Casimir forces between nano-structured particles

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Abstract. We develop a computational study of Casimir forces between three
dimensional (3D) finite objects with an internal granular structure. The objects
in the model consist of a finite arrangement of nanometer sized spherical particles
having a dipolar interaction. In this model system one can both study the basic
properties of the Casimir forces, and the effects from changing the parameters
of the nano-structured materials that constitute the particles; this last type of
study leads to a form of control of the Casimir force and an insight into possible
technological applications. We present examples of both kinds of study.

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In the last 20 years an increased interest in nano-systems has revealed a new realm
of physical phenomena. These studies have gained special attention due to the
possibility of technological applications. For example, at nano-scale distances the
dispersion forces play an important role and one has considered the possibility to
employ them in the development of nano-mechanical devices. Some first attempts
have been performed and several others have been proposed [1, 2]. Another special
interest in nano-systems comes from the fact that in nano-meter scale the physical
properties of the objects change with their size. Nano particles are currently used as
building blocks of macroscopic materials that will have properties not found in nature.
With the most modern techniques it has been possible to produce arrangements of
nano particles in 2D or 3D patterns with great control of shape, size, and spacing. With
the control of these parameters it has been feasible to accurately engineer the optical
properties of these so called metamaterials. Some of the most amazing examples of
new artificial materials are those with negative refractive index. They have come in
focus in the area of Casimir forces due to the possibility of obtaining repulsive forces.
The use of this or other kind of Casimir interactions for technological applications
requires a deep understanding of the basics of the phenomena and the experience of
a wide range of ways to control the interaction.

Here we consider a model of finite 3D objects consisting of ordered arrangements
of spherical particles with dipolar interaction. This system could be interpreted as a
model of objects made of metamaterials. We present results of how the characteristics
of the arrangement affects the Casimir forces. In particular we present examples of
the use of metamaterials to obtain Casimir rotational forces. This model system can
also be used as a basic research tool to study the phenomenon of Casimir forces due
to a connection with a computational method called discrete dipole approximation
(DDA)[3]. In conditions where the granularity of the material is not of relevance
the results of the study of this system could be applied to normal materials. We
present several results that are consistent with well known results obtained from other theoretical models.

The successful measurement of Casimir forces brought back new attention to this effect predicted by the earlier quantum field theory. Some studies have been motivated by the possibility of technological application in the form of nano-mechanical devices. Different possible interactions have been considered: lateral forces have already been measured and rotational forces have been proposed in different configurations. The Casimir forces show a complex behaviour due to the material and surface geometry dependences. An important insight into the basics of the phenomena of Casimir forces has been obtained from the various theoretical models. However, these models rely on important simplifications that limit their applicability to actual devices: perfect metal assumption, the translational invariance (2D problem) or non-retarded interactions. Although a computational model exists for the Casimir energy between arbitrary 3D objects of real materials, due to the numerical complexity of the problem, similar assumptions have been needed in order to produce results. The unique results that exist at the moment for these kind of systems, obtained with a general multipolar scattering formalism, are the interaction between two spheres and a sphere above a substrate. This kind of formalism gives results of high accuracy for highly symmetric systems like pair of spheroids or cylinders; for other geometries the description becomes much more complex and the numerical calculations slow and with low precision. These problems hamper the use of these models in a general study of how the Casimir forces depend on geometrical shapes, configurations, materials, temperature, etc. In what follows we present a system that can be useful in the understanding and the application of Casimir forces.

Consider a system of $N$ spherical particles, made of a homogeneous isotropic material characterized by the dielectric function $\varepsilon(\omega)$, immersed in the vacuum. An electric field $E_{inc}(r, \omega)$ applied to the system induces a dipole moment in each sphere as a consequence of its polarizability, $\alpha(\omega)$.

$$p_j(\omega) = \alpha(\omega) \left[ E_{inc}(r_j, \omega) - \sum_{k \neq j} A_{j,k}(\omega) \cdot p_k(\omega) \right].$$  \hspace{1cm} (1)

The so called interaction tensor $A_{j,k}(\omega)$ gives the electric field at the position $r_j$ of particle $j$ due to the dipole moment $p_k$ of particle $k$ at position $r_k$.

$$A_{j,k}(\omega) \cdot p_k(\omega) = \frac{e^{iqr_{jk}}}{r_{jk}} \left\{ q^2 r_{jk} \times (r_{jk} \times p_k(\omega)) + \left[ \frac{1 - iq^2}{r_{jk}^3} \right] \left[ r_{jk}^2 [r_{jk} \cdot (r_{jk} \times p_k(\omega))] \right] \right\},$$

where $q = \omega/c$, with $c$ the speed of light, and $r_{jk} = r_j - r_k$, with $r_{jk}$ its magnitude. The polarizability of a sphere with radiative corrections due to the retarded propagation of the electromagnetic waves in its interior is given by

$$\alpha(\omega) = a^3 \frac{\varepsilon(\omega) - 1}{3 + [\varepsilon(\omega) - 1] \left[ 1 + (qa)^2 - 2i(qa)^3/3 \right]}.$$
The electromagnetic resonances are obtained as those frequencies $\omega_s$ that make the determinant of the linear system of equations for $p_k$, obtained from Eq. (1), vanish, i.e.,

$$0 = G(\omega_s) = \det \left( \frac{1}{\alpha(\omega_s)} \delta_{\beta,\gamma} \delta_{j,k} + A_{j\beta,k\gamma}(\omega_s) \right),$$

where, $\beta, \gamma = x, y, z$, the coordinates of a cartesian system. Using the argument theorem one obtains the formula for the zero point energy $[11]$

$$U(\omega) = -\frac{\hbar}{i2\pi} \int_{i0}^{i\infty} d\omega \log G(\omega).$$

We calculate the interaction energy numerically by first considering the whole system and then subtracting the result when the objects do not interact.

In the figures that follow we present results for cubes and cylinders of rectangular or circular cross sections. All these objects are made up from an ordered inner structure of small spheres. In Fig. 1 we show results of direct forces between two cubes of side length $L$. We consider cubes of different sizes but with the same number of gold spheres (1000) and filling fraction ($4\pi/3^3$). We also present non-retarded van der Waals results ($c \to \infty$) and of two interacting circular cylinders with their bases aligned. The area of the cylinder base is the same as for the cube of side length $5\, \mu m$ but the height is $4\, \mu m$. The experimental dielectric function of gold has been taken from $[13]$. In the non-retarded calculations it is possible to choose one of the dimensions of the system as a scale parameter due to the independence of the problem with the dimensions of the system; we choose the side length of the cube, $L$. The retarded calculations are presented in the same way, but here one obtains one curve for each cube size. We observe that as expected the bigger objects present bigger deviations from the vdW results due to the bigger retardation effects within them, and also that the retardation effects produce a weakening of the force even for the smallest cubes. We find for the bigger cubes at large distances the calculations including retardation present the behavior of a retarded dipolar interaction $F \sim z^{-8}$ $[11]$. The non-retarded calculations show the known power law behaviour of the form $F \sim z^{-7}$ $[11]$. At short distances we see that the smaller cubes present values similar to the non-retarded calculations. They vary as $F \sim z^{-3}$, consistent with a pair of semi-infinite slabs $[11]$. 

**Figure 1.** Effect of the object size on the normal Casimir force.
We refrain from doing comparisons with vdW results at small distances for the bigger cubes because of the increasing effects of granularity. These effects become severe when the separation distance is of the same order as the structural parameters of the cubes. Finally, we observe that, for the cylinder and the cube of 5 μm the force is very close. This result is similar to that found for vdW forces in case of homogeneous media where at shorter distances the force is independent of the shape of the base of the cylinder.35.

In Fig. 2 we explore the effects that the modification of the parameters of the objects’ nano-structure could have on the Casimir forces. In panel (a) we show the effects of the material of the spheres that constitute the cubes and in panel (b) some of the geometry parameters of the arrangement. First we show the results for gold and aluminum spheres without considering retardation. As can be seen the forces are different at all distances. However, in cubes of 0.5 μm when retardation is taken into account one obtains differences only at smaller distances. At larger distances both materials show the same force. We also compare with results from using the perfect metal approximation for the spheres. We observe that with the perfect metal assumptions the forces show bigger differences than those existing between real metals but eventually at larger distances the differences go away. We have observed that those
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differences are smaller for bigger cubes. Interestingly, the short distance forces do not have the power law behavior corresponding to homogeneous perfect metal objects, $F \sim z^{-4}$; instead, they show that of objects made of normal dielectric materials. Finally we show in the same panel results for non-metallic materials [14]. One observes differences at all distances. Smaller forces are obtained with silicon spheres and even much smaller forces with poly-styrene spheres.

