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 [H. B. Chan, Y. Bao, J. Zou, R. A. Cirelli, F. Klemens, W. M. Mansfield, and C. S. Pai, Phys. Rev. Lett. **101**, 030401 (2008)] 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 proximity force approximation predictions.

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Introduction.—The availability of experimental setups 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, 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 mirror 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., [2–5]), for most other geometries exact calculations exist only for perfectly reflecting boundaries (see, e.g., [6]). 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 Letter [7], 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 [7].

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 formulas. 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%. 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 electric and magnetic fields can be written in the form

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

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

respectively. Let us first suppose the upper grating to be absent and consider a generalized conical diffraction prob-

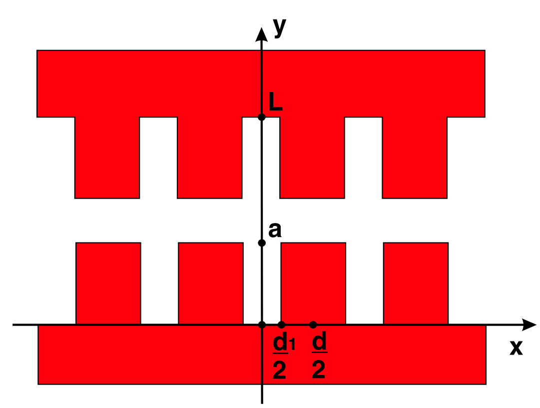

FIG. 1 (color online). Rectangular gratings geometry.

lem 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:

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

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

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

$$\alpha_n = k_x + 2\pi n/d, \qquad \beta_n^{(1)2} = \omega^2 - k_z^2 - \alpha_n^2, \quad (6)$$

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 and H_z. This solution is valid outside any periodic one-dimensional structure.

We now have to determine the coefficients $R_{np}^{(e)}$ and $R_{np}^{(h)}$ 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 $8N + 4$, $A^T = (E_z, E_x, H_z, H_x)$, 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 following expansions, valid for $y \leq 0$:

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

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

$$\beta_n^{(2)2} = \epsilon\mu\omega^2 - k_z^2 - \alpha_n^2. \quad (9)$$

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) and (4) at $y = a$ and expansions (7) and (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:

$$R_1(\omega) = \begin{pmatrix} R_{n_1 q_1}^{(e)}(I_p^{(e)} = \delta_{pq_1}, I_p^{(h)} = 0) & R_{n_2 q_2}^{(e)}(I_p^{(e)} = 0, I_p^{(h)} = \delta_{pq_2}) \\ R_{n_3 q_3}^{(h)}(I_p^{(e)} = \delta_{pq_3}, I_p^{(h)} = 0) & R_{n_4 q_4}^{(h)}(I_p^{(e)} = 0, I_p^{(h)} = \delta_{pq_4}) \end{pmatrix}. \quad (10)$$

Performing a change of variables $y = -y' + L$, $x = x' - s$ ($s < d$) in (3) and (4), it is possible to obtain the reflection matrix $R_{2\mathrm{up}}$ 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 Ref. [9], 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 Ref. [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

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

where ω_0 are zeros and ω_∞ are poles of the function $f(\omega)$ inside the contour of integration. Degenerate eigenvalues are summed over 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

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

Here $r_{1\mathrm{TE}}(\omega)$ is the reflection coefficient of a downward plane wave which reflects on a dielectric surface of slab 1 at $y = 0$, while $r_{2\mathrm{TEup}}(\omega)$ 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 $r_{2\mathrm{TEup}}(\omega) = r_{2\mathrm{TE}}(\omega) \exp(2ik_y L)$ [$r_{2\mathrm{TE}}(\omega)$ is a reflection coefficient of a downward TE plane wave which reflects on a dielectric slab 2 now located at $y < 0$].

From (12) and the analogous equation for TM modes, one immediately obtains the Lifshitz formula by making use of the argument principle (11).

For two periodic dielectrics separated by a vacuum slit, one has to consider a reflection of downward and upward waves from a unit cell $0 < k_x < 2\pi/d$. Because of 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 that

$$R_1(\omega_i)R_{2\mathrm{up}}(\omega_i)\psi_i = \psi_i, \tag{13}$$

where ψ_i is an eigenvector describing the normal mode with a frequency ω_i. Instead of Eq. (12), one obtains from (13) the following condition for eigenfrequencies:

$$\det[I - R_1(\omega)R_{2\mathrm{up}}(\omega)] = 0. \tag{14}$$

For every k_x and k_z the solution of (14) yields possible eigenfrequencies ω_i of the solutions of Maxwell equations that should be substituted into the definition of the Casimir energy $E = \sum_i \hbar\omega_i/2$. 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 (11), which yields the Casimir energy of two parallel gratings on a "unit cell" of period d and unit length in the z direction:

$$E = \frac{\hbar c d}{(2\pi)^3}\int_0^{+\infty} d\omega \int_{-\infty}^{+\infty} dk_z \int_0^{2\pi/d} dk_x \ln\det[I - R_1(i\omega)R_{2\mathrm{up}}(i\omega)], \tag{15}$$

where 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

$$R_{2\mathrm{up}}(i\omega) = K(i\omega)R_2(i\omega)K(i\omega), \tag{16}$$

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

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

with matrix elements $e^{-L\sqrt{\omega^2+k_z^2+[k_x+(2\pi m/d)]^2}}$, $m = -N, \ldots, N$, on a main diagonal of a matrix G. Note that in all Rayleigh expansions the Fourier basis is taken symmetrically around $m = 0$. When changing the maximum value of m from $N-1$ to N, each Rayleigh coefficient $R_{Np}(i\omega)$ appearing in the reflection matrices is multiplied by a factor $\simeq e^{-2\pi NL/d}$ coming from the matrix $K(i\omega)$. As a consequence, when $2\pi NL/d \gg 1$ is satisfied, the contribution of the coefficients $R_{Np}(i\omega)$ 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 $a = 100$ nm by making use of the formulas (15)–(17) and a Drude-Lorentz model for the dielectric permittivity of intrinsic silicon [5]. 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, $F_{\mathrm{PFA}} = \frac{1}{2} \times [F_{\mathrm{PP}}(L) + F_{\mathrm{PP}}(L-2a)]$. In particular, it is independent of the corrugation period d. To assess quantitatively the validity of the PFA, we plot the dimensionless quantity $\rho = \frac{F}{F_{\mathrm{PFA}}}$ [12]. The ratio is presented on Fig. 2. Exact and PFA results differ for silicon by up to 24% for a corrugation period of 100 nm, 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.* [7], who measured the Casimir force gradient between a silicon grating with nanostructured trenches and a gold sphere of radius $R = 50$ μm. 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 $F'_{\mathrm{PS}} = 2\pi R F_{\mathrm{PP}}$. This is why we show in Fig. 3 the zero temperature result for the absolute force values evaluated for a grating with the experimental parameters $a = 980$ nm, $d = 400$ nm, and $d_1 = 196$ nm placed in front of a gold plate (we used a plasma model

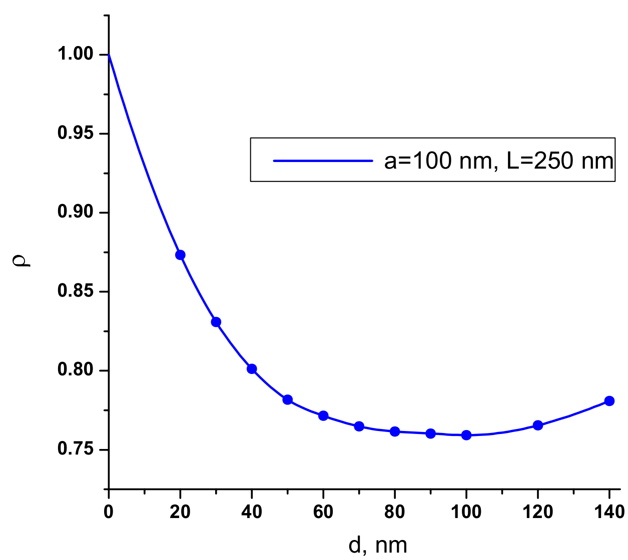

FIG. 2 (color online). Casimir force normalized by its PFA value for two Si gratings with $a = 100$ nm and $d_1 = \frac{d}{2}$ as a function of d at a fixed distance $L = 250$ nm.

