Surface Screening in the Casimir Force

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Abstract

We calculate the corrections to the Casimir force between two metals due to the spatial dispersion of their response functions. We employ model-independent expressions for the force in terms of the optical coefficients. We express the non-local corrections to the Fresnel coefficients employing the surface $d_\perp$ parameter, which accounts for the distribution of the surface screening charge. Within a self-consistent jellium calculation, spatial dispersion increases the Casimir force significantly for small separations. The nonlocal correction has the opposite sign than previously predicted employing hydrodynamic models and assuming abruptly terminated surfaces.

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The Casimir force between two ideal mirrors a small distance apart is a manifestation of the quantum fluctuations of the electromagnetic field confined to the cavity within [1]. The study of vacuum forces among real materials began with Lifshitz [2] in 1956, who obtained a formula for the force between semi-infinite homogeneous isotropic local systems characterized by a frequency $\omega$ dependent dielectric function $\epsilon(\omega)$. Developments in micro- and nano-technologies have stimulated a renewed attention on the Casimir force. Deviations from the force between ideal mirrors are now measurable experimentally. The pioneering measurements of Lamoreux [3] had a 5% precision and 1% precision has now become common [4–7]. Distances down to $\approx 60\text{nm}$ have been explored [8]. Due to alignment difficulties, most experiments have involved spherical surfaces, while most theories have concentrated on the force between flat parallel surfaces for simplicity, so comparisons have resorted to the proximity theorem [9] which relates approximately the force between curved surfaces to that between flat parallel surfaces. Nevertheless, measurements of the force between flat surfaces have already been performed [10]. We expect that in the near future even better measurements at smaller distances will be produced. Therefore, manifold corrections have to be carefully evaluated in theoretical calculations, such as the finite conductivity of the metals [11–14], surface roughness [15, 16], finite temperatures [17, 18], grain structure [8], etc. In this paper we calculate non-local effects in the Casimir force. We employ density functional jellium calculations [19, 20] of the surface response functions which are consistent with realistic electronic density profiles that decay smoothly to zero beyond the nominal surface of the metal, instead of being artificially truncated abruptly [21, 22]. At very small distances the non-local corrections can be remarkably large. Within simple hydrodynamic models with abrupt surfaces [21, 22] nonlocal effects yield a diminution of the force apparently due to the possibility of exciting bulk plasmons at the surface of spatially dispersive metals. However, nonlocal corrections within self-consistent jellium theories have the opposite sign and yield an increase in the Casimir force, as most of the surface screening charge accumulates outside of the body of the conductor, as characterized with $d_\perp$ theory [19, 20].

It has been shown [21, 23] that Lifshitz formula [2], when written in terms of the exact surface impedances [24, 25] of the system, or equivalently, in terms of its optical reflection amplitudes [26],

$$F(L) = \frac{hc}{2\pi^2} \int_0^\infty dQQ \int_{Q>0} dk \frac{k^2}{q} \text{fRe} \left[ \frac{1}{\xi_s - 1} + \frac{1}{\xi_p - 1} \right], \quad (1)$$
is applicable to any system with translational invariance along the surfaces and isotropy around their normal [21, 23]. Here, \( F(L)/A \) is the force per unit area between two slabs with flat parallel faces a distance \( L \) apart, \( c \) the speed of light, \( q = \omega/c \) the wavenumber, \( \vec{Q} \) the projection of the wavevector parallel to the surface and \( k = \sqrt{q^2 - \vec{Q}^2} \) its component normal to the surface, \( \xi_\alpha = (r_\alpha^1 r_\alpha^2 e^{2 i k L})^{-1} \), \( r_\alpha^a \) the reflection amplitude of slab \( a = 1, 2 \) corresponding to the polarization \( \alpha = s, p \), and \( f = \coth(\beta \omega/2)/2 \) the photon occupation number at temperature \( T = 1/k_B \beta \). The integral over \( k \) in Eq. (1) goes from \( iQ \) towards 0 along the imaginary axis and then towards \( \infty \) just above the positive real axis, although it may be easily manipulated into a more convenient path along the imaginary axis.

