CASIMIR FORCES BETWEEN NANOPARTICLES AND SUBSTRATES

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ABSTRACT

We study the Casimir force between a nanoparticle and a substrate using a spectral representation formalism. We consider the interaction of metal nanoparticles with different substrates within the dipolar approximation. The force is calculated as a function of the distance between the particles and the substrate. The particles are made of gold or potassium spheres, and the substrate is titanium dioxide, sapphire or a perfect conductor.

INTRODUCTION

Recent advances in micro and nano devices have opened the possibility of studying quantum phenomena that occurs at these length scales. Such is the case of Casimir forces [1] predicted by the theory of quantum electrodynamics. The textbook example [2] consist of two parallel neutral conducting plates separated by a fixed distance. The plates will attract each other with a force per unit area of roughly one atmosphere when the plates are 35 nm apart. This force has been measured accurately in different ways. However, a truly parallel plate configuration has been measured only by Bressi *et al.* [3]. The difficulty of keeping the two plates parallel at separations of few nanometers makes it easier to measure the Casimir force between a large conducting sphere and a plane using microtorsional balances [4] or atomic force microscopes [5,6]. In this cases, comparison with the theoretical results obtained for the parallel plates is done using the proximity theorem [7]. The proximity theorem is a geometrical approximation that states that if the free energy per unit area E at a given distance between two parallel plates is known, the force between a sphere and a plane is $2\pi ER$, where R is the radius of the sphere. This approximation is valid provided the minimum separation between the sphere and the plane is much smaller than R. The theorem does not quantify or gives bounds for the ratio between R and the separation with the plane. Thus, the question improving the theoretical description of the proximity theorem is important from the theoretical and experimental point of view.

In this work we present a calculation of the Casimir force between a sphere and a conducting plane using a spectral representation approach [8]. The Casimir force is calculated as a function of z, the minimum separation between the sphere and the plane. The force is studied as a function of the sphere's radius, and the dielectric functions of the sphere and the substrate.

THEORY

Consider a homogeneous sphere of radius R, electrically neutral and with a local dielectric function $\epsilon_s(\omega)$. The sphere is suspended over a substrate which is also electrically neutral and with a local dielectric function $\epsilon_p(\omega)$. The space above the substrate, where the sphere is immersed, is also electrically neutral and characterized by a dielectric function $\epsilon_a(\omega)$. The quantum fluctuations of the electromagnetic field in vacuum induce a dipole moment $\mathbf{p}_s$ on the sphere. If the sphere is close to a substrate, the charge distribution on the sphere generates a field which also induces a charge distribution on the substrate, given by a image-dipole moment $\mathbf{p}_p$. The latter also alters the charge distribution on the sphere through the so-called local-field. The dipole moment of the sphere is affected by the presence of the substrate through the local-field such that

$$\mathbf{p}_s = \alpha \left[\mathbf{V}^{\text{vac}} + \mathbf{A} \cdot \mathbf{p}_p \right], \tag{1}$$

where α is the polarizability of the sphere, $\alpha = R^3[(\epsilon_s - 1)/(\epsilon_s + 2)]$, $\mathbf{V}^{\text{vac}}$ is the electromagnetic field in vacuum, and $\mathbf{A}$ is the dipole-dipole interaction matrix given by

$$A_m^{m'} = \frac{4\pi(-1)^m}{(d/R)^3} \frac{2}{3} \left[\frac{1}{(1+m)!(1-m)!(1+m')!(1-m')!} \right]^{1/2}, \tag{2}$$

where d is the distance from the center of the sphere to the substrate, and m and m' indicate the cartesian component of the dipole of the sphere and substrate, respectively. Given the symmetry of the system m and m' only have two independent components: one perpendicular ($m = 0$) and one parallel ($m = \pm 1$) to the surface of the substrate. Finally, using the method of images we can calculate the dipole moment on the substrate, as

$$p_p^{m'} = (-1)^{m'} f_c p_s^{m'}. \tag{3}$$

Here f_c is a dielectric contrast factor relating the dielectric properties of the ambient and the substrate. This is,

$$f_c = \frac{\epsilon_a - \epsilon_p}{\epsilon_a + \epsilon_p}. \tag{4}$$

For example, if the substrate is a perfect conductor ($\epsilon_p(\omega) \to \infty$), then $f_c = -1$. Let us define a variable which relates the dielectric properties of the sphere and the ambient as $u = [1 - \epsilon_s/\epsilon_a]^{-1}$. Also, we define $x_m = p_s^{m'}/R^{3/2}$ and $g_m = -R^{3/2} V_m^{\text{vac}}/4\pi$. Now, we can rewrite each component m of Eq. (1) as

$$[-u\delta_{mm'} + H_m^{m'}] x_{m'} = g_m, \tag{5}$$

where

$$H_m^{m'} = n^0 \delta_{mm'} + f_c \frac{R^3}{4\pi} (-1)^m A_m^{m'}, \tag{6}$$

with $n^0 = 1/3$.

We observe that $H_m^{m'}$ is a hermitian matrix if f_c is real. In this case, we can find a unitary matrix $\mathbf{U}$, such that, $\mathbf{U}^{-1} H \mathbf{U} = 4\pi n_s$, and using the Green's function, we can obtain a density of states of the variable u for a given direction m, as

$$\rho_m(u) = \frac{-1}{\pi} \text{Im} \left[\sum_s \frac{(U_{1s} U_{s1}^{-1})_m}{u - n_s} \right]. \tag{7}$$

Then, the total density of states is given by $\rho(u) = \sum_m \rho_m(u) = \rho_0(u) + 2\rho_1(u)$.

The energy difference U between the sphere and substrate system and an isolated sphere gives rise to the Casimir energy. This is,

$$U = \int_0^\infty \frac{\hbar\omega}{2}[\rho^{sp}(\omega) - \rho^{s}(\omega)]d\omega, \tag{8}$$

where $\rho^{sp}(\omega)$ is the density of the states of the system sphere-substrate, while $\rho^{s}(\omega)$ is the density of the states of the isolated sphere ($f_c = 0$ or $\epsilon_p = \epsilon_a$).

The Casimir force is given by $F = -dU/dz$, where z is the distance of separation between the sphere and the substrate (i.e.$z = d - R$). Notice that for a given model of the dielectric function of the sphere and the ambient, we can find a relation between $\rho(\omega)$ and $\rho(u)$, as we will show in the next section.

RESULTS AND DISCUSSION

In this section we present the results for the Casimir force for metal spheres of radius 10 nm, 100 nm and 1000 nm. The dielectric function of the sphere is given by a Drude model,

$$\epsilon_s(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i/\tau)}, \tag{9}$$

where ω_p is the plasma frequency and τ is the relaxation time of a given material. Then, the density of states as a function of frequency is derived from Eq. 7, and is given by

$$\rho_m(\omega) = \frac{2\omega_p^2}{\pi}\sum_s \sqrt{n_s}\left(U_{1s}U_{s1}^{-1}\right)_m \left[\frac{\omega/\tau}{(\omega^2 - n_s\omega_p^2)^2 + (\omega/\tau)^2}\right]. \tag{10}$$

The parameters used in our calculations are for spheres made of potassium (K), $\hbar\omega_p =$ 3.8 eV and $1/\tau = 0.105\omega_p$, and for gold (Au) with $\hbar\omega_p = 8.55$ eV and $1/\tau = 0.0126\omega_p$. To achieve the condition of f_c to be real, we have considered substrates whose dielectric function is real and constant in a wide range of the electromagnetic spectrum such as TiO_2 (titanium dioxide), Al_3O_2 (sapphire), and a perfect conductor ($f_c = -0.773$, -0.516, and $-$ 1.0 respectively). If $\epsilon_p > 1$ then $f_c < 0$ always. In this work, we only consider the case where the sphere is in vacuum, $\epsilon_a = 1$. Our theory does not consider retardation effects, therefore we have to work in the limit when R and z are smaller than c/ω_p, being c the speed of light.

In Fig. 1, we present the energy calculated from Eq. 8 as a function of the separation in units of the radius of the sphere, z/R. The left panel shows the results for spheres of potassium (K) over different substrates, while the right panel are the results for spheres of gold (Au) over the same substrates. In general, we observe that the energy is negative in both cases, and its absolute value is two times larger for gold particles than for potassium particles. We also observe that as the absolute value of f_c is larger, then the absolute value of energy is also larger.

