New geometries in the Casimir effect: dielectric gratings

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Abstract. An exact solution for the Casimir force between two arbitrary dielectric gratings with the same period $d$ is presented. The Casimir energy for two dielectric gratings or periodic dielectrics is expressed in terms of Rayleigh coefficients. The theory is applied to calculate the Casimir force in several cases of interest.

1. Introduction

In 1948 H. B. G. Casimir showed that two electrically neutral, perfectly conducting plates, placed parallel in vacuum, modify the vacuum energy density with respect to the unperturbed vacuum[1]. The vacuum energy density varies with the separation between the mirrors and leads to the Casimir force, which scales with the inverse of the fourth power of the mirrors separation.

The Casimir force is highly versatile. Changing materials and shape of the boundaries can modify its strength and even its sign. For example the role of surface plasmons to tailor the Casimir force [2, 3, 4, 5] and the possible interest of metamaterials [6, 7, 8, 9] in order to produce repulsive forces have been studied during the last years. The modification of the Casimir force between a silicon membrane and a gold coated sphere due to the illumination of the silicon membrane with laser light was demonstrated recently [10]. Modifying the Casimir force could potentially be useful in the design and control of micro- and nanomachines.

The availability of experimental set-ups that allow accurate measurements of surface forces between macroscopic objects at submicron separations has recently stimulated a renewed interest in the Casimir effect. While the material dependence of the Casimir force has been thoroughly studied between two plane mirrors (see e.g. [11, 12, 13, 14]), for most other geometries exact calculations exist only for perfectly reflecting boundaries (see e.g. [15]). If finite conductivity effects are taken into account, the shape dependence of the Casimir force is usually treated using the proximity force approximation (PFA) which amounts to summing up contributions at different distances as if they were independent. PFA is known to be valid if the typical length scale of geometric deviation from the plane-plane configuration is much larger than the distance between the two bodies. However, for periodic metallic or dielectric gratings such as manufactured in nanotechnology PFA is expected to fail as all important length scales are of the same order.
The first measurement of the Casimir force between an aluminium grating with small sinusoidal corrugations and an aluminium sphere was performed by Roy and Mohideen [16]. In a recent paper [17], Chan et al. present the first measurement of the Casimir force between a rectangular silicon grating of high aspect ratio and a gold sphere and demonstrate the violation of the PFA in this geometry. Corresponding calculations taking into account the periodic structure beyond PFA, but only for perfect mirrors [18], turn out to lead to a too large deviation from PFA [17].

In this paper we present a novel exact theory of the Casimir effect between gratings of arbitrary periodic structure, where we take explicitly into account the (arbitrary) dielectric permittivity of the material. First we describe the Rayleigh basis and outline the way to calculate the Rayleigh coefficients for an arbitrary grating. Then we present the derivation of the Casimir energy in terms of Rayleigh coefficients for two dielectric gratings or periodic dielectrics with the same period $d$. This derivation generalizes the idea of the argument principle method in the Casimir effect, which was used for plane geometries before (see e.g. [19, 20]). We insert the reflection matrices for two separated gratings into the argument principle explicitly and express the formula for the Casimir energy in terms of them. Our general derivation can be applied to various Casimir systems. We apply our formulation to the situation of two rectangular silicon gratings and show that our calculation yields deviation of the real force from the PFA prediction up to 24 percents. We also performed calculations corresponding to the measurement by Chan et al. allowing therefore a first quantitative theory-experiment comparison. The result taking into account the finite conductivity gives a smaller deviation of the exact force from the PFA prediction than the calculation for perfect mirrors.

2. General method

We consider two periodic dielectric gratings of arbitrary form separated by a vacuum slit. The special case of lamellar (or rectangular) gratings is depicted in Fig.1. The geometrical parameters of the grating are the corrugation depth $a$, the period $d$ and the gap $d_1$. The gaps of both gratings are separated by a distance $L$. For simplicity we will suppose the space between the two gratings to be filled with vacuum with $\epsilon = \mu = 1$.