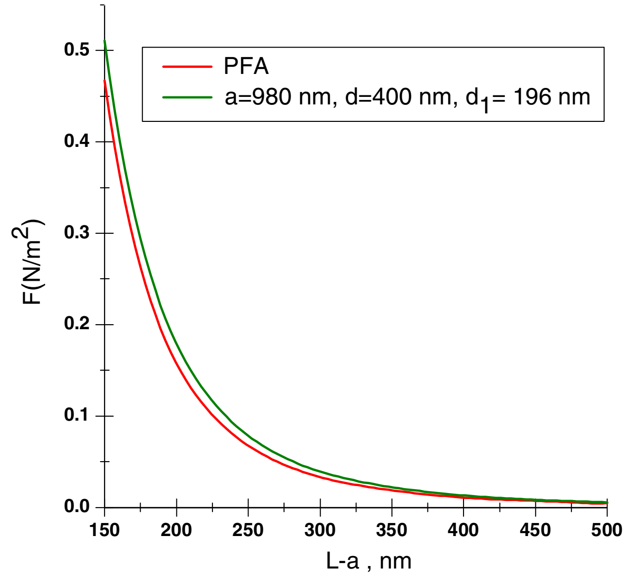

FIG. 3 (color online). Casimir force between a Si grating and a gold plate as a function of distance.

with a plasma frequency $\omega_p = 9$ eV for gold and a Drude-Lorentz model for intrinsic silicon [5]).

From our calculation, we obtain a force $F_{\mathrm{PP}} = 0.51\ \mathrm{N/m^2}$ for a plate separation of 150 nm. With the experimental parameters, this leads to a prediction for the Casimir force gradient of $F' = 160.8$, 56.4, and 24.6 pN/μm at, respectively, $L - a = 150$, 200, and 250 nm. The absolute values of the force are thus in good agreement with the measured values depicted in Fig. 3(c) of [7].

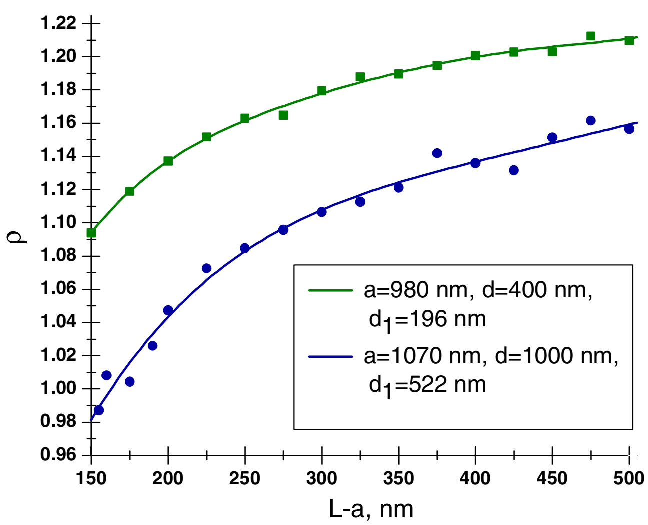

FIG. 4 (color online). Casimir force normalized by the PFA value between a Si grating and a gold plate as a function of distance for two different gratings. Solid curves are calculated by making use of the least square method from the theoretical points on the figure.

We finally present ratios of our results for the force to the predictions of PFA for two different gratings. Figure 4 shows ρ as a function of $L - a$ for two gratings corresponding to the experiment with $a = 980$ nm, $d = 400$ nm, and $d_1 = 196$ nm (green line) and $a = 1070$ nm, $d = 1000$ nm, and $d_1 = 522$ nm (blue line) and gives reasonable agreement with experimental points and the fit in Fig. 3(d) of [7].

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 [13–16]; 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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