In Fig. 2 we show the force for gold and potassium nanoparticles over a perfect conductor for spheres of radius of 10^1 nm, 10^2 nm and 10^3 nm. The force is attractive in both cases

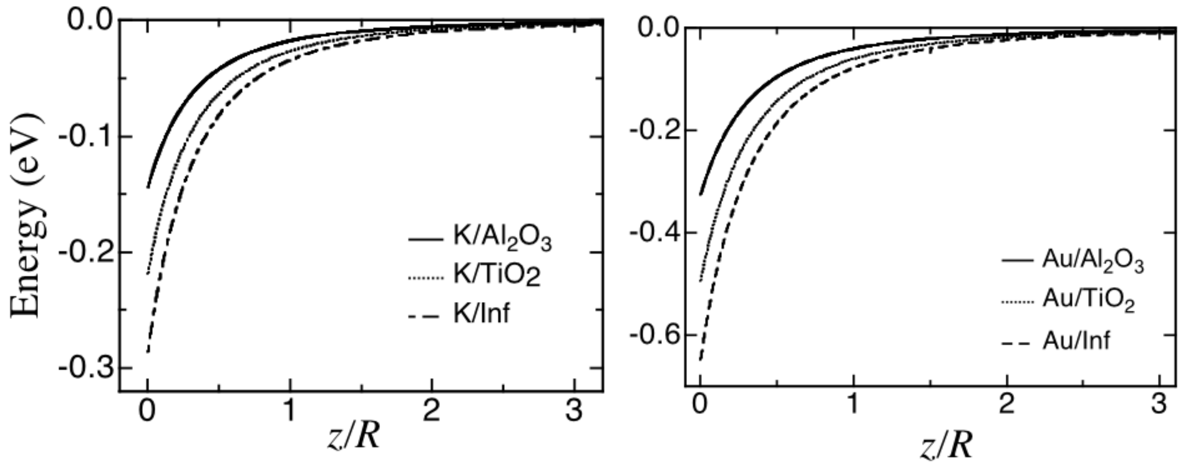

Figure 1: *Energy as a function of the separation in units of radius (z/R) for K and Au spheres over substrates of Al_2O_3, TiO_2, and a perfect conductor (Inf).*

and is smaller as the radius of the sphere becomes larger at small separations. In particular, at $z = 0$ nm the force on a sphere with $R = 10$ nm is ten times larger than the one with $R = 10^2$ nm, and it is two orders of magnitude larger than the force of the sphere with $R = 10^3$ nm. We also observe that as the radius of the sphere increases the force decreases slowly as function of z. Thus, the force for the larger sphere with $R = 10^3$ nm is almost flat as the separation increases from 0 to 40 nm. On the other hand, for a sphere of radius $R = 10$ nm the force decreases very fast as a function of z, in this case the force decreases about three orders of magnitude as the separation of the sphere goes from 0 to 40 nm.

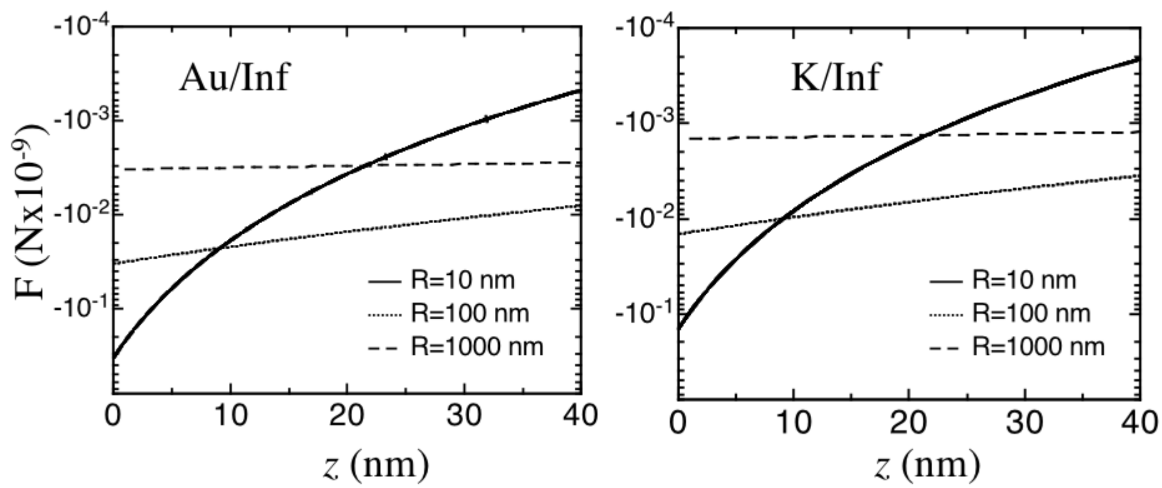

Figure 2: *Casimir force as a function of the separation for K and Au spheres over a perfect conductor (Inf) substrate and spheres of different radius.*

