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The role of geometry on dispersive forces

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Abstract
The role of geometry on dispersive forces is investigated by calculating the energy between different spheroidal particles and planar surfaces, both with arbitrary dielectric properties. The energy is obtained in the non-retarded limit using a spectral representation formalism and calculating the interaction between the surface plasmons of the two macroscopic bodies. The energy is a power-law function of the separation of the bodies, where the exponent value depends on the geometrical parameters of the system, like the separation distance between bodies, and the aspect ratio among minor and major axes of the spheroid.

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1. Introduction

The Casimir effect is one of the macroscopic manifestations of the fluctuations of the quantum vacuum [1]. Casimir showed that the energy $\mathcal{U}(z)$ between two parallel perfect conductor plates can be found from the change of the zero-point energy of the classical electromagnetic field, as

$$\mathcal{U}(z) = \frac{\hbar}{2}\sum_i [\omega_i(z) - \omega_i(z \to \infty)], \qquad (1)$$

where $\omega_i(z)$ are the proper modes that satisfy the boundary conditions of the electromagnetic field at the plates which are separated by the distance z. The energy obtained by Casimir is a power-law function of z, and at large distances $\mathcal{U}(z) \propto z^{-3}$, while at short distances $\mathcal{U}(z) \propto z^{-2}$. Later, Lifshitz obtained a formula to calculate the force between two parallel half-spaces with arbitrary dielectric properties [2]. The Lifshitz formula depends only on the reflection amplitude coefficients of the half-spaces and the separation between them, finding the same dependence of the energy with z. In 1968, van Kampen *et al* [3] showed that the Lifshitz formula, in the non-retarded limit, is obtained from the zero-point energy resulting from the Coulomb interaction of the surface plasmons of the plates. After, Gerlach [4] did an extension showing that also in the retarded limit, the Lifshitz formula is obtained by solving the proper electromagnetic modes with the appropriate boundary conditions, which he called erroneously, surface plasmons, to all the proper modes. Recently, these formulations in terms of surface plasmons have been revisited, and the proper modes have been identified correctly, showing that the Casimir energy is given by the contributions from (i) the interacting surface plasmons (evanescent waves), and (ii) propagating modes in the cavity formed by the parallel plates [5]. Furthermore, it has been shown that the contribution from the surface plasmons is essential to calculate the Casimir energy, and that they dominate the effect at short distances, where retardation effects are insignificant [5].

Surface plasmons are evanescent electromagnetic waves that propagate along the surface of conductors, and vanish elsewhere. By altering the surface, i.e., modifying size, shape, and/or environment of the conductor, the properties of surface plasmons can be tailored [6, 7]. Therefore, if the shape of at least one of the bodies is modified, we would expect to observe changes in the energy due to the interaction between surface plasmons. In this paper, we study the influence of the geometry on the zero-point energy due to the interaction between macroscopic bodies. Using a method based on a spectral representation formalism [8], which determines the proper frequencies of the system, we calculate the zero-point energy of all the interacting surface plasmons between a spheroidal particle and a flat plate, both with arbitrary dielectric functions. We find that the geometry plays an important role in the determination of the energy. This latter can be very important for experiments using atomic force microscopy, where very small separation can be reached and the shape of the tip can be substantially changed.

2. Interacting surface plasmons

We consider a spheroidal particle located near a flat substrate. The particle is generated by the rotation around one of the axes of an ellipse with lengths $2r_>$ and $2r_<$, with $r_> > r_<$. The symmetry axis of the particle is perpendicular to the substrate, and its centre is located at a distance d from the substrate, which has a dielectric constant $\epsilon_{\rm sub}$. The particle has a dielectric function $\epsilon_{\rm part}$ and is embedded in an ambient of dielectric constant $\epsilon_{\rm amb}$, which is equal to 1 for vacuum. We consider that the three media, particle, substrate and ambient, are non-magnetic. We are not considering nonlocal effects; therefore, all the variables are functions of the frequency only. The explicit dependence of the following equations on the frequency is omitted here for simplicity. The charge distribution on the particle's surface, in the presence of a substrate, depends on the components of the external electromagnetic excitations, through the so-called effective polarizability tensor $\bar{\alpha}_{\rm eff}$. When the particle is far from the substrate the effective polarizability becomes the polarizability of the isolated particle. But, when the particle is close to the substrate the induced multipolar interactions modify the electromagnetic response of the system because more surface plasmon resonances of the particle interact with those in the substrate [13].

The quantum vacuum fluctuations induce a charge distribution on the particle which also induces a charge distribution in the substrate. These charge distributions are due to the induced surface plasmons on the particle and substrate. In the non-retarded limit, the induced lmth multipolar moment on the particle is given by [8]

$$Q_{lm}(\omega) = \alpha_{\rm eff}^{lm}(\omega)\left[V_{lm}^{\rm vac}(\omega) + V_{lm}^{\rm sub}(\omega)\right], \tag{2}$$

where $V_{lm}^{\rm vac}(\omega)$ is the field associated with the quantum vacuum fluctuations at the zero-point energy, $V_{lm}^{\rm sub}(\omega)$ is the induced field due to the presence of the half-space and $\alpha_{\rm eff}^{lm}(\omega)$ is the lmth component of the effective polarizability of the particle. It is known that the poles of $\bar{\alpha}_{\rm eff}$

yield the frequencies of the proper modes of the system [9–11]. In the non-retarded limit, the spheroidal radius of the major axis and the minimum separation between the particle and the substrate are much smaller than the characteristic length of the system given, in this case, by $\lambda_p = 2\pi c/\omega_p$, with c being the speed of light and ω_p the plasma frequency of the metallic particle.

The analysis of $\bar{\alpha}_{\text{eff}}$ for the system described above was done as follows. First, the electric potential induced in the system at any point in space was calculated to all multipolar orders. To find the solution for the induced potential a spectral representation of the Fuchs–Bergman–Milton type [9–11] was developed [12]. By identifying the multipolar moments $Q_{lm}(\omega)$ induced in the particle, the components of $\bar{\alpha}_{\text{eff}}$ were obtained. Then, the frequencies of the proper modes for different shapes and locations of the particles are calculated by choosing a model for the dielectric function of the particle. For a detailed description of the method, see [13].

Within the spectral representation formalism, we can write the component of $\bar{\alpha}_{\text{eff}}$ in the following form:

$$\alpha_{\text{eff}}^{lm}(\omega, z) = -\frac{v}{4\pi}\sum_{s,q}\frac{C_{sq}^{lm}(z)}{u(\omega) - n_{sq}^{lm}(z)}, \tag{3}$$

where v is the volume of the particle, z is the minimum separation distance from the particle to the substrate such that $z = d - r_>$ for prolate spheroids while $z = d - r_<$ for oblate spheroids. Here,

$$u(\omega) = [1 - \epsilon_{\text{part}}/\epsilon_{\text{amb}}]^{-1} \tag{4}$$

is the so-called spectral variable and the strengths $C_{sq}^{lm} = \left(U_{sq}^{lm}\right)^2$ are the so-called spectral functions where U_{sq}^{lm} is the unitary matrix that satisfies the relation

$$\left(U_{sq}^{l'm'}\right)^{-1} H_{l'm'}^{s'q'}(z) U_{s'q'}^{lm} = 4\pi n_{sq}^{lm}(z). \tag{5}$$

The matrix $H_{l'm'}^{s'q'}(z)$ depends only on the geometrical properties of the model and on the dielectric properties of substrate and ambient, through the contrast parameter

$$f_c = (\epsilon_{\text{amb}} - \epsilon_{\text{sub}})/(\epsilon_{\text{amb}} + \epsilon_{\text{sub}}). \tag{6}$$

Furthermore, $H_{l'm'}^{s'q'}(z)$ is a real and symmetric matrix which is given by [8]:

$$H_{lm}^{sq}(z) = n_{sq}^{lm}(z \to \infty)\delta_{sl}\delta_{qm} + f_c D_{sq}^{lm}(z), \tag{7}$$

where $n_{sq}^{lm}(z \to \infty)$ are the depolarization factors of an isolated spheroid, and $D_{sq}^{lm}(z)$ is a matrix given by the multipolar coupling due to the presence of the substrate; this later vanishes when $z \to \infty$. Note that $H_{l'm'}^{s'q'}(z)$ contains all the information of the geometry of the system and the dielectric constant of the substrate, and is independent of the dielectric properties of the particle. In equation (3), $\bar{\alpha}_{\text{eff}}(\omega, z)$ is given as the sum of terms which show resonances at frequencies ω given by the poles of the equation, i.e., when $u(\omega) = n_{sq}^{lm}(z)$. As a consequence, an explicit and exact procedure to calculate the strength and position of the resonances was obtained. In the next section we present results for the energy between a spheroid and a plate due to the interaction of all the induced multipolar surface plasmons.

3. Zero-point energy of a spheroid near a substrate

As follows, we present a systematic study of the energy for oblate and prolate particles with different asymmetries and considering different kinds of substrates. The energy is calculated by

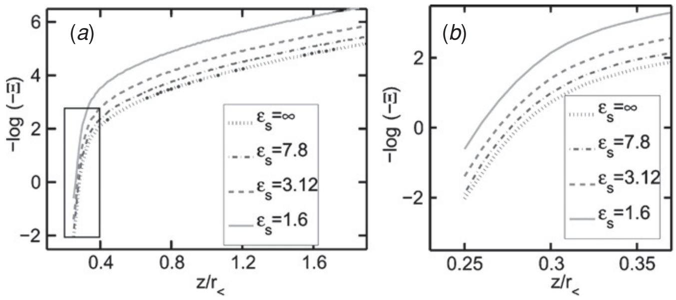

Figure 1. Dimensionless energy as a function of $z/r_<$ for an oblate spheroid with $r_>/r_< = 1.4$ and different substrates. (*b*) Magnification of the boxed area in (*a*).

substituting the frequencies of the proper modes, obtained as described above, in equation (1). Using the spectral representation, a systematic study of the energy in terms of the geometrical parameters, $r_>$, $r_<$ and z, and the dielectric properties of the substrate, can be done.

In the presence of a dielectric half-space, the proper modes, given by $\bar{\alpha}_{\rm eff}(\omega, z)$, are always red shifted as the particle approaches the substrate, and this shift depends on the separation distance z. In general, the interaction energy is negative for any z, and is proportional to $(1+z)^{-\beta}$, with $\beta = 2L + 1$. Here L is a positive integer which labels the highest order of the multipolar interaction, and depends on the geometrical parameters $r_>$, $r_<$ and z [13]. For example, when $r_> = r_< = a$, and $z > 5a$, then the relevant multipolar excitations are given by $L = 1$, i.e., only surface plasmons with dipolar distributions are important. On the other hand, if $5a > z > 2a$ the interactions among surface plasmons with dipolar and quadrupolar charge distributions become relevant and $L = 2$, such that the energy, when $z \approx 2a$, is proportional to $(1+z)^{-4}$. As $z \to 0$, more and more multipolar charge distributions must be taken into account, and when the spheroid is touching the substrate, one would expect that $L \to \infty$, so that the interaction energy also does.

As a case study, we employ the plasma model for the dielectric function of the particle, $\epsilon_{\rm part}(\omega) = 1 - \omega_{\rm p}^2/\omega^2$, where $\omega_{\rm p}$ is the plasma frequency, which is different for different metals. Therefore, the frequencies of the proper modes, obtained from the relation $u(\omega) = n_{sq}^{lm}(z)$, are

$$\omega_{sq}^{lm}(z) = \omega_{\rm p}\sqrt{n_{sq}^{lm}(z)}, \tag{8}$$

and according to equation (1), the zero-point energy is given by

$$\mathcal{U}(z) = \frac{\hbar\omega_{\rm p}}{2}\sum_{sq,lm}\left[\sqrt{n_{sq}^{lm}(z)} - \sqrt{n_{sq}^{lm}(z\to\infty)}\right], \tag{9}$$

where $n_{sq}^{lm}(z \to \infty)$ denotes the proper modes of the isolated spheroid. From equation (9), we can define a dimensionless energy $\Xi = \mathcal{U}(z)/\hbar\omega_p$, and study in detail the behaviour of the system independently of the plasma frequency of the metallic spheroid. Let us first analyse the influence of the dielectric properties of the substrate on the energy as a function of the dimensionless distance $z/r_<$. In figure 1, we show $-\log(-\Xi)$ for an oblate spheroid with an aspect ratio among the semi-axes of the spheroid, $r_>/r_< = 1.4$, and different substrates. Here, $\epsilon_{\rm sub} = \infty$ corresponds to a perfect conductor, while $\epsilon_{\rm sub} = 7.8$ and 3.12 correspond to TiO_2 and sapphire, respectively. The case of $\epsilon_{\rm sub} = 1.6$ is just for illustration. The interaction strength between the particle and the substrate is modulated by the contrast factor given by equation (6), which is a function of $\epsilon_{\rm sub}$. For distances $z/r_< > 1$, the energy goes to 0 faster, the smaller the value of $\epsilon_{\rm sub}$, as shown in figure 1(*a*). At small distances, $z/r_< < 0.4$, the

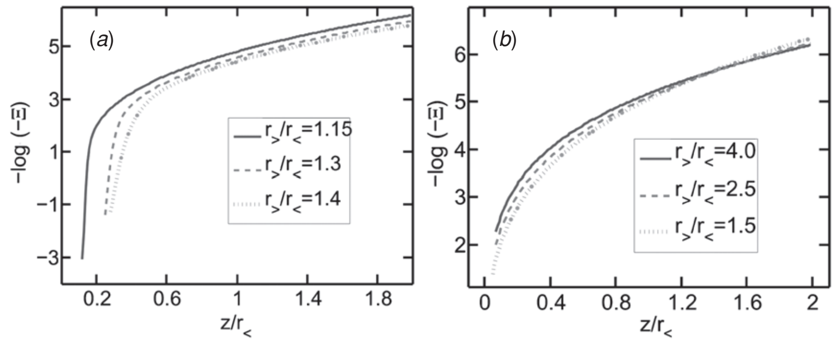

Figure 2. Dimensionless energy as a function of $z/r_<$ for (a) oblate, and (b) prolate spheroids with different aspect ratios $r_>/r_<$.

interaction between the particle and substrate increases considerably, because the largest value of the multipolar interaction L becomes larger, as shown in figure 1(b). However, the value of L is independent of $\epsilon_{\rm sub}$, and the observed differences at a given distance are due to the fact that the strength of the multipolar surface plasmon interactions is modulated with the factor f_c, such that, for larger values of the substrate dielectric constant, the force strength increases. In figure 1, we observe that the energy at a given distance is larger for greater values of $\epsilon_{\rm sub}$. The same general behaviour of the energy as a function of the dielectric function of the substrate is also found for prolate spheroids.

Now let us examine in detail the influence of the geometrical parameters on the energy between different spheroidal particles and a sapphire substrate, as a function of the dimensionless distance $z/r_<$. In figure 2(a), the dimensionless energy for oblate spheroids with different aspect ratios between the semi-axes, $r_>/r_<$, is shown. At a fixed distance, the energy for oblate spheroids is larger when the aspect ratio $r_>/r_< \to 1$, i.e., when the spheroids tend to the spherical shape. Since the substrate is always the same, this means that the value of L becomes larger when $r_>/r_< \to 1$ at any distance. In figure 2(b), the same is shown for prolate spheroids; however, we observe two different regimes in this case. When $z/r_< < 1.2$, the value of L becomes larger when $r_>/r_< \to 1$, but the contrary occurs when $z/r_< > 1.2$. This means that the value of L not only depends on the separation distance, but also on the axes aspect ratio $r_>/r_<$, and the specific symmetry of the particle. From figure 2, we also observe that the energy behaviour is different for oblate and prolate spheroids, which is more evident when $z/r_< < 0.4$. The energy for oblate particles becomes more negative faster than for prolate ones, because the value of L is larger for oblates. In conclusion, the exponent β of the power-law behaviour of the energy depends on the specific geometrical parameters z, $r_>$ and $r_<$.

To examine in detail the energy dependence with the geometry of the system, let us consider different spheroidal particles at a fixed distance z and all with the axis normal to the surface $r_\perp$, such that, $z/r_\perp = 0.25$ is a constant. In figure 3(a) is shown the dimensionless energy as a function of the aspect ratio $r = r_{||}/r_\perp$ between the axis parallel to the surface ($r_{||}$) and the one normal to it. The case when $r < 1$ corresponds to prolate particles, while $r = 1$ is the value for spheres, and when $r > 1$ we have oblate ones, as illustrated in the inset of figure 3(a). Here, one can observe clearly the energy reliance on the geometry. For prolate spheroids the relevant multipolar interactions do not change dramatically with the aspect ratio of the axes. This means that the value of L increases smoothly as the aspect ratio goes to $r = 1$. On the other hand, for oblate particles the number of multipolar interactions is more

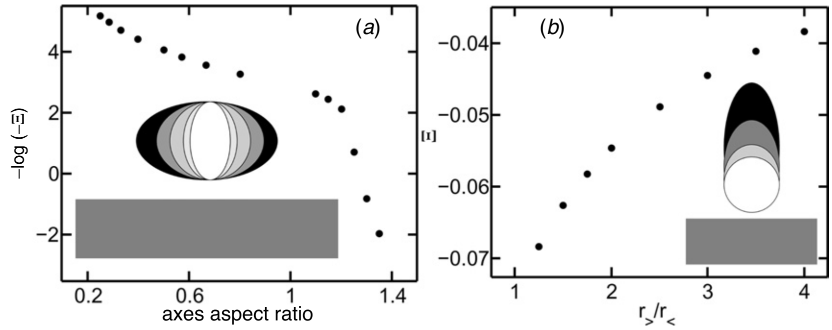

Figure 3. (*a*) Dimensionless energy of spheroidal particles at a fixed distance z, as a function of the aspect ratio between the axes. (*b*) Dimensionless energy of prolate spheroids at a fixed z and $r_<$ constant, as a function of $r_>/r_<$.

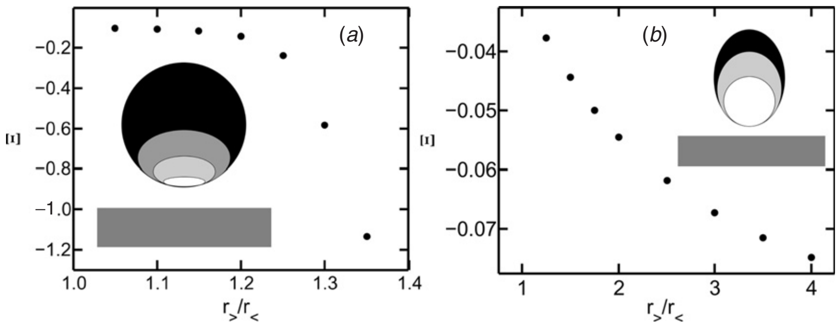

Figure 4. Dimensionless energy as a function of $r_>/r_<$ for (*a*) oblate and (*b*) prolate spheroids with the same curvature, at a fixed distance.

sensitive to r, and the value of the largest multipolar interaction rises dramatically with small increments of r.

In figure 3(*b*), the energy of prolate particles, at a fixed z and $r_<$ constant, with $z/r_> = 0.1$, as a function of $r_>/r_<$ is shown. In this case, the projected area of the particle over the substrate is always the same, since the minor axis is constant for all cases (see the inset in figure 3(*b*)). Here, we observe that when the major axis increases the energy decreases because the reduction of number of relevant multipolar interactions involved, yielding different exponents of the power-law function of z for the energy. Therefore, we have shown that the energy is very sensitive to the geometry of the system. In our formulation, the force is proportional to $(1 + z)^{-\gamma}$, where $\gamma = 2L + 2$ and the value of L depends on z itself, and $r_>$, and $r_<$. A direct comparison of the proximity theorem approximation [14] with our formalism will be presented in a more extended paper [12].

In figure 4, we show the dimensionless energy as a function of the aspect ratio $r_>/r_<$, for (*a*) oblate and (*b*) prolate particles. We consider the case when all oblate (prolate) particles have the same curvature and are at a distance $z/r_> = 0.25$ (0.1). The energy for oblate, as well as for prolate particles is a power-law function of z, which depends on the geometrical parameters, even when the curvature of the particle is not changed. In the case of prolate particles, the value L increases smoothly as the aspect ratio also does. On the other hand, for oblate particles the number of multipolar interactions is more sensitive to the axes aspect ratio, and the value of the largest multipolar interaction increases dramatically as $r_>/r_<$ also does.

4. Conclusions

The role of geometry in dispersive forces in the non-retarded limit is studied by calculating the energy from the interacting surface plasmon of macroscopic bodies. We analyse in detail the interaction of oblate and prolate particles with a substrate. When the particle is close to the substrate the multipolar interactions induced by the substrate modify the electromagnetic response of the system. In general, we find that the energy is described by a power-law function whose exponent depends on the minor and major axes of the spheroid, as well as on the separation between bodies. The influence of the geometry on dispersive forces can be very important for experiments using atomic force microscopy.

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