Numeric corrections to the proximity-force approximation for lateral Casimir forces

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Abstract

We report a numeric investigation on the proximity-force approximation (PFA) for lateral Casimir forces between a sphere and a grating. Near-unity force correlations are found between the approximated force and the exact values, due to geometric effects. A minimal model yields a best-fit expression of the numeric correction to the PFA, for gratings in the dilute limit. Our results are not restricted to specific material of the sphere, and allows simple estimation of Casimir interactions for micro-scale spheres, and thus shall be useful in relevant experimental and engineering Casimir applications.

Keywords: Casimir effect, proximity-force approximation, electromagnetic scattering, lateral Casimir force

(Some figures may appear in colour only in the online journal)

1. Introduction

The Casimir force, resulted from the variation of the zero-point energy when fluctuating electromagnetic (EM) fields are perturbed by materials, is becoming increasingly important in micro- or nano-scale systems [1]. While it is originally predicted between two neutral parallel plates [2], the Casimir force is usually measured in sphere-plate configurations to avoid the problem of maintaining parallelism [3–5], where the gently curved sphere is theoretically modeled as a series of patches parallel to the plate and each patch is assumed to interact only with the part of the plate in its close proximity. This so-called proximity-force approximation (PFA) [6] relates the normal force between curved surfaces to the Casimir energy per unit area \(\mathcal{E}\) between corresponding parallel plates via

\[
F^\text{PFA}_n = 2\pi r \mathcal{E},
\]

and accurately describes the interaction strength in the small-curvature limit [7], i.e. \(\epsilon \equiv d/r \ll 1\), where \(r\) is the radius of the sphere and \(d\) is the surface-to-surface separation between the sphere and the plate. Since contributions of oblique waves to the Casimir force and the non-additivity property of the force are not taken into account directly (but through \(\mathcal{E}\)), the PFA is generally thought of as a rough treatment with uncontrolled errors [5, 8–11], especially for large \(\epsilon\) and for lateral Casimir forces [12]. There are evidences, however, that have put equation (1) on a firm ground. For instance, the semi-classical approximation in [13, 14] evaluates the Casimir energy based on classical periodic orbits like in geometrical optics, and recovers equation (1) within quantum field theory. References [15, 16] use multiple scattering formalism, confirm equation (1), and obtain the first-order correction beyond the PFA, \(F \equiv \eta_\alpha \times F^\text{PFA}_n\), \(\eta_\alpha = 1 + \frac{\alpha}{2} + \mathcal{O}(\epsilon^2)\). Describing a curved surface by a function \(\psi\) and regarding the Casimir energy as a functional of \(\psi\), [17] shows that the PFA coincides with the leading term of the derivative expansion of the Casimir energy, and also obtains the general form of the next-to-leading-order curvature correction. The coefficient \(\alpha\) varies, though, from \(-1.4\) [18, 19] obtained by fitting numeric data, to \(-1.69\) [16, 20] and to \(-5.2\) [21] obtained by different analytic approaches, for EM fields with perfect-conductor boundary conditions.

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Quantifying \( \eta \) allows simple and fast evaluation of Casimir interactions based on the PFA. This is important not only in cases of \( \epsilon < 0.1 \) where most experiments are involved and exact calculations become almost impractical [21], but also in emerging applications, such as probing field fluctuations using nanospheres [22] and Casimir transport of nanoparticles [23], where complicated plates (e.g. gradient gratings) are considered and rigorous computations become cumbersome. Modern methods including the scattering approach [24], the path-integral approach [25, 26] and the stress-tensor approach [27–29], in principle permit exact calculations of Casimir forces between arbitrary three-dimensional objects. While to the best of our knowledge, exact Casimir interactions between a sphere and a non-periodic inhomogeneous plate have not yet been reported. A recent attack [23] on that problem utilizes the re-construction technique which constructs a series of virtual metasurfaces and obtains the desired Casimir forces in an asymptotic manner. It is found that the convergence is especially slow for lateral Casimir forces at large separations, as shall also be detailed below. Exploring the link between lateral Casimir forces and the PFA, \( F_l \equiv \eta_l \times F_l^{PFA} \), hence becomes both fundamentally interesting and technically useful.

