Casimir interaction of dielectric gratings.

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We derive an exact solution for the Casimir force between two arbitrary periodic dielectric gratings and illustrate our method by applying it to two nanostructured silicon gratings. We also reproduce the Casimir force gradient measured recently$^{1}$ between a silicon grating and a gold sphere taking into account the material dependence of the force. We find good agreement between our theoretical results and the measured values both in absolute force values and the ratios between the exact force and PFA predictions.

INTRODUCTION

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. 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$^{2}$. The vacuum energy density varies with the separation between the mirrors and leads to the Casimir force, which scales with the inverse of the forth power of the mirrors separation $L$.

The Casimir force is highly versatile and tailoring it could potentially be useful in the design and control of micro- and nanomachines. While the material dependence of the Casimir force has been thoroughly studied between two plane mirrors (see e.g.$^{3,4,5}$, for most other geometries exact calculations exist only for perfectly reflecting boundaries (see e.g.$^{7}$). If material properties 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.

In a recent paper$^{1}$, Chan et al. present the first measurement of the Casimir force between a silicon grating of high aspect ratio and a gold sphere and demonstrate the violation of PFA in this geometry. Corresponding calculations taking into account the periodic structure beyond PFA, but only for perfect mirrors$^{8}$, turn out to lead to a too large deviation from PFA$^{1}$.

In this Letter we present the first exact calculation of the Casimir force between gratings of arbitrary periodic structure, where we take explicitly into account the (arbitrary) dielectric permittivity of the material. We first present formulations for the Casimir energy between two periodic dielectric gratings and outline the derivation of these formulae. We then apply our formulation to the situation of two rectangular silicon gratings and show that our calculation yields deviations 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.

GENERAL PROCEDURE

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 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 electro and magnetic fields can be written in the form:

\[ E_i(x, y, z, t) = E_i(x, y) \exp(ik_z z - i\omega t), \]

\[ H_i(x, y, z, t) = H_i(x, y) \exp(ik_z z - i\omega t). \]

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

\[ E_z(x, y) = I_p^{(c)} \exp(i\alpha_p x - i\beta_p^{(1)} y) + \sum_{n=-\infty}^{+\infty} R_{np}^{(c)} \exp(i\alpha_n x + i\beta_n^{(1)} y), \]

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

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

\[ \alpha_n = k_x + 2\pi n/d, \quad \beta_n^{(1)2} = \omega^2 - k_z^2 - \alpha_n^2, \]

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.

We now have to determine the coefficients $R_{np}^{(c)}, R_{np}^{(h)}$ for a specific periodic geometry profile. For this purpose we 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 $8N + 4$, $AT = (E_z, E_x, H_z, H_x)$ 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 following expansions, valid for $y \leq 0$:

$$E_z(x, y) = \sum_{n=-\infty}^{+\infty} T_{np}^{(c)} \exp(i\alpha_n x - i\beta_n^{(2)} y),$$  \hspace{1cm} (7)

$$H_z(x, y) = \sum_{n=-\infty}^{+\infty} T_{np}^{(h)} \exp(i\alpha_n x - i\beta_n^{(2)} y),$$  \hspace{1cm} (8)

$$\beta_n^{(2)^2} = \epsilon_j \omega^2 - k_z^2 - \alpha_n^2.$$  \hspace{1cm} (9)

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 [7, 8] at $y = 0$. Everywhere in the calculations we assumed $\mu = 1$.

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:

$$R_1 = \begin{pmatrix}
R_{11,11}^{(c)}(I_p^{(c)} = \delta_{pq}i, I_p^{(h)} = 0) & R_{11,22}^{(c)}(I_p^{(c)} = 0, I_p^{(h)} = \delta_{pq}) \\
R_{12,12}^{(c)}(I_p^{(c)} = \delta_{pq}i, I_p^{(h)} = 0) & R_{12,22}^{(c)}(I_p^{(c)} = 0, I_p^{(h)} = \delta_{pq})
\end{pmatrix}. \hspace{1cm} (10)$$

Performing a change of variables $y = -y' + L, x = x' - s$ (s < d) in [3, 4], it is possible to obtain the reflection matrix $R_{2np}$ for the reflection of an upward 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 [3] 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 [10]. The path integral method was used to obtain multipole expansion of the Casimir energy between the two compact objects [11], exact results in spherical geometries [11, 12] 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 gratings separated by a gap-gap distance $L$. These eigenfrequencies can be summed up by making use of an argument principle, which states:

$$\frac{1}{2\pi i} \oint \phi(\omega) \frac{d}{d\omega} \ln f(\omega) d\omega = \sum \omega_0 - \sum \omega_\infty,$$  \hspace{1cm} (11)

where $\omega_0$ are zeroes and $\omega_\infty$ are poles of the function $f(\omega)$ inside the contour of integration. Degenerate eigenvalues are summed up according to their multiplicities. For the Casimir energy we have $\phi(\omega) = \hbar \omega/2$. 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:

$$f(\omega) = 1 - r_{1TE}(\omega) r_{2TEup}(\omega) = 0.$$  \hspace{1cm} (12)

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 $r_{2TEup}(\omega)$ is the reflection coefficient of an upward plane wave which reflects on a dielectric surface...
waves from a unit cell 0
one has to consider a reflection of downward and upward
the argument principle (11).

Immediately obtains the Lifshitz formula by making use of
the condition for eigenfrequencies:

\[ k = \text{anymore, but they are coupled by the diffraction process.} \]

The equation for normal modes states:

\[ R_1(\omega_i)R_{2up}(\omega_i)\psi_i = \psi_i, \tag{13} \]

where \( \psi_i \) is an eigenvector describing the normal mode
with a frequency \( \omega_i \). Instead of equation (12) one obtains

\[ \omega = \text{coupled by the diffraction process.} \]

For every \( k_x, k_z \) the solution of (14) yields possible eigen-
frequencies \( \omega_i \) of the solutions of Maxwell equations that
should be substituted into the definition of the Casimir
energy \( E = \sum \omega_i/2 \). These solutions should tend to
zero for \( y \to \pm \infty \). The summation over the eigen-
frequencies is performed by making use of the argument
principle (11), which yields the Casimir energy of two
parallel gratings on a “unit cell” of period \( d \) and unit length in \( z \) direction:

\[
E = \frac{\hbar c d}{(2\pi)^3} \int_0^{+\infty} \omega \int_{-\infty}^{+\infty} k_z \int_0^{2\pi} dk_x \left[ \ln \left| I - R_1(\omega)R_{2up}(\omega) \right| \right], \tag{15}
\]

c is the speed of light in vacuum. This is an exact expression
valid for two arbitrary periodic dielectric gratings
separated by a vacuum slit. It can be applied to calculate
the Casimir energy of any parallel periodic gratings made
of a material described by a dielectric function,
with surface corrugations of arbitrary geometry.

Consider the particular case \( s = 0 \), depicted in Fig 1.
From the derivation sketched above it follows that

\[ R_{2up}(\omega) = K_0(\omega)K_2, \tag{16} \]

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

\[ K(\omega) = \begin{pmatrix} G & 0 \\ 0 & G \end{pmatrix}, \tag{17} \]

with matrix elements \( e^{-L/\sqrt{\omega^2+k_z^2+(k_x^2+4\pi^2k_z^2)}} \) \((m = -N, \ldots, N) \) on a main diagonal of a matrix \( G \). Note that
in all Rayleigh expansions the Fourier basis is taken sym-
metrically around \( m = 0 \). When changing the maximum
value of \( m \) from \( N - 1 \) to \( N \), each Rayleigh coefficient

\[ R_{Np}(\omega) \]

appearing in the reflection matrices is multi-
plied by a factor \( e^{-2\pi NL/d} \) coming from the matrix \( K(\omega) \).
As a consequence, when \( 2\pi NL/d \gg 1 \) is satisfied,
the contribution of the coefficients \( R_{Np}(\omega) \) is suppressed
exponentially. Therefore for large enough \( N \) changing \( N \)
has only a little impact on the final result.

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 \( a = 100 \text{ nm} \) by making use of the formu-
as (15, 16, 17) and a Drude-Lorentz model for the
dielectric permittivity of intrinsic silicon [3]. We
compare our exact results of the Casimir force for differ-
ent 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 \( F_{PPA} = F_{PP}(L) + F_{PP}(L - 2a) \). In particular it is
independent of the corrugation period \( d \). To assess qua-
titatively the validity of PFA, we plot the dimensionless
quantity \( \rho = \frac{F_{PPA}}{F_{PFA}} \) [12]. The ratio is presented on Fig 2.

Exact and PFA results differ for silicon by up to 24 per-
cents for a corrugation period of 100 nm and the PFA vi-
olation could thus be demonstrated experimentally. We
recover the PFA result in two limiting cases, for a van-
ishing 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

\[ \rho \]

FIG. 2: Casimir force normalized by its PFA value for two Si
gratings with \( a = 100 \text{ nm} \) and \( d_1 = d/2 \) as a function of \( d \) at a
fixed distance \( L = 250 \text{ nm} \).
force is always larger than the PFA prediction.

We will now apply our method to the recent experiment by Chan et al.\cite{1}, 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 \( F'_{PS} = 2 \pi R F_{PP} \). 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 \( a = 980 nm, d = 400 nm, d_1 = 196 nm \) placed in front of a gold plate (we used a plasma model with a plasma frequency \( \omega_p = 9 eV \) for gold and a Drude-Lorentz model for intrinsic silicon \cite{6}).

From our calculation we obtain a force \( F_{PP} = 0.51 N/m^2 \) for a plate separation of 150nm. With the experimental parameters this leads to a prediction for the Casimir force gradient of \( F' = 160.8, 56.4, 24.6 \) pN/\( \mu m \) at respectively \( L - a = 150, 200, 250 \) nm. The absolute values of the force are thus in good agreement with the measured values depicted in Fig.3c of \cite{1}.

We finally 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 \( a = 980 nm, d = 400 nm, d_1 = 196 nm \) (green line) and \( a = 1070 nm, d = 1000 nm, d_1 = 522 nm \) (blue line) and gives reasonable agreement with experimental points and the fit in Fig. 3d of \cite{1}.

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 \cite{13, 14, 15, 16}, 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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