Nonlocal effects [25] in the Casimir force have been calculated approximately [27] employing expressions for the surface impedance [13] which are only valid for good conductors at low frequencies [28], and they have been calculated from the density response function of semiinfinite metals within a semiclassical infinite barrier model [22]. However, they may be fully incorporated simply by plugging the appropriate reflection amplitudes into Eq. (1). The polarization induced at a given position \( \vec{r} \) within a non-local or spatially dispersive medium depends on the field that is applied at nearby positions \( \vec{r}' \) [25, 29], instead of depending exclusively on the field at \( \vec{r} \). Within the bulk of a homogeneous system, non-locality manifests itself as a dependence of the response functions on the wavevector besides their usual dependence on the frequency. Thus, spatial dispersion is expected to become important as the length scales associated to the field become small. A few consequences of spatial dispersion at metal surfaces, such as the anomalous skin effect [30], the excitation at surfaces of propagating plasmons [21], and the finite screening distance [22] of low frequency fields, have been studied in relation to the Casimir force, which they modify substantially at very small distances.

The most simple non-local model for the response of a metal is the hydrodynamic model [31, 32], in which a negative semiclassical electronic fluid is confined within a uniform positively charged region. The electrons interact with the macroscopic electric field and with the hydrodynamic forces derived from the pressure of the fluid. The longitudinal contribution to the bulk dielectric response in this model is

\[
\epsilon^L((\vec{Q}, k_t), \omega) = 1 - \frac{\omega_p^2}{\omega^2 + i \omega/\tau - \beta^2 (Q^2 + k_t^2)}, \tag{2}
\]

where the compressibility, related to \( \beta^2 = 3 v_F^2/5 \), is the source of the spatial dispersion.
Here, $v_F$ is Fermi’s velocity, $\omega_p$ the plasma frequency, $\tau$ a phenomenological lifetime, and $k_l$ is the component of the wavevector of the longitudinal wave normal to the surface, given by the longitudinal dispersion relation $\epsilon^L(\omega) = 0$. In this model, the reflection amplitude $r_s$ for $s$ polarized light agrees with that, $r^0_s$, of a local metal described by the Drude dielectric function $\epsilon^T(\omega) = 1 - \omega_p^2/(\omega^2 + i\omega/\tau)$. To calculate the reflection amplitude $r_p$ for $p$ polarized waves, the excitation of longitudinal waves at the surface has to be accounted for. This might be done by postulating the continuity of the component $E_\perp$ of the electric field normal to the surface as a physically reasonable additional boundary condition (meaning there is no singularity in the induced charge density), beyond the usual conditions derived from electromagnetic theory, and solving them for the amplitudes of the longitudinal transmitted field as well as the transmitted and reflected transverse waves, yielding

$$r_p = \frac{\epsilon^T k - k_m + Q^2(\epsilon^T - 1)/k_l}{\epsilon^T k + k_m - Q^2(\epsilon^T - 1)/k_l},$$

where $k_m = \sqrt{\epsilon^T q^2 - Q^2}$ is the normal component of the wavevector of the transverse wave transmitted into the metal [33]. The reflection amplitude $r_p^0$ for a local metal may be obtained from Eq. (3) by taking the limit $\beta \to 0, k_l \to \infty$.

In order to use more realistic models of metallic surfaces, we require expressions for the reflection amplitudes that may also be employed beyond the hydrodynamic model. We remark that non-local effects are expected to be important mostly within a thin region close to the surface of the metal, where the electric field varies rapidly from its value in vacuum to its bulk value. As the width of the selvedge is typically much smaller than the wavelength $\lambda$, $r_p$ may be calculated perturbatively[34]. Applying boundary conditions across the selvedge and employing the long wavelength approximation we obtain [19, 20]

$$r_p = r_p^0 \left[ 1 + \frac{2ik\epsilon^T}{\epsilon^Tk^2/Q^2 + 1}d_\perp \right],$$

where $d_\perp/\lambda$ is the small perturbative parameter and

$$d_\perp(\omega) \equiv \frac{\int dz(z\delta\rho(z))}{\int dz\delta\rho(z)},$$

is the position of the centroid of the induced charge density $\delta\rho(z)$ measured towards vacuum from the nominal surface of the metal [19], defined by the edge of the positive background. In a local model with an abrupt interface, there is a singular charge induced right at the surface, so $d_\perp = 0$. In non-local models with an abrupt termination the screening charge
occupies a finite region within the metal, so that \( d_\perp < 0 \), as may be confirmed within the hydrodynamic model, for which

\[
d_\perp = -\frac{i}{k_l}.
\]

(6)

In this case, \(-d_\perp\) may be regarded as the finite frequency generalization of the Thomas-Fermi screening distance. However, within more sophisticated models such as the self consistent jellium model [19, 20] with a smoothly terminated charge density profile, the screening charge may be localized on the outside of the surface, so \( d_\perp \) may become positive. Furthermore, surface dissipation yields a complex valued \( d_\perp \).