This paper focuses on lateral Casimir forces between a nanosphere and a one-dimensional grating, as schematically shown in figure 1, and reports an investigation on \( \eta_l \) for various filling factors \( f \) and radius-to-period ratios \( r/p \), in the deep-grating limit \( h \rightarrow \infty \) as in [23]. We restrict ourselves to \( \epsilon \geq 0.06 \) throughout this paper, and we decompose the lateral position of the sphere \( x \) by unit-cell period \( p \) as \( x \equiv j \times p + \bar{x} \), where \( j \) is the number of unit cells and \( \bar{x} < p \) is the relative position within a unit cell. \( f(j) \) is thus constant for periodic gratings and varying for gradient gratings. We confirm that \( F_l^{PFA} (x) \) severely deviates from \( F_l (\bar{x}) \), as previously reported for periodic gratings [12, 22], but find in a wide region in the parameter space near-unity correlations of them which suggests weak \( \bar{x} \) dependence of \( \eta_l \). This surprising result allows simple numeric corrections to the PFA. The outline of this paper is as follows. We start in section 2 by explaining how lateral Casimir forces are evaluated in both the scattering approach and the PFA. And we present the results of force correlations in section 3. Section 4 is devoted to the numeric corrections to the PFA for lateral Casimir forces. Section 5 discusses the case of gradient gratings. And we conclude in section 6.

2. Evaluation of the force

In the range of \( \epsilon \geq 0.06 \), the multiple scattering effect is negligible and the exact lateral Casimir force in the system under consideration could be simplified to the single-round scattering formula

\[
F_l = \frac{1}{\beta} \sum_{n=0}^{\infty} \sum_{\gamma} \int_{-\infty}^{\infty} (\mathbf{k}_\gamma, \mathbf{in}[\mathbf{R}_4 \cdot \partial_0 R_g \mathbf{k}_\gamma, \mathbf{in}]_\eta) d^3 \mathbf{k}.
\]

where \( \beta = 1 / k_0 T \), \( k_0 \) is the Boltzmann constant, \( T = 300 \) K is the room temperature, and \( \gamma = \text{TE or TM} \) represents polarization. The prime on the summation over Matsubara frequencies \( i \eta_n \equiv i \cdot 2 \pi n / \hbar \beta (h \text{ the reduced Planck constant}) \) indicates that the \( n = 0 \) term is weighted by 1/2. \( \mathbf{k} \) in the plane-wave basis \( |\mathbf{k}_\gamma, \mathbf{in}\rangle \) is the lateral wave vector in the \( x-y \) plane. And \( \mathbf{in} \) represents the propagation direction along the negative(positive) \( z \) axis. \( \mathbb{R} \) is the reflection operator, and from the translational transformation of \( \mathbb{R} \) we have

\[
\partial_0 R_g = i \mathbf{k} R_g - R_g \mathbf{k}.
\]

Equation (2) originates from the well-known trace-log formula of Casimir energy for a given system, \( \mathcal{E} = -\frac{1}{\beta} \sum_{\gamma} \text{trln}[\mathbb{I} - \mathbb{R}_g] \). And in the single-round scattering formula, the Fabry–Pérot factor \( 1/(1 - R_g) \) is ignored in calculations within 5% numeric error. The reflection operator of the sphere, observed in plane-wave states, is obtained by partial-wave transformations

\[
\langle \mathbf{k}_\gamma, \mathbf{in}| \mathbb{R}_g | \mathbf{k}' \mathbf{\gamma}', \text{out}\rangle = \frac{1}{2|k|} \frac{1}{K} \sum_{m=0}^{m_0} r \sum_{m=-l}^{l} \langle \mathbf{k}_\gamma, \text{out}|m Q, \mathbf{in}|k' \mathbf{\gamma}', \text{out}\rangle,
\]

where \( K = \omega_0 / c \) (c the speed of light in vacuum), \( |k| = \sqrt{K^2 + k^2} \), \( Q = E(M) \) in the spherical-wave basis \( |m Q, \mathbf{\gamma}\rangle \) denotes electric(magnetic) multipoles, \( \varphi = \text{in(out)} \) represents the inward(outward) propagation wave, and \( l \) and \( m \) represent angular momenta. \( r \) is the Mie coefficient, and \( \langle \mathbb{m} Q, \mathbf{in}|k' \mathbf{\gamma}', \text{out}\rangle \) can be found in [22, 30] (attention should be paid to different notations and different normalizations of bases). The reflection operator of the periodic grating is obtained by the modal approach (or rigorous coupled-wave analysis) [31]. With the help of the super-cell technique, modal approach can also be applied to gradient gratings [23]. For a given gradient grating, we re-construct a series of virtual metasurfaces (of super-cell dimension \( L_p \), as shown in figure 1) which asymptotically approach the gradient grating. Explicitly, in \( \alpha_\mathbb{R} (j = 1, 2, 3, \ldots) \)
run of computation, we cut a small patch (of dimension \(L_j = j \times p\), nearest to the sphere) of the gradient grating, and define it as a virtual super cell and periodically duplicate it to construct a virtual metasurface, based on which we can calculate the lateral Casimir force exerted on the sphere come from a small area of where

\[
g_{1} \text{ runs over all edges, and } F_{g} \text{ is determined by }
\]