The physical problem is time and $z$ invariant, so electric and magnetic fields can be written in the form:

$$E_i(x, y, z, t) = E_i(x, y) \exp(ik_z z - i\omega t), \quad (1)$$
$$H_i(x, y, z, t) = H_i(x, y) \exp(ik_z z - i\omega t). \quad (2)$$

Let us suppose for the moment that the upper grating is absent. We consider a generalized conical diffraction problem on the lower grating. The longitudinal components of the electromagnetic field outside the corrugated dielectric region ($y > a$) may be written by making use of a generalization of the Rayleigh expansion for an incident monochromatic wave:

$$E_z(x, y) = I_p^{(e)} \exp(i\alpha_p x - i\beta_p^{(1)} y) + \sum_{n=-\infty}^{+\infty} R_{np}^{(e)} \exp(i\alpha_n x + i\beta_n^{(1)} y), \quad (3)$$

$$H_z(x, y) = I_p^{(h)} \exp(i\alpha_p x - i\beta_p^{(1)} y) + \sum_{n=-\infty}^{+\infty} R_{np}^{(h)} \exp(i\alpha_n x + i\beta_n^{(1)} y), \quad (4)$$

$$\alpha_p = k_x + 2\pi p/d, \quad \beta_p^{(1)} = \omega^2 - k_z^2 - \alpha_p^2, \quad (5)$$

$$\alpha_n = k_x + 2\pi n/d, \quad \beta_n^{(1)} = \omega^2 - k_z^2 - \alpha_n^2. \quad (6)$$
with an integer $p$, the sums are performed over all integers $n$. All other field components can be expressed via the longitudinal components $E_z, H_z$. This solution is valid outside any periodic one-dimensional structure. Note that the expansions should satisfy the quasi-periodicity conditions:

$$E_z(x + d, y) = e^{ik_z d} E_z(x, y),$$  \hspace{1cm} (7)  

$$H_z(x + d, y) = e^{ik_z d} H_z(x, y).$$  \hspace{1cm} (8)  

We now have to determine the coefficients $R^{(e)}_{np}, R^{(h)}_{np}$ for a specific periodic geometry profile. For this purpose it is convenient to rewrite the Maxwell equations inside the corrugation region $0 < y < a$ in the form of first order differential equations, $\frac{\partial A}{\partial y} = MA$, where $M$ is a square matrix of dimension $8N + 4$, $A^T = (E_z, E_x, H_z, H_x)$ and $2N + 1$ is the number of Rayleigh coefficients considered in every Rayleigh expansion. For a rectangular dielectric grating the matrix $M$ is a constant matrix. At $y = 0$ the solution has to satisfy the expansions

$$E_z(x, y) = \sum_{n=-\infty}^{+\infty} T^{(e)}_{np} \exp(i\alpha_n x - i\beta^{(2)}_{n} y),$$  \hspace{1cm} (9)  

$$H_z(x, y) = \sum_{n=-\infty}^{+\infty} T^{(h)}_{np} \exp(i\alpha_n x - i\beta^{(2)}_{n} y),$$  \hspace{1cm} (10)  

$$\beta^{(2)}_{n} = \epsilon \mu \omega^2 - k_z^2 - \alpha^2_n,$$  \hspace{1cm} (11)  

which are valid for $y \leq 0$. We then determine the unknown Rayleigh coefficients by matching the solution of equations $\frac{\partial A}{\partial y} = MA$ inside the corrugation region with Rayleigh expansions (3),(4) at $y = a$ and expansions (9),(10) at $y = 0$. Everywhere in the calculations we assumed $\mu = 1$.  

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**Figure 1.** Rectangular gratings geometry.
The fields $E_z$ and $H_z$ are not decoupled for $k_z \neq 0$. This is why the reflection matrix $R_1$ for a reflection from a lower grating can be defined as follows:

$$
R_1(\omega) = \begin{cases}
R_{11}^{(e)}(i_p^e) = \delta_{p,q}, I_p^{(h)} = 0 & \text{if } y > L \\
R_{13}^{(e)}(i_p^e) = \delta_{p,q}, I_p^{(h)} = 0 & \text{if } y < L
\end{cases}
R_{13}^{(e)}(i_p^e) = \delta_{p,q}, I_p^{(h)} = 0 & \text{if } y < L,
\\
R_{13}^{(e)}(i_p^e) = \delta_{p,q}, I_p^{(h)} = 0 & \text{if } y > L.
$$

(12)

Performing a change of variables $y = -y' + L$, $x = x' - s$ ($s < d$) in (3), (4), it is possible to obtain the reflection matrix $R_{2up}$ for the reflection of an upward plane wave from a grating with the same profile turned upside-down, displaced from the lower grating by $\Delta x = s$, $\Delta y = L$. Note that for the upper grating in Fig.1 the special case $s = 0$ is depicted.

Up to now we considered a diffraction problem on a single grating. In [21] the Casimir energy between two bodies, the diffraction properties of which can be described by a scattering matrix, has been derived in plane geometries on the basis of canonical quantization. Roughness corrections were derived on the basis of a scattering approach in [22, 23]. The path integral method was used to obtain multipole expansion of the Casimir energy between the two compact objects [24], exact results in spherical geometries [24, 25] were also derived.

We outline a novel derivation here, which can be applied to various Casimir systems. To obtain the Casimir energy we need to determine the eigenfrequencies of all stationary solutions of the generalized diffraction problem of subsequent diffraction of the electromagnetic field on two periodic dielectrics separated by a gap-gap distance $L$. These eigenfrequencies can be summed up by making use of an argument principle, which states:

$$
\frac{1}{2\pi i} \oint \phi(\omega) \frac{d}{d\omega} \ln f(\omega) d\omega = \sum \phi(\omega_0) - \sum \phi(\omega_{\infty}),
$$

(13)

where $\omega_0$ are zeroes and $\omega_{\infty}$ are poles of the function $f(\omega)$ inside the contour of integration, degenerate eigenvalues are summed over according to their multiplicities (see e.g. [19, 20]). For the Casimir energy we have $\phi(\omega) = h\omega/2$. The equation for eigenfrequencies of the corresponding problem of classical electrodynamics is $f(\omega) = 0$.

Consider first the plane-plane geometry when two dielectric parallel slabs (slab 1: $y < 0$, slab 2: $y > L$) are separated by a vacuum slit ($0 < y < L$). In this case $TE$ and $TM$ modes do not couple. The equation for $TE$ eigenfrequencies is:

$$
f(\omega) = 1 - r_{1TE}(\omega)r_{2TE}(\omega) = 0.
$$

(14)

Here $r_{1TE}(\omega)$ is the reflection coefficient of a downward plane wave which reflects on a dielectric surface of slab 1 at $y = 0$, while $r_{2TE}(\omega)$ is the reflection coefficient of an upward plane wave which reflects on a dielectric surface of slab 2 at $y = L$. One can deduce from Maxwell equations that $r_{2TE}(\omega) = r_{2TE}(\omega) \exp(2ik_y L)$ ($r_{2TE}(\omega)$ is a reflection coefficient of a downward $TE$ plane wave which reflects on a dielectric slab 2 now located at $y < 0$). From (14) and the analogous equation for $TM$ modes one immediately obtains the Lifshitz formula [11] by making use of the argument principle (13).

For two gratings or periodic dielectrics separated by a vacuum slit one has to consider a reflection of downward and upward waves from a unit cell $0 < k_x < 2\pi/d$. Due to the structure of the surface, $TE$ and $TM$ modes do not decouple anymore, but they are coupled by the diffraction process. The equation for normal modes states:

$$
R_1(\omega_1)R_{2up}(\omega_1)\psi_1 = \psi_1,
$$

(15)

where $\psi_1$ is an eigenvector describing the normal mode with a frequency $\omega_1$. Instead of equation (14) one obtains from (15) the following condition for eigenfrequencies:

$$
\det(I - R_1(\omega)R_{2up}(\omega)) = 0.
$$

(16)
For every $k_x, k_z$ the solution of (16) yields possible eigenfrequencies $\omega_i$ of the solutions of Maxwell equations that should be substituted into the definition of the Casimir energy $E = \sum_i \frac{\hbar \omega_i}{2}$. These solutions should tend to zero for $y \to \pm \infty$. The summation over the eigenfrequencies is performed by making use of the argument principle (13), which yields the Casimir energy of two parallel dielectrics on a "unit cell" of period $d$ and unit length in $z$ direction:

$$E = \frac{\hbar c d}{(2\pi)^3} \int_0^{+\infty} d\omega \int_{-\infty}^{+\infty} dk_z \int_0^{2\pi} dk_x \ln \det \left( I - R_1(i\omega)R_{2up}(i\omega) \right),$$

(17)

c is the speed of light in vacuum. This is an exact expression valid for two arbitrary gratings or periodic dielectrics with the same period $d$ separated by a vacuum slit. It can be applied to calculate the Casimir energy of any parallel gratings or periodic dielectrics made of a material described by a dielectric function.

Consider the particular case $s = 0$, which is depicted in Fig.1. From the derivation sketched above it follows that

$$R_{2up}(i\omega) = K(i\omega)R_2(i\omega)K(i\omega),$$

(18)

where $K(i\omega)$ is a diagonal $2(2N + 1)$ matrix of the form:

$$K(i\omega) = \begin{pmatrix} G & 0 \\ 0 & G \end{pmatrix},$$

(19)

with matrix elements $e^{-L\sqrt{\omega^2 + k_x^2 + (k_z + \frac{2\pi m}{d})^2}}$ ($m = -N \ldots N$) on a main diagonal of a matrix $G$. Note that in all Rayleigh expansions the Fourier basis is taken symmetrically around $m = 0$.

3. Rectangular gratings

We have numerically calculated the exact Casimir force for two rectangular gratings at zero temperature in the geometry of Fig.1 for silicon for different values of $d$, $d_1 = d/2$ and $a = 100$ nm.
by making use of the formulas (17, 18, 19) and a Drude-Lorentz model for a dielectric permittivity of an intrinsic silicon obtained in [14]. We compare our exact results of the Casimir force for different values of $d$ to the PFA results. Calculated with the proximity force approximation, the Casimir force between the two gratings is just the geometric sum of two contributions corresponding to the Casimir force between two plates $F_{PP}$ at distances $L$ and $L - 2a$, that is $F_{PFA} = \frac{1}{2}(F_{PP}(L) + F_{PP}(L - 2a))$. In particular it is independent of the corrugation period $d$. To assess quantitatively the validity of PFA, we plot the dimensionless quantity $\rho = \frac{F}{F_{PFA}}$. The ratio is presented on Fig.2. Exact and PFA results differ for silicon by up to 24 percents for a corrugation period of 100nm and the PFA violation could thus be demonstrated experimentally. We recover the PFA result in two limiting cases, for a vanishing corrugation period and for very large corrugation periods. In between the exact result for the Casimir force is always smaller than the PFA prediction, in contrast to calculations for perfect conductors, where the resulting force is always larger than the PFA prediction.

We will now apply our method to the recent experiment by Chan et al.[17], who measured the Casimir force gradient between a silicon grating with nanostructured trenches and a gold sphere of radius $R = 50\mu$m. The force gradient $F'_{PS}$ between a sphere of radius $R$ and a plate can be expressed via the force $F_{PP}$ in the plane-plane configuration as $F'_{PS} = 2\pi RF_{PP}$. This is why we show in figure 3 the zero temperature result for the absolute force values evaluated for a grating with the experimental parameters $a = 980\text{nm}$, $d = 400\text{nm}$, $d_1 = 196\text{nm}$ placed in front of a gold plate (we used a plasma model with a plasma frequency $\omega_p = 9$eV for gold [14] and a Drude-Lorentz model for intrinsic silicon [14]).

From our calculation we obtain a force $F_{PP} = 0.51\text{N/m}^2$ for a plate separation of 150nm. With the experimental parameters this leads to a prediction for the Casimir force gradient of $F' = 160.8, 56.4, 24.6 \text{pN/\mu m}$ at respectively $L - a = 150, 200, 250 \text{nm}$. The absolute values of the force are thus in good agreement with the measured values depicted in Fig.3c of [17].

Now we present ratios of our results for the force to the predictions of PFA for two different gratings. Figure 4 shows $\rho$ as a function of $L - a$ for two gratings corresponding to the experiment with $a = 980\text{nm}$, $d = 400\text{nm}$, $d_1 = 196\text{nm}$ (green line) and $a = 1070\text{nm}$, $d = 1000\text{nm}$,
Figure 4. Casimir force normalized by the PFA value between a Si grating and a gold plate as a function of distance for two different gratings. Solid curves are calculated by making use of the least square method from the theoretical points on the figure.

$d_1 = 522\,\text{nm}$ (blue line). One can compare our results with the experimental points and the fit shown in Figure 3d of [17], there is a reasonable agreement between the theoretical results and experimental data. Possible improvements in future may include calculations with more detailed models of dielectric permittivities of silicon and gold performed at finite temperature.

The fact that the perfect conductor model fails might be due to the influence of surface plasmons, as the grating affects their dispersion relation. Surface plasmons contribute essentially and at all distances to the Casimir force [2, 3, 4, 5], the Casimir force thus has to change considerably when structured surfaces are considered. These changes are not visible in a perfect conductor model which ignores the existence of surface plasmons.

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References
[1] Casimir H B G 1948 Proc. K. Ned. Akad. Wet. 51 793
[2] Barton G 1979 Rep. Prog. Phys. 42 65
[3] Intravaia F and Lambrecht A 2005 Phys. Rev. Lett. 94 110404
[4] Henkel C, Joulain K, Mulet J Ph and Greffet J J 2004 Phys. Rev. A 69 023808