Linearizing the Casimir force (1) with respect to \( d_\perp \), we obtain an expression for the non-local correction

\[
\frac{\delta F(L)}{A} = \frac{2hc}{\pi^2} \int_0^\infty dQQ \int_{k>0} dk \frac{k^2}{q} f \text{Im} \left[ \left( \frac{e^T k d_\perp}{e^{T k^2 / Q^2} - 1} \right) \frac{\xi_p^0}{(\xi_p^0 - 1)^2} \right],
\]

(7)

where \( \xi_p^0 \) is the local limit of \( \xi_p \). This expression may be simplified at small distances for which retardation may be neglected, yielding

\[
\frac{\delta F(L)}{A} = \frac{2hc}{\pi^2} \int_0^\infty dQQ \int_0^\infty dq f \text{Im} \left[ \left( \frac{e^T d_\perp}{e^{T} + 1} \right) \frac{\xi_p^0}{(\xi_p^0 - 1)^2} \right],
\]

(8)

where we may further approximate \( \xi_p^0 = [(\epsilon + 1)/(\epsilon - 1)]^2 e^{2QL} \).

Fig. (1), calculated within the hydrodynamic model using the density parameter \( r^s = 1.59\text{Å} \) and the lifetime \( \tau = 400/\omega_p \) corresponding to Au[35], shows that the non-local correction decreases the Casimir force within the hydrodynamic model. At \( L = 60\text{nm} \approx 3c/\omega_p \), the closest distance for which measurements are available, the non-local correction amounts to \( \delta F/F \approx 0.5\% \), which is smaller [33] than the experimental error estimate of 1.75\% [8]. However, \( \delta F/F \) increases for shorter distances approximately as \( L^{-1} \) and may become of the order of 100\% at a few Å. Although non-local corrections seem too small to be noticeable in current experiments, they will become much more important at closer range.

We use now the hydrodynamic model as a test ground to appraise the results of the perturbative theory. In order to enhance the differences between the different approximations discussed above, in the right panel of Fig. 1 we show the corresponding nonlocal corrections scaled by the separation \( L \). For distances larger than \( L \approx 2nm \approx 0.1c/\omega_p \) there is a very good agreement between the perturbative and the exact hydrodynamic calculations; for that distance perturbative calculation produces a \approx 12\% error on the \approx 15\% nonlocal correction.
FIG. 1: Nonlocal correction to the Casimir force between Au flat surfaces (a-d) and between a flat and a curved surface (e), calculated within the hydrodynamic model using the exact (a) reflection amplitudes, retarded $d$-parameter theory using the dynamical values of $d_{\perp}(\omega)$ (b, e) and its static limit $d_{\perp}(0)$ (c), and the non-retarded $d$-parameter theory (d) as a function of the separation $L$ between plates. The left panel shows the normalized correction $-\delta F/F$ and the right panel shows the correction $(-\delta F/F)(L\omega_p/c)$ scaled by the separation $L$.

We also show in Fig. 1 that the corrections to the force between a plane and a sphere [8] are similar to those for flat surfaces.

The non retarded calculation also yields similarly good results up to distances $L \approx 20\text{nm} \approx c/\omega_p$, and although it overestimates the corrections by up to $\approx 20\%$ at larger distances $L \approx 10c/\omega_p$, they are themselves negligible $\delta F/F < 0.1\%$ at those distances. Finally, we calculated the nonlocal corrections employing the perturbative theory but substituting the static value $d_{\perp}(0)$ instead of the dynamic value $d_{\perp}(\omega)$. In this case, the nonlocal correction is further overestimated but by not more than $20\%$ if $L > 0.1c/\omega_p$.

As the vacuum fluctuations of the electromagnetic field within a cavity are correlated to fluctuations in the charges and currents induced at the surfaces, the $p$-polarization contribution to the Casimir force may be interpreted as due to the force between fluctuating
charges in one surface and their images charges at the opposite surface. Within nonlocal optics, the charges induced at a surface are not at the nominal surface, but are actually spread over a finite region whose centroid lies a distance $d_{\perp}$ from the nominal surface. At low frequencies, the position of the centroid corresponds to the effective image plane [19]. Thus, we may expect that the force between nonlocal media is similar to the force between local media but separated by an effective distance $L' = L + \delta L$. As $F \propto L^{-3}$ at small distances, $\delta F/F \approx -3\delta L/L$, which allows to identify $\delta L \approx -0.006c/\omega_p \approx -2d_{\perp}(0)$ from Fig. 1. Thus, nonlocal effects amount to displacing each surface a distance $\sim d_{\perp}$ towards each other. Since in the hydrodynamic model $d_{\perp} < 0$, the effective separation is larger than the nominal separation and nonlocality decreases the force.