In panel (b) of Fig. 2, we first consider cubes of side length 5 $\mu$m made with different number of spheres ($10^3, 8^3, 6^3$) but keeping the same filling fraction ($4\pi/3^3$). We observe that at smaller distances, when one expects stronger granularity effects, the forces in the three different systems are different. However, at larger distances their values coincide. This indicates that in this model at large distances the Casimir force depends on the filling fraction of the material and not on the actual size of the spheres. A similar situation appears in the DDA model when the convergence of the calculations is reached [5]. This fact is also compatible with some of the results of the effective medium approximation (EMA) [15]. In the EMA the objective is to determine the optical properties of the system based on geometrical and material parameters of a composite material. Some of the simplest models of the EMA have the filling fraction and the dielectric function of the materials as the only information of their internal structure. We show results from using the formalism of Ref. [5] to calculate the vdW force for homogeneous objects with the dielectric function from an EMA formalism, the Maxwell-Garnett model [15], based on similar assumptions as our model. Note that they coincide in a wide range of distances, and differ only at smaller distances where the effects of the granularity of the model are stronger. In Fig. 2(b) we also present results for cubes of $10^3$ spheres with smaller radii ($L/50$). A great reduction of the force is observed.

In Fig. 3 we show calculations of rotational forces between two finite rectangular cylinders. The lengths of the base are $L(1 \mu m)$ and $2L$ and the height is $0.5L$. They are kept at a distance $d_s$ and considered initially with their bases aligned. Then we consider a rotation around a perpendicular axis that goes throughout their geometrical center. With a numerical derivation we calculate the torque on the system. We consider results for objects of different lengths $L$ and also different separations $d_s$ and compare with the homogeneous model of [5] using the Maxwell-Garnett dielectric function model. Note that the homogeneous and discrete model present similar shapes, despite of the different approaches. As we see in panel (b) for the bigger value of $d_s$ the numerical differences of both non-retarded calculations are smaller; this is expected from the experience of normal forces at greater separation distances. These last results are another evidence for that the model produces results that are compatible with those obtained from accurate models of homogeneous objects. In the following we present an example of Casimir rotational forces between two cylinders made of anisotropic metamaterials. The effect of rotational interaction between two birefringent material slabs has been studied in [1]. In this phenomenon it is interesting to, instead of being limited by the availability of natural birefringent materials, consider metamaterials as a way to increase or control these forces. In Fig. 4 we show results for different kinds of anisotropic metamaterials obtained from our model by changing the parameters of the constituents. Two anisotropic arrangements of particles produce a difference of energy when their axes are not aligned; and as a consequence a rotation. A pair of finite cylinders of height 0.43 $\mu$m are positioned so that their circular bases of area $A(1 \mu m^2)$ are kept parallel at a distance of $0.4A^{1/2}$. We consider three different anisotropic inner structures: one with spheres of radii $A^{1/2}/42$
Figure 3. Torque between rectangular cylinders: (a) $d_s = 0.35L$; (b) $d_s = 0.35L$ in Casimir and $d_s = 0.5L$ in vdW.

Figure 4. Torque between circular cylinders of anisotropic metamaterials. (a) spheres in asymmetric lattice; (b) prolate in symmetric lattice; (c) prolate in asymmetric lattice.
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in a lattice obtained from a cubic one by increasing one of its lattice parameters \((A^{1/2}/14)\) by a factor of 1.2; the second arrangement considers prolate spheroids with aspect ratio 1.2 and the bigger semi-axis of \(A^{1/2}/42\) in a cubic lattice; the third is a combination of both with the long axis of the spheroid in the direction of the modified lattice direction. This last case resembles the production of prolate nanoparticles by stretching a sample of metallic spheres immersed in a dielectric matrix. The prolate polarizability was taken from [9]. We see that the maximum torque is obtained with the prolaters in a cubic lattice, while the smaller is obtained with the spheres in the stretched lattice. However the combinations of both geometries do not show a greater anisotropy. The effect of the stretched lattice compensates the effect of the prolate spheroids.

In summary, we have introduced a simple model system of two nano-structured 3D objects for the study of dispersion forces with the inclusion of retardation and material effects. This system could be interpreted as a model of objects made of metamaterials, in which it is possible to control the magnitude and direction of Casimir forces through the modification of the internal structure. Furthermore, it can be used to study the effects of shape, size, temperature and materials on the Casimir forces between compact 3D objects; due to the complexity of the theoretical models available, this has not been possible until now. This letter is just a very brief summary of our results. A more detailed publication will follow.

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