The effects of surface electronic structure on Casimir interaction at short range

Hua-Yao Wu
Department of Physics, SUNY Oswego, Oswego, NY 13126, United States of America
E-mail: huayaowu@oswego.edu
Keywords: Casimir effect, van der Waals force, nonlocal effect, divergence, Jellium model, tunneling effect, subwavelength

Abstract
We present a comprehensive model for analytically investigating the nonlocal and tunneling effects on Casimir interaction at short range for two metallic planes. The plates in this approach are described by free-electron gases constrained in semi-finite potential wells without imposing any macroscopic permittivity properties. Charge density distributions corresponding to the potential wells are calculated analytically to include the effects of spatial dispersion. We show that the Casimir energy in this limit highly depends on the electronic structure near the surface boundary. The usual Lifshitz’s formula with macroscopic permittivity models can be recovered in the limit of bulk density function while the interaction appears to be largely suppressed as incorporating the nonlocal (real) density function. We also show that the divergences for zero distance can be eliminated in this model. A finite and sensible result is then obtained. Finally, the results are compared with the well-known Lifshitz’s formula at zero temperature.

1. Introduction
In 1948, Casimir [1] obtained his famous result that the attractive force between two neutral parallel conducting plates arises due to electromagnetic zero-point fluctuations. His approach was soon generalized to a unified description of both the van der Waals (vdW) interaction, London dispersion force, between atoms and the Casimir interaction between planar dielectrics by Lifshitz [2] and Schwinger [3]. The theory has had enormous success in describing this fluctuation-induced force in the long-wavelength, large separation, limit based on the local description of the dielectric functions. Nevertheless, at short distances, the idealization of bulk permittivity is not adequate to describe the electronic responses. Naively calculating the Casimir/vdW interaction with such macroscopic models is therefore not physically sound and leads to divergences as the separation $a \to 0$.

The Ultraviolet (UV) problems arose at short-wavelength, small separation, limit can be traced to the unphysical boundary conditions utilized at high energy regime. The energy scale of the local dielectric function, i.e. plasma or Drude model, is the plasma frequency $\omega_p$. Descriptions of electromagnetic interactions with materials by employing these bulk dielectric responses are therefore not reasonable and justified for momentum and energy transfers much above the plasma frequency $\omