphere. In section 4, we present our final remarks.

2. A brief review of the perturbative calculation

In [13], it was considered the vdW interaction between a plane surface ($z = 0$) with a single slight protuberance, and a neutral polarizable particle located at $r_0$, and kept constrained to move on a plane $z = z_0 > 0$, as illustrated in figure 1. Such constraint is just a theoretical artifice intending to neutralize the normal component of the force, enabling us to focus only on the behavior of the lateral force. To investigate the vdW interaction, it was took as basis the analytical perturbative formula presented in [11], related to the vdW interaction between the particle and a grounded conducting corrugated surface described by $z = h(r_0)$, with $h(r_0)$ describing a general small modification $|\max h(r_0)| = a \ll z_0$ of a planar surface at $z = 0$ (in [13], this modification is represented by a single protuberance on the surface). The vdW interaction energy $U_{vdW}$, between the particle and the corrugated surface, was written as
Figure 1. Illustration of a neutral anisotropic polarizable particle (elliptic figures), kept constrained to move on the plane \( z = z_0 \) (horizontal dotted lines), interacting with a perfectly conducting plane with a single slight Gaussian protuberance with characteristic width \( d \). Due to the presence of the protuberance, the particle feels a lateral force (arrows). In (i), the particle at \( A' \) (or \( A'' \)) feels a lateral force that takes it back to \( A \); in (ii), for a decreased ratio \( d/z_0 \), the lateral force moves the particle away from \( A \). This sign inversion in the lateral force was predicted in [13].

\[ U_{\text{vdW}} \approx U^{(0)}_{\text{vdW}} + U^{(1)}_{\text{vdW}}, \]

where the first term \( U^{(0)}_{\text{vdW}} \) is the vdW potential for the case of a grounded conducting plane [17], whereas \( U^{(1)}_{\text{vdW}} \) is the first perturbative correction of \( U^{(0)}_{\text{vdW}} \) due to the presence of the corrugation, and is given by equations (1)–(3) in [13]. This approach requires no demand on the smoothness of the rough surface, so that the results are valid beyond the PFA.

The main situation discussed in [13] was the case of a Gaussian protuberance of height \( a \) and width \( d \), given by \( h(r_1) = a \exp\left[-\left(|r_1|/d\right)^2\right] \). It was shown that when the PFA is considered \( (d/z_0 \to \infty) \), the lateral vdW force always leads the particle towards the peak of the protuberance. On the other hand, for a generic value of \( d/z_0 \), nontrivial geometric effects arise when considering an anisotropic polarizable particle and manipulating the ratio \( d/z_0 \). In this situation, the main prediction is that as \( d/z_0 \) decreases, the minimum value of the vdW energy can no longer coincide with the peak of the protuberance, which means that, instead of being attracted to the peak, the particle can be moved away from it (see figure 1). It was also shown in [13] that such a sign inversion in the lateral vdW force is affected by the particle orientation and its anisotropy, so that, depending on them, the mentioned effects can be suppressed.

As mentioned, in [13] these nontrivial behaviors of the lateral vdW force were predicted by means of a perturbative approach with \( a/z_0 \ll 1 \), and investigated using only the first perturbative correction \( U^{(1)}_{\text{vdW}} \). Differently from this, in the next section, we study such nontrivial effects by means of an exact calculation, considering a perfectly conducting plane with a hemispherical protuberance.

### 3. Exact calculation

Let us start considering a point charge \( Q \), located at the position \( r' = (\rho', \phi', z') \) (with \( z' > 0 \)), interacting with a grounded perfectly conducting plane surface \( (z = 0) \) that has a protuberance with the shape of a hemisphere of radius \( R \), as shown in figure 2(a). The potential \( \Phi(r) \), related to the Poisson’s equation of this problem, can be obtained, exactly, by means of the image method. For this case, one can obtain that only three image charges are necessary to obtain \( \Phi(r) = 0 \) at the plane \( z = 0 \) and the hemisphere [15, 16]. In figure 2(b), we illustrate the
Figure 2. (a) Illustration of a charge $Q$ located at $\mathbf{r}' = (\rho', \phi', z')$ (with $z' > 0$), interacting with a conducting plane surface ($z = 0$) that has a protuberance with the shape of a hemisphere of radius $R$. (b) Illustration of the charge $Q$ and its three image charges $\tilde{Q}, Q$, and $\tilde{Q}$, which are located at $\tilde{\mathbf{r}}'$, $\mathbf{r}'$, and $\tilde{\mathbf{r}}'$, respectively.

The physical charge $Q$ together with its image charges $\tilde{Q}, Q$, and $\tilde{Q}$, which are situated, respectively, at [we are using the cylindrical coordinates $(\rho, \phi, z)$]

\[
\tilde{\mathbf{r}}' = (\rho', \phi', -z'),
\]

\[
\mathbf{r}' = \left(\frac{R^2}{\rho'' + z'^2} \rho', \phi', \frac{R^2}{\rho'' + z'^2} z'\right),
\]

\[
\tilde{\mathbf{r}}' = \left(\frac{R^2}{\rho'' + z'^2} \rho', \phi', -\frac{R^2}{\rho'' + z'^2} z'\right),
\]

and can be written in terms of $Q$, as $\tilde{Q} = -Q$, $\overline{Q} = -Q R / \sqrt{\rho''^2 + z'^2}$, and $\overline{\overline{Q}} = QR / \sqrt{\rho''^2 + z'^2}$ [15]. Note that, together with the physical charge $Q$, the image charge $\overline{Q}$ cancels the potential at the hemisphere, but we still have $\Phi(\mathbf{r}) \neq 0$ at the plane $z = 0$. In this way, in order to cancel the potential at $z = 0$, we also have to insert the image charges $\tilde{Q}$ and $\overline{Q}$, which are, respectively, the images of $Q$ and $\overline{Q}$ due to the plane. Thus, the four charges $Q, \tilde{Q}, Q$, and $\overline{Q}$ together guarantee $\Phi(\mathbf{r}) = 0$ over the entire surface, so that the solution of the Poisson’s equation for this problem is given by

\[
\Phi(\mathbf{r}) = \frac{Q}{|\mathbf{r} - \mathbf{r}'|} + \frac{\tilde{Q}}{|\mathbf{r} - \tilde{\mathbf{r}}'|} + \frac{Q}{|\mathbf{r} - \mathbf{r}'|} + \frac{\overline{Q}}{|\mathbf{r} - \overline{\mathbf{r}}'|},
\]

where, from equations (1)–(3), one can write [15]

\[
|r - r'| = \sqrt{\rho^2 + \rho'^2 - 2 \rho \rho' \cos(\phi - \phi') + (z - z')^2},
\]

\[
|r - \tilde{r}'| = \sqrt{\rho^2 + \rho'^2 - 2 \rho \rho' \cos(\phi - \phi') + (z + z')^2},
\]

\[
|r - r'| = \frac{1}{(\rho''^2 + z'^2)} \times \sqrt{\rho^2 (\rho''^2 + z'^2)^2 + R^2 \rho'^2 + 2R^2 (\rho''^2 + z'^2) \rho \rho' \cos(\phi - \phi') + z (\rho''^2 + z'^2) - R^2 z'^2},
\]
\[ |\mathbf{r} - \mathbf{r}'| = \frac{1}{(\rho^2 + z^2)^2} \]
\[
\times \sqrt{(\rho^2 (\rho^2 + z^2)^2 + R^4 \rho'^2 - 2R^2 (\rho^2 + z^2) \rho \rho' \cos(\phi - \phi') + [z(\rho^2 + z^2) + R^2 z']^2)}.
\]

(8)

Note that, as expected, the difference between equations (5) and (6) (and also between equations (7) and (8)) is only that \(z' \leftrightarrow -z'\), which just affects the last term inside the roots in these equations. Since \(\Phi(\mathbf{r}, \mathbf{r}') = QG(\mathbf{r}, \mathbf{r}')\), the Green’s function \(G(\mathbf{r}, \mathbf{r}')\) is given by
\[
G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} - \frac{1}{R} \frac{1}{\sqrt{\rho^2 + z^2}} \left( \frac{1}{|\mathbf{r} - \mathbf{r}'|} - \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right).
\]

(9)

Now that we have the Green’s function related to a point charge in the presence of a conducting plane with a hemisphere, we can compute the vdW interaction \(U_{vdW}\) between a neutral polarizable point particle located at \(\mathbf{r}_0\) and this surface, by using the formula proposed by Eberlein and Zietal in [14], which is given by
\[
U_{vdW}(\mathbf{r}_0) = \frac{1}{8\pi\varepsilon_0} \sum_{i,j} \langle \hat{d}_i \hat{d}_j \rangle \nabla_i \nabla_j \left. G_H(\mathbf{r}, \mathbf{r}') \right|_{\mathbf{r} = \mathbf{r}' = \mathbf{r}_0},
\]

(10)

where \(\hat{d}_i\) are the components of the dipole moment operator, and the expectation value \(\langle \hat{d}_i \hat{d}_j \rangle = \frac{1}{2} \int_0^\infty d\xi \alpha_{ij}(\xi)\), where \(\alpha_{ij}\) are the components of the polarizability tensor of the particle. Besides this, the function \(G_H\) is the homogeneous part of the Green’s function \(G\) of the Laplacian operator, so that it satisfies the Laplace’s equation \(\nabla^2 G_H(\mathbf{r}, \mathbf{r}') = 0\), and can be written as
\[
G_H(\mathbf{r}, \mathbf{r}') = G(\mathbf{r}, \mathbf{r}') - \frac{1}{|\mathbf{r} - \mathbf{r}'|}.
\]

(11)

In this way, one can note that the Eberlein–Zietal formula relates the quantum problem of finding the vdW interaction between a polarizable particle and a surface, with the classical one of finding the solution for the Laplace’s equation. We remark that the function \(G_H\) contains all the information about the geometry of the surface, and that equation (10) can be applied to nondispersive materials or ideal conductors. This means that, in principle, equation (10) can describe the vdW interaction of a polarizable particle with a surface of any geometry, as long as we know the \(G_H\) function associated with the surface in question. As examples, one can find the application of equation (10) for a cylindrical wire and a 2D semi-infinite half plane in [14], a nondispersive dielectric slab in [18], a 2D perfectly conducting plate with a hole in [3], a 2D perfectly conducting disk in [19] (the investigation of the interaction between a particle and a 2D surfaces is of relevance, and one can see, for instance, [20–22]), a perfectly conducting toroid in [5], a corrugated surface in [11, 12].

Depending on the geometry of the surface, the function \(G_H\) can be obtained by means of the image method. As previously discussed, the problem of a point charge \(Q\) in the presence of a conducting plane with a hemisphere admits an exact solution by the image method, which is given by equation (9). Thus, using equation (9) in equation (11), and substituting in equation (10), one obtains that \(U_{vdW} = U_{vdW}^{(0)} + U_{vdW}^{(0)} + U_{vdW}^{(0)}\) [15]. The first term \(U_{vdW}^{(0)}\) is the vdW potential for the case of a grounded conducting plane [17], and is given by
\[
U_{vdW}^{(0)} = -\frac{1}{64\pi\varepsilon_0 c^2} \left[ \langle \hat{d}_6^2 \rangle + \langle \hat{d}_6^2 \rangle + 2\langle \hat{d}_6^2 \rangle \right].
\]

(12)
The second term, $U_{\text{vdW}}^{(b)}$, is the term of the energy that arises due to the presence of the hemisphere, and can be written as

$$U_{\text{vdW}}^{(b)} = -\frac{1}{64\pi\varepsilon_0 z_0^5} \left[ \langle d^2 \rangle R_{\rho\rho} + \langle d^2 \rangle R_{\phi\phi} + \langle d^2 \rangle R_{zz} + \langle d^2 \rangle R_{\rho\phi} \right],$$

(13)

where

$$R_{\rho\rho} = -8\overline{R} \left\{ \frac{\overline{R}^2 + 2\overline{R}^2 (1 + \overline{R}^2) + (1 + \overline{R}^2)^2}{(\overline{R}^2 - \overline{R}^2 - 1)^3} \right\},$$

(14)

$$R_{\phi\phi} = -8\overline{R} \left\{ \frac{1}{(\overline{R}^2 - \overline{R}^2 - 1)^3} \right\},$$

(15)

$$R_{zz} = -8\overline{R} \left\{ \frac{\overline{R}^2 + 1}{(\overline{R}^2 - \overline{R}^2 - 1)^3} - \frac{\overline{R}^2}{(\overline{R}^2 - \overline{R}^2 - 1)^3} \right\},$$

(16)

$$R_{\rho\phi} = -16\overline{R} \left\{ \frac{1}{(\overline{R}^2 - \overline{R}^2 - 1)^3} \right\},$$

(17)

with $\overline{R} = R/z_0$ and $\overline{\rho}_0 = \rho_0/z_0$. Note that the lateral vdW force that acts on the particle arises due to the dependence of $U_{\text{vdW}}^{(b)}$ on the variable $\rho_0$. Since we are interested only in the behavior of this force, hereafter we focus our attention only on $U_{\text{vdW}}^{(b)}$. We remark that the behavior of the lateral force just depends on $\overline{R}$ and $\overline{\rho}_0$, and we investigate the behavior of $U_{\text{vdW}}^{(b)}$ in relation to $\overline{\rho}_0$ for fixed values of $\overline{R}$. Here, we only consider values of $\overline{R}$ such that $0 < \overline{R} < 1$, but, we highlight that equations (13)–(17) are valid even for $\overline{R} > 1$, with the condition that $\overline{\rho}_0 > \sqrt{\overline{R}} - 1$, since the particle has to be located outside the hemisphere. In addition, as a consistency check, it is direct to see that in the absence of the hemisphere ($R = 0$), one has $U_{\text{vdW}}^{(b)} = 0$, and we just have the interaction between the particle and a grounded conducting plane, which is described by $U_{\text{vdW}}^{(d)}$ in equation (12) [15].

From equations (13)–(17), there are also some limiting cases that can give us some insight about the behavior of $U_{\text{vdW}}^{(b)}$ next to $\overline{\rho}_0 = 0$. To investigate these limits, let us start considering, for instance, the idealized case of a particle with a strong anisotropy in the $\rho$-direction, so that one has $U_{\text{vdW}}^{(b)} = -\langle d^2 \rangle R_{\rho\rho}/(64\pi\varepsilon_0 z_0^5)$. For this case, the second derivative of $U_{\text{vdW}}^{(b)}$ at $\overline{\rho}_0 = 0$ is given by

$$\frac{\partial^2 U_{\text{vdW}}^{(b)}}{\partial \overline{\rho}_0^2} |_{\overline{\rho}_0 = 0} = \frac{2 \langle d^2 \rangle}{64\pi\varepsilon_0 z_0^5} \left\{ \frac{32\overline{R}^3 (4\overline{R}^4 - 5\overline{R}^4 + 56\overline{R}^2 - 34\overline{R}^2 + 36\overline{R}^2 - 9)}{(\overline{R}^2 - 1)^4(\overline{R}^2 + 1)^5} \right\},$$

(18)

From this result, the limit $\overline{R} \to 1$ (particle close to the hemisphere) leads to $\partial^2 U_{\text{vdW}}^{(b)}/\partial \overline{\rho}_0^2|_{\overline{\rho}_0 = 0} \approx 3\langle d^2 \rangle/(64\pi\varepsilon_0 z_0^5 (\overline{R} - 1)^4) > 0$. This means that the peak of the hemisphere is a minimum point and, thus, under the action of the lateral vdW force, the particle is
associated to this point. Another situation is the limit $R \to 0$ (particle far from the hemisphere) in equation (18), which leads to $\frac{\partial^2 U_{vdW}^{(h)}}{\partial \rho_0^2}|_{\rho_0=0} \approx -288 \langle \hat{d}^2_\rho \rangle R^3 / (64 \pi \epsilon_0 z_0^5) < 0$. This means that the peak of the hemisphere is a maximum point and, thus, under the action of the lateral vdW force, the particle is moved away from this point. This change from a minimum to a maximum point in these limit cases shows that the particle can feel a sign inversion in the lateral vdW force by changing $R$.

In [13], the geometric effects due to the presence of the protuberance are regulated by the ratio between the characteristic width $d$ of the protuberance and the distance $z_0$ from the particle to the plane. Similarly, from the previous discussion, one can already see that the geometric effects due to the presence of the hemisphere are regulated by the ratio $R/z_0$, which is also discussed later in a more general way. Moreover, unlike the perturbative approach discussed in [13], by manipulating the width of the hemisphere we alter its size as a whole, and therefore the geometric effects predicted here are related to a change in the entire size of the protuberance, and not just in its width.

We can also show that the occurrence of a sign inversion in the lateral vdW force depends on the particle orientation and anisotropy. Next, we make a more detailed discussion on this, but, let us first investigate some special cases to obtain some insight about it. The dependence on the particle orientation can be shown, for instance, by considering a particle with a strong anisotropy in the $\phi$-direction, so that one has $U_{vdW}^{(h)} = -\langle \hat{d}^2_\phi \rangle R_{\phi\phi}/(64 \pi \epsilon_0 z_0^5)$. In this situation, we obtain that

$$\frac{\partial^2 U_{vdW}^{(h)}}{\partial \rho_0^2}|_{\rho_0=0} = \langle \hat{d}^2_\rho \rangle \frac{96 R^5 (R^8 + 10 R^4 + 5)}{64 \pi \epsilon_0 z_0^5 (R^2 + 1)^5 (R^2 - 1)^4}.$$  \hspace{1cm} (19)

Note that $\frac{\partial^2 U_{vdW}^{(h)}}{\partial \rho_0^2}|_{\rho_0=0} > 0$ for any value of $R$, which means that, in this situation, the peak of the hemisphere is always a minimum point and, thus, under the action of the lateral vdW force, the particle is attracted to this point independently on $R$. Note that, by only changing the direction in which the particle is strongly anisotropic (from $\rho$- to $\phi$-direction), which can be interpreted as a change on its orientation, the occurrence of a sign inversion in the lateral force is suppressed, indicating that such effect depends on the orientation of the particle. Now, the dependence on the particle anisotropy can be shown, for instance, by considering an isotropic particle ($\langle \hat{d}^2_\rho \rangle = \langle \hat{d}^2_\phi \rangle = \langle \hat{d}^2_z \rangle = \langle \hat{d}^2_i \rangle$). In this situation, we obtain that

$$\frac{\partial^2 U_{vdW}^{(h)}}{\partial \rho_0^2}|_{\rho_0=0} = \langle \hat{d}^2_i \rangle \frac{32 R^3 (7 R^8 + 12 R^6 + 50 R^4 + 12 R^2 + 15)}{(R^2 - 1)^4}.$$  \hspace{1cm} (20)

Note that $\frac{\partial^2 U_{vdW}^{(h)}}{\partial \rho_0^2}|_{\rho_0=0} > 0$ for any value of $R$, which means that, under the action of the lateral vdW force, an isotropic particle is always attracted to the peak of the hemisphere. This shows that the occurrence of a sign inversion on the lateral vdW force demands anisotropy on the polarizability of the particle.

To investigate the behavior of $U_{vdW}^{(h)}$ in a more general way, let us start considering a class of particles whose tensor $\langle \hat{d}_i \hat{d}_j \rangle$ diagonalized, in cylindrical coordinates, is represented by the matrix

$$\langle \hat{d}_i \hat{d}_j \rangle = \begin{pmatrix} \langle \hat{d}^2_\rho \rangle & 0 & 0 \\ 0 & \langle \hat{d}^2_\phi \rangle & 0 \\ 0 & 0 & \langle \hat{d}^2_z \rangle \end{pmatrix},$$  \hspace{1cm} (21)
which represents cylindrically symmetric polarizable particles, and thus the subscript $p$ and $n$ refer to the directions parallel and normal to the symmetry axis of the particle (here, we consider $\langle d_p^2 \rangle \geq \langle d_n^2 \rangle$). For a general orientation of this particle, we can write

\begin{align}
\langle d_p^2 \rangle &= \langle d_n^2 \rangle + [\langle d_p^2 \rangle - \langle d_n^2 \rangle] \sin^2(\theta) \cos^2(\gamma - \phi_0), \quad (22) \\
\langle d_p^2 \rangle &= \langle d_n^2 \rangle + [\langle d_p^2 \rangle - \langle d_n^2 \rangle] \sin^2(\gamma - \phi_0), \\
\langle d_z^2 \rangle &= \langle d_n^2 \rangle + [\langle d_p^2 \rangle - \langle d_n^2 \rangle] \cos^2(\theta), \\
\langle d_n d_z \rangle &= \frac{\langle d_p^2 \rangle - \langle d_n^2 \rangle}{2} \sin(2\theta) \cos(\gamma - \phi_0), \quad (25)
\end{align}

where the angles $\theta$ and $\gamma$ describe the particle orientation, as illustrated in figure 3. It is convenient to describe the particle anisotropy by means of the ratio $\beta = \langle d_n^2 \rangle / \langle d_p^2 \rangle$ ($0 < \beta \leq 1$), so that equations (22)–(25) can be rewritten as

\begin{align}
\langle d_p^2 \rangle &= \langle d_n^2 \rangle \left[ \beta + (1 - \beta) \sin^2(\theta) \cos^2(\gamma - \phi_0) \right], \quad (26) \\
\langle d_p^2 \rangle &= \langle d_n^2 \rangle \left[ \beta + (1 - \beta) \sin^2(\gamma - \phi_0) \right], \\
\langle d_z^2 \rangle &= \langle d_n^2 \rangle \left[ \beta + (1 - \beta) \cos^2(\theta) \right], \\
\langle d_n d_z \rangle &= \langle d_p^2 \rangle \left[ \frac{1 - \beta}{2} \sin(2\theta) \cos(\gamma - \phi_0) \right]. \quad (29)
\end{align}

As a first case, let us consider a particle, kept constrained to move on the plane $z = z_0$, characterized by $\beta = 0.2$ and oriented with $\theta = \pi/2$ and $\gamma = 0$ (its symmetry axis is along the x-direction). As mentioned in section 2, the consideration of the particle being constrained to move in a plane above the surface is just a theoretical artifice intending to neutralize the normal component of the force, which enables us to focus only on the behavior of the lateral force. In figure 4, we show the behavior of $U_{vdW}^{(b)}$ for $R/z_0 = 0.6$ (figure 4(a)) and $R/z_0 = 0.2$ (figure 4(b)). In figure 4(a), note that the minimum point of $U_{vdW}^{(b)}$ is over the origin, which means that the lateral vdW force always leads the particle to the peak of the hemisphere. On the other hand, in figure 4(b), we decrease the value of the ratio $R/z_0$ and one notes that $U_{vdW}^{(b)}$ now has two minimum points, and none of them coincide with the peak of the hemisphere. This change in the minimum points means that a particle slightly displaced from the origin can
Figure 4. Behavior of $U_{\text{vdW}}^{(b)}/U$, with $U = \langle \Delta E \rangle/(64\pi\varepsilon_0z_0^2)$, versus $x_0/z_0$ and $y_0/z_0$, for a particle fixed at $z = z_0$. In each panel, we consider this particle characterized by $\beta = 0.2$ and oriented such that $\theta = \pi/2$ and $\gamma = 0$ (its symmetry axis is along the $x$-direction). From panels (a), (b), we change the value of the ratio $R/z_0$ from $R/z_0 = 0.6$ to $R/z_0 = 0.2$. The insets on the right show the behavior of $U_{\text{vdW}}^{(b)}/U$ with respect to $x_0$ ($y_0 = 0$), and illustrate that the change in the behavior of the energy results in a sign inversion of the lateral vdW force (represented by the arrows).

feel a sign inversion in the lateral force, in the sense that instead of being attracted towards the hemisphere, the particle can be moved away from it. These examples show that such a sign inversion in the lateral vdW force, which is a nontrivial geometric effect of the presence of the hemisphere on the conducting plane, is regulated by the ratio $R/z_0$. Moreover, the existence of this effect is now confirmed by means of an exact calculation, with no restriction on the size of the hemisphere or the particle position, differently from [13].

The change in the minimum points by manipulating the ratio $R/z_0$, as shown in figure 4, also occurs for other values of $\beta$. But, we remark that, above a certain value of $\beta$, $U_{\text{vdW}}^{(b)}$ will always have only one minimum point over the peak of the hemisphere, independently on the ratio $R/z_0$. This means that the mentioned sign inversion in the lateral vdW force is affected by the particle anisotropy. In this way, for a particle free to move along the $x$-axis ($y_0 = 0$) and oriented with $\theta = \pi/2$ and $\gamma = 0$, in figure 5(a) we show the configurations of $\beta$ and $R/z_0$ such that the peak of the hemisphere ($x_0 = 0$) is a minimum (dark region) or a maximum (light region) point of $U_{\text{vdW}}^{(b)}$. The sign inversion in the lateral force is obtained when a transition from the dark to the light region occurs, and, thus, one can note that for $\beta > 3/8$ there are no manipulation of the ratio $R/z_0$ that makes possible the sign inversion in the lateral force. In addition, the regions shown in figure 5(a) change depending on the orientation of the particle in the $xy$ plane, which is given by the angle $\gamma$ (see figure 3), and, thus, we show these regions for other values of $\gamma$ in figures 5(b) and (c). This means that behaviors similar to that shown in figure 4 also occur for other values of $\gamma$, but with the change in the minimum points occurring for different
Figure 5. For a particle free to move along the x-axis ($y_0 = 0$) and oriented with $\theta = \pi/2$, it is shown the configurations of $\beta$ and $R/z_0$ for which $x_0 = 0$ is a minimum (dark region) or a maximum (light region) point of $U_{vdW}$. These configurations are shown for (a) $\gamma = 0$, (b) $\gamma = \pi/6$ and (c) $\gamma = \pi/3$. We remark that, we just have a dark region when $\beta > 3/8$ in (a), $\beta > 9/29$ in (b), and $\beta > 3/23$ in (c).

Figure 6. Behavior of $U_{vdW}^{(h)}/U$, with $U = \langle d_p^2 \rangle/(64\pi \epsilon_{0} \varepsilon_0 z_0^3)$, versus $x_0/z_0$ and $y_0/z_0$, for a particle fixed at $z = z_0$. In each panel, we consider $R/z_0 = 0.2$, and the particle characterized by $\beta = 0.2$ and oriented with $\gamma = 0$ and different values of $\theta$ (its symmetry axis is along the $xz$-plane). We consider $\theta = \pi/3$ in panel (a), $\theta = \pi/6$ in panel (b), and $\theta = 0$ in panel (c).

configurations of $\beta$ and $R/z_0$. This not occur when we reorient the particle by changing the angle $\theta$. In this situation, we have an asymmetric behavior of $U_{vdW}^{(h)}$ when $0 < \theta < \pi/2$, as shown in figures 6(a) and (b). When $\theta = 0$ (symmetry axis of the particle along the $z$-direction),
For a particle free to move along the $x$-axis ($y_0 = 0$) and oriented such that $\langle \hat{d} \hat{d} \rangle = \langle \hat{d}_p^2 \rangle \text{diag}(1, \beta, \beta)$, it is shown the configurations of $\beta$ and $R/z_0$ for which $x_0 = 0$ is transitioning between a minimum and a maximum point of $U^{(b)}_{\text{vdW}}$. The solid line is obtained by means of the exact calculation presented here, and corresponds to the transition border between the dark and light regions in figure 5(a). The dashed line is obtained by means of the first order perturbative calculation shown in [13]. The hatched region shows the configurations of $\beta$ and $R/z_0$ such that the perturbative and exact calculations predict different behavior for the lateral vdW force.

The minimum point of $U^{(b)}_{\text{vdW}}$ is always over the origin (see figure 6(c)), independent on the value of $\beta$ or the ratio $R/z_0$. All of this show us that the sign inversion in the lateral vdW force is also affected by the particle orientation.

It is interesting to make a comparison between the exact approach discussed here and the perturbative one shown in [13]. For this, let us consider, for instance, a particle kept constrained to move on the $x$-axis ($y_0 = 0$), with $z = z_0$, and oriented such that $\langle \hat{d} \hat{d} \rangle = \langle \hat{d}_p^2 \rangle \text{diag}(1, \beta, \beta)$, with $\beta = \langle \hat{d}^2_n \rangle / \langle \hat{d}_p^2 \rangle$. Also considering that a surface with the shape of a plane with a hemisphere, as shown in figure 2(a), is described by the function

$$h(x, y) = \sqrt{R^2 - x^2 - y^2} \Theta \left( R^2 - x^2 - y^2 \right),$$

(30)

using equations (1)–(3) of [13], we obtain that the first perturbative correction in the energy ($U^{(1)}_{\text{vdW}}$), due to the presence of such hemisphere, is given by

$$U^{(1)}_{\text{vdW}}(r_0) = -\frac{3R(d_p^2)}{512\pi\epsilon_0c_0} \int_0^\infty duu \left[ \frac{\sin(uR)}{uR} - \cos(uR) \right]$$

$$\times \left\{ \left[ 1 + \frac{5\beta}{3} \right] aK_3(u) + \frac{16\beta}{3} aK_2(u) \right\} J_0(u|x_0|) - (1 - \beta)aK_2(u)$$

$$\times \left[ uJ_0(u|x_0|) - \frac{J_1(u|x_0|)}{|x_0|} \right].$$

(31)

From this equation, we can obtain the configurations of $\beta$ and $\bar{R}$, such that the peak of the hemisphere ($x_0 = 0$) is a minimum or a maximum point of $U^{(1)}_{\text{vdW}}$. The diagram of these configurations is similar to that in figure 5(a), which was obtained by means of the exact calculation. However, there is a significant difference in the transition border between the dark and light regions when comparing the predictions from the exact and the first order perturbative approach. In figure 7, we show the transition borders obtained by means of the exact calcu-
lation, and the perturbative one. Note that, for small values of $\mathcal{R}$, the prediction from the first order perturbative calculation is very close to the exact one, but, as $\mathcal{R}$ increases, they become distant from each other. The hatched region in figure 7 shows the configurations of $\beta$ and $\mathcal{R}$ such that, from the point of view of the first order perturbative calculation, $x_0 = 0$ is a maximum point of $U^{(h)}_{vdW}$. However, from the exact calculation, such hatched region corresponds, in fact, to $x_0 = 0$ as being a minimum point of $U^{(h)}_{vdW}$. Moreover, to obtain better predictions from the perturbative calculation, it is necessary to consider higher order corrections, which demands a considerable effort in the calculations. Thus, in comparison to the perturbative method shown in [13], the exact calculation presented here provides precise results in a much simpler way.

4. Final remarks

Using the well known solution for the Green’s function for the problem of a perfectly conducting plane with a hemispherical protuberance with radius $R$ (equation (9)), we investigated the vdW interaction (equations (12)–(17)) between an anisotropic particle interacting with a perfectly conducting plane containing a protuberance with the shape of a hemisphere. We verified, via an exact calculation, the sign inversion in the lateral vdW force, so that, instead of pointing to the protuberance (figure 4(a)), in certain situations the lateral vdW force points to the opposite direction (figure 4(b)). In the literature, such prediction considered that the height of the protuberance was very small when compared to the distance between the particle and the plane [13]. In contrast, here we discussed such effect with no restriction on the particle position and on the size of the hemisphere, obtaining the lateral vdW force for any value of the ratio $R/z_0$. We investigated how such nontrivial geometric effect depends on this ratio, and how the particle orientation and anisotropy affect the sign inversion (figures 5 and 6).

We remark that our investigations of the behavior of the interaction energy were made by considering an anisotropic particle with a fixed orientation. As a further investigation, it could also be interesting to consider the particle free to rotate, since in this situation a torque acts on the particle in order to orientate it to a stable orientation in which the energy is minimized (see, for instance, [8–10]). Thus, in the same way that the presence of the hemisphere on the conducting plane can change the sign of the lateral vdW force, we expect that a similar change can also occur in the sign of the torque.

The investigation of such nontrivial geometric effects on the lateral vdW force, presented here, contributes to a better understanding and control of the interaction between a neutral anisotropic polarizable particle and a non-planar surface.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Acknowledgments

The authors thank Alexandre P da Costa and Stanley S Coelho for careful reading of this paper and fruitful discussions. L Q and E C M N were supported by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior—Brasil (CAPES), Finance Code 001.
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