Although very simple and amenable to analytical solutions, the hydrodynamic model for an abruptly terminated electron gas is not considered a realistic model of metal surfaces. It doesn’t account for the fact that electrons spill across the nominal surface, giving rise to a static surface dipole which is the source of the confinement potential, nor the density oscillations due to the quantum interference between the incoming and outgoing wavefunctions of electrons reflected at the surface. Landau damping due to excitation of electron-hole pairs and many body effects such as exchange and correlation are also absent. Nevertheless, much more sophisticated models of metal surfaces have been developed [19, 20], and have been employed to calculate $d_{\perp}$ for manifold metals. In the jellium model, the Schrödinger-like Kohn-Sham equations [36] of density functional theory are solved within the local density approximation (LDA) to obtain the selfconsistent wavefunctions and ground state density of electrons which interact with an abruptly terminated semiinfinite homogeneous positive background. Their response to a perturbing electric field may then be obtained using time dependent LDA, and $d_{\perp}$ may be calculated from the ensuing density-density response function [20] using Eq. (5).

In Fig. (2) we show the nonlocal corrections to the Casimir force for metals of various density parameters $\sigma^a$ [35] calculated within the self consistent jellium model obtained by plugging the corresponding known values of $d_{\perp}(0)$ [20] into Eq. (7). In contrast to the previous hydrodynamic results, in this model the nonlocal effects increase the Casimir force since most of the screening takes place in the low density region on the outside of the nominal surface, i.e., $d_{\perp} > 0$ and the effective distance $L'$ is smaller than the nominal distance $L$. We remark that in the hydrodynamic model the ground state electronic density is constant up
FIG. 2: Normalized nonlocal corrections to the Casimir force calculated for the selfconsistent semiinfinite jellium model using the LDA for different densities corresponding to $r^*/a_B = 2, 3, 4,$ and 5.

In summary, we have calculated the nonlocal corrections to the Casimir force between metals using a generalization of Lifshitz formula in terms of reflection amplitudes which has been proved to be applicable to arbitrary materials that are homogeneous and isotropic along the surface. A perturbative theory in which the width of the selvedge divided by the relevant wavelengths plays the role of small parameter is a useful approximation for distances that are not too small, and yields an interpretation of the nonlocal effect in terms of an effective separation between the metal surfaces. The exactly solvable hydrodynamic model predicts a diminution in the force as the effective separation increases due to the finite screening.
length of spatially dispersive metals. Contrariwise, the jellium model yields an increase of the Casimir force due to the spilling of electrons out of the metals and into vacuum, and to the fact that most of the screening takes place in the resulting low density region outside of the nominal surfaces, thus reducing the effective separation. \( |\delta F/F| \) grows roughly as \( L^{-1} \) and thus becomes very important at distances smaller than \( \sim 100 \text{nm} \). As the surface screening may be manipulated through the adsorption of overlayers [20], our results suggest that the Casimir force at small distances may be tailored. Other surface corrections, such as the surface local field effect [37] may easily be incorporated into Casimir force calculations simply by replacing the Fresnel coefficients \( r_p \) and \( r_s \) in Eq. (1) by the appropriate nonlocal, surface-corrected expressions [34] instead of Eqs. (3) or (4). We hope our results stimulate experiments exploring such small distances.

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[33] Notice that that Eq. (14) of Ref. [21] is wrong. Furthermore, the horizontal axis in Fig. 2 of Ref. [21] is mislabeled and off by a factor of 2\pi; it should have been L\omega_p/c. Additionally, the
results for Au in Fig. 2 of Ref. [21] were calculated with the parameter $\beta = \sqrt{1/3}v_F$ instead of $\sqrt{3/5}v_F$ as in the present manuscript. See Raul Esquivel, Carlos Villarreal, and W. Luis Mochán, *Erratum: Exact surface impedance formulation of the Casimir force: application to spatially dispersive metals [Phys. Rev. A 68, 052103 (2003)],* Phys. Rev. A. 71, 029904 (2005).