Eventually we can recover the gradient grating when \(L_j \rightarrow L_p\), and obtain the desired force \(F_j\). Since major contributions of the Casimir force exerted on the sphere come from a small area of the grating nearest to the sphere, one can expect that the convergence is slower for patches of the sphere opposing flat areas of the grating give the same Casimir energy during virtual lateral shifts.

3. Force correlations

Starting with periodic gratings. By computing equations (2) and (10), we observe that \(F_j^{\text{PFA}}(\tilde{\eta})\) and \(F_j^{\text{PFA}}(\tilde{\eta})\) have near-unity correlations, in a wide region in the parameter space. Figure 3 shows \(\xi = \log_{10}(1 - \text{corr}(f_j(\tilde{\eta}), F_j^{\text{PFA}}(\tilde{\eta})))\), for various \(\epsilon\) and \(f_j\) and for different materials in the dense (we use gold for implementation) or dilute (we set \(\xi = 1.001\) limit). Data is obtained at \(r/p = 0.6\). It can be seen that, for dilute gratings \(\xi\) is widely below \(-3\) and for dense gratings \(\xi\) is widely below \(-2\). High correlations indicate weak \(\tilde{\eta}\) dependence of \(\eta\). This feature could partially be attributed to the geometry of the sphere. In fact, the correlation would drop if the sphere is replaced, for example, with a cube, since in that case the PFA would yield square-wave force profiles. In the sphere-grating case, \(\xi\) is found to increase with \(r/p\), as shown in figure 4. This is also irrelevant to specific materials and is a geometric effect, because when \(r/p\) increases, more edges contribute to the approximated lateral force. The dominant contribution comes from the edge which is nearest to the sphere, while contributions from other edges are the reason of complex force profiles and low correlations. Their relative weight of the side-edge contributions, compared with the dominant contribution, increases with \(d\) but decreases with \(p, d/p = r/p \times d/r = \text{const.}\) qualitatively characterizes the

\[
F_j^{\text{PFA}} = \lim_{b \rightarrow 0} \rho \partial_\rho l^{\rho} E = -\sum_i \hbar g_i \partial_\rho l^{\rho} E,
\]
Gold sphere and silica grating are used in these calculations. In all the above computations, the Au permittivity is obtained from a Drude model, 

\[ \varepsilon_{\text{Au}} = 1 + \frac{\Omega^2}{\varepsilon_0} (\varepsilon_\infty + \Gamma), \]

with plasma frequency \( \Omega = 1.28 \times 10^{16} \text{ rad s}^{-1} \) and damping constant \( \Gamma = 6.60 \times 10^{13} \text{ rad s}^{-1} \). The silica permittivity is fitted by Lorentz terms from tabular data [32]. In following cases where silicon shall be used, the Drude–Lorentz model is adopted to describe the permittivity with parameters given in [31]. The highest order of Matsubara frequency is set to be \( n \leq \frac{4000}{d_{\text{nm}}} \), and the highest order of angular momentum is set to be \( l \leq \frac{4}{\epsilon} \), to ensure convergence of \( F_l \).

4. Numeric corrections

We introduce two different functionals to characterize relative numeric errors of Casimir forces. Considering lateral Casimir forces, \( F_l(\xi) \) obtained by rigorous computations and \( F_l^{\text{PFA}}(\xi) \) obtained based on the PFA, the first functional describes the force residue

\[ \delta_1[F_l^{\text{PFA}}(\xi)] = \left| \frac{\langle F_l - F_l^{\text{PFA}} \rangle}{\langle F_l \rangle} \right|, \]

where \( \langle F \rangle \equiv \left( \int_0^\infty F^2 \, d\xi \right)^{1/2} \) is the norm of the considered force. For nanospheres, the lateral Casimir force is usually of the order of femto-Newton or even smaller and thus more feasible to be revealed by the dynamics of a sphere under its influence. The travel time of the sphere across a unit cell defines the second functional

\[ \delta_2[F_l^{\text{PFA}}(\xi)] = \left| \frac{t[F_l] - t[F_l^{\text{PFA}}]}{t[F_l]} \right|, \]

where \( t[F] = \int_0^\infty v^{-1}(\xi) \, d\xi, \quad v[F] = \sqrt{2(\langle E \rangle - E) / m}, \) and Casimir energy \( E(\xi) = -\int_\xi^\infty F(\tau) \, d\tau. \) \( E_0 \) is an initial energy and \( m \) is the mass of the sphere. This paper aims to study \( \eta_l \) numerically in the context of the above two types of errors.

We further restrict ourselves to dilute gratings. By computing \( F_l/F_l^{\text{PFA}} \) at a rising edge of a periodic grating, we show numeric values of \( \eta_l \) in figure 6. Dense or dilute spheres yield similar topography of \( \eta_l \), and this even holds for silica gratings with static permittivity up to \( \epsilon = 3.9 \). For the weak \( \xi \) dependence, we search a numeric correction to the PFA of the form

\[ \eta_l = 1 + (\chi_1 + \chi_2 f) \epsilon, \]

where \( \chi_1 = 0.2 \) and \( \chi_2 = 0.01 \) for silica gratings.
where coefficients £ may vary for different materials. The best fit of £ to equation (13) leads to (£1, £2) = 
(-1.32, -1.48 × 10^{-3}) for the dilute–dilute (sphे-
grating) case with at most (£1[£ PFA], £2[£ PFA]) =
(6.67%, 3.37%) in the ξ ≤ -3 region, and (£1, £2) =
(-1.26, -1.71 × 10^{-3}) for the dense–dilute case with at most
(£1[£ PFA], £2[£ PFA]) = (4.47%, 3.50%). For practical
purposes, averaging £1 and ignoring £2 (since f ≤ 1), i.e.

\( (\chi_1, \chi_2) \approx (-1.29, 0), \)  

(14)

should be the desired result for dilute gratings, which yields in
the ξ ≤ -3 region at most (£1[£ PFA], £2[£ PFA]) =
(7.50%, 3.67%) for the dense–dilute case, and at most
(£1[£ PFA], £2[£ PFA]) = (6.09%, 3.26%) for the dilute–
dilute case. Without the correction, we have, for example,
(£1[F PFA], £2[F PFA]) = (180.32%, 28.18%) for the dilute–
dilute case in the ξ ≤ -3 region, which reflects the effec-
tiveness of our numeric correction. In comparison, we find for
the Au–silica case (£1, £2) = (-0.98, -0.48) which yields in
the ξ ≤ -3 region, where we see apparent material dependence of £. In evaluating £2, we have set E0 as one percent of the Casimir energy barrier. Larger E0 leads to smaller £2.

5. Discussions

We then turn to gradient gratings of slow varying f(t), where lateral Casimir forces include displacement-induced and inhomogeneity-induced two components [23]

\[ F_i = A \cdot H(x/p) + B, \]  

(15)

where H is a certain periodic function of period 1 and of magnitude 1. The inhomogeneity-induced force B is of partic-
ular interest in transport applications. In such cases, f in £ could approximately take the value associated with the unit cell opposing the center of the sphere. And in this way, results of periodic gratings may also apply to gradient gratings at first glance. However, component B turns out to be beyond the proposed numeric corrections. Figure 7 shows sample data as comparisons of lateral Casimir forces based on the PFA with exact values, for both periodic (upper two panels) and gradient (lower two panels) gratings, before (left two panels) and after (right two panels) our numeric corrections. Relative errors are: (a): £1[F PFA] = 8.43%; (b): £1[F PFA] = 0.04%; (c): £1[F PFA] = 19.1%; and (d): £1[F PFA] = 5.76%, respectively. £2 is not discussed here for gradient gratings because the travel time may not be well defined. Though £ still minimizes the force residue, B predicted by the correction (0.078) is of 22.9% relative error, compared with the exact value (B = 0.1014). In fact, to model the inhomogeneity-induced lateral Casimir force, r/p ≫ 1 should be met so that the information of the gradient of f can enter into the PFA. This immediately leads to d/r ≫ 1, according to the above analysis, which is outside the £ > 0.06 range under consideration.

6. Conclusions

In conclusion, we have studied lateral Casimir forces between a nanosphere and a one-dimensional grating, with special attention paid to the PFA. We have observed high force correlations between approximated and exact forces, and proposed a numeric correction to the PFA in the dilute limit of gratings. This work extends the application of the PFA to previously unexpected regions, and can benefit future exper-
imental and engineering Casimir researches. Our findings also invite future investigations on the analytic expression of £ and its underlying physics.
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