In Fig. 3 we compare the force between nanoparticles of radius $R = 10$ nm and made of different materials (potassium and gold), over a substrate. The left panel shows the results for a sapphire substrate, while on the right the substrate is a perfect conductor. As before, the force is larger for the perfect conductor substrate than for sapphire. On the other hand, for both substrates, we observe that the force between gold particles and the substrate is larger than the force with potassium particles. This is consistent with the fact that the gold particles have a plasma frequency more than two times larger than the plasma frequency of potassium particles.

The magnitude of the forces calculated here are within the resolution of current measuring systems such as atomic force microscopes. Measurements with different size of spheres can provide bounds for the validity of the proximity thorem.

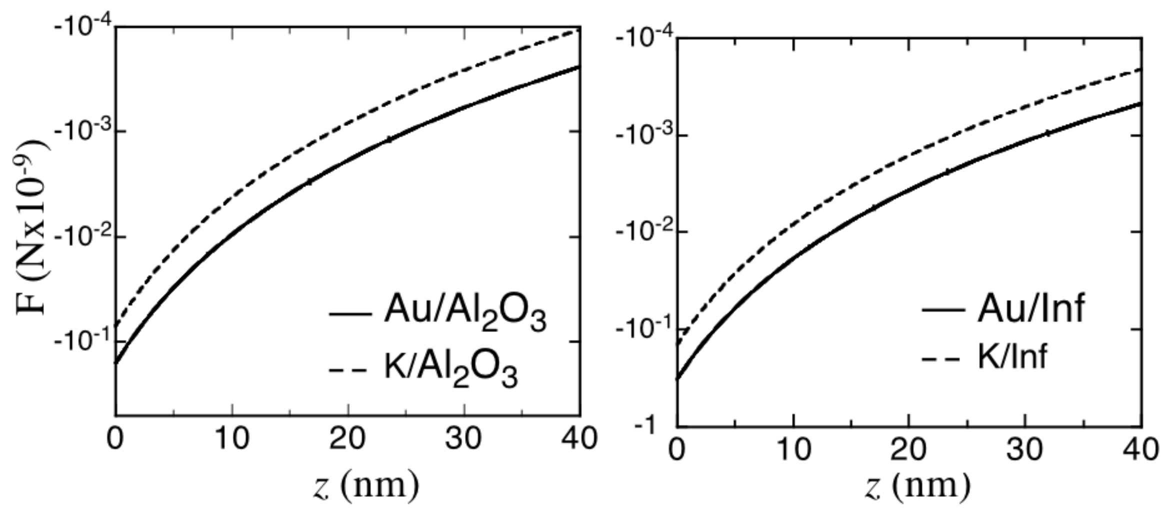

Figure 3: *Casimir force as a function of the separation for K and Au spheres over Al_2O_3 (left) and perfect conductor (right) substrates. Spheres with radii of $R = 10$ nm.*

Finally, in Fig. 4, we show as a function of energy (eV), the difference of the density of states between the sphere near a substrate and the isolated sphere, $\rho(\omega) = \rho(\omega)^{\rm sp} - \rho(\omega)^{\rm s}$. We show results for potassium (upper plots) and gold nanoparticles (lower plots) over a substrate of sapphire (left) and a perfect conductor (right). Different curves correspond to different separations of the sphere and the substrate on units of the radius of the nanoparticle (z/R). We found that for gold particles over a perfect conductor, ρ shows three different peaks, two positive and one negative, when the sphere is touching the substrate $(z/R = 0)$. At $z/R = 0$, the positive peak at lower energies (at about 4.25 eV) corresponds to electromagnetic modes (EM) on the sphere which are perpendicular to the substrate plane, while the positive peak at about 4.6 eV corresponds to EM modes on the sphere which are parallel to the substrate plane. The latter peak is about two times larger than the one corresponding to perpendicular modes. At larger energies we found a negative peak that corresponds to the EM modes of the isolated sphere. As the separation z/R increases, the strength of all the peaks decreases and the positive peaks are blue-shifted and overlap, while the negative peak does not shift its position. For large separations, the density of states is almost null. The same is observed for Au/Al_2O_3, however the positive peaks are at higher energies. On the other hand, we found that K particles show a smaller density of states than Au particles, and ρ only has two peaks, one negative and one positive. The positive peak corresponds to all the EM modes (perpendicular and parallel to the substrate plane) which have the same energy, while the negative peak also corresponds to the EM modes of the isolated sphere. Notice that these peaks are wider than those show for Au particles, this fact is due to the difference in τ of K and Au.

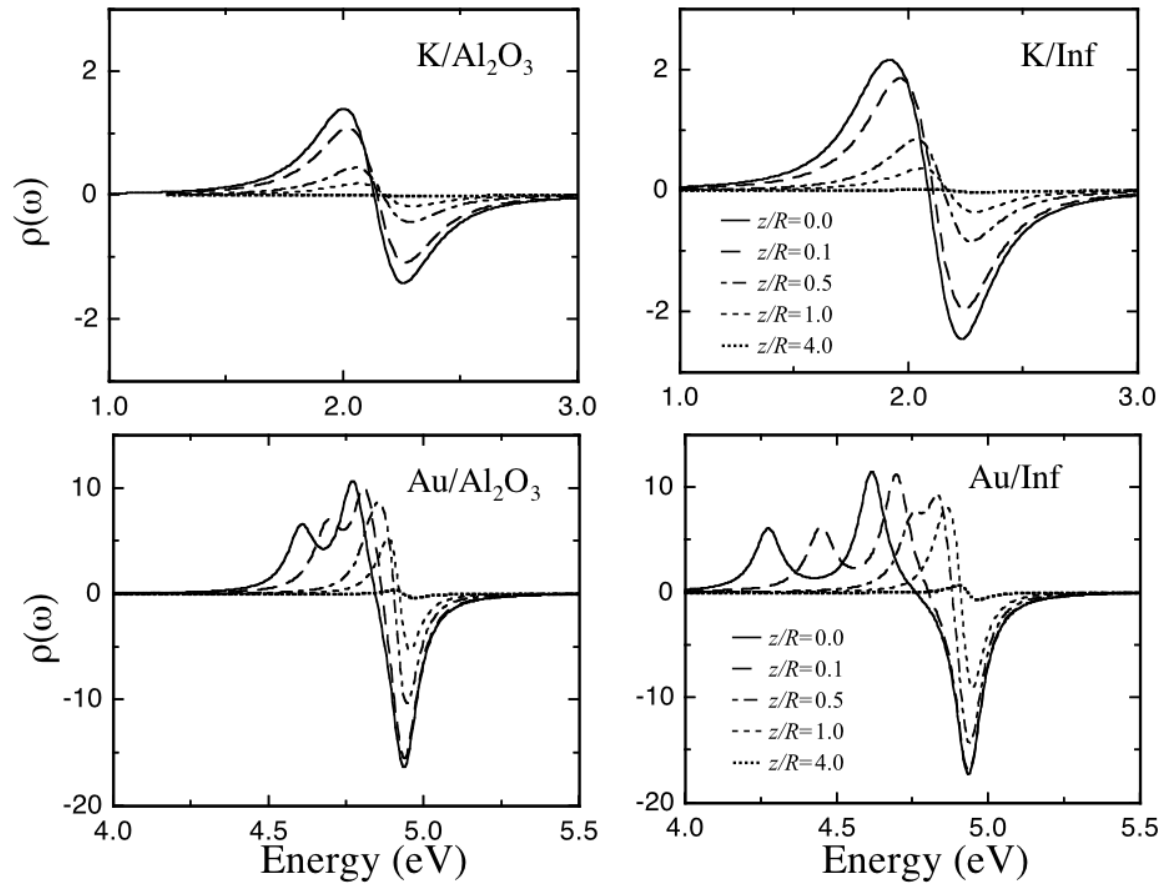

Figure 4: *Density of states ρ for Au and K nanoparticles over a substrate of sapphire (left panel) and a substrate made of a perfect conductor (right panel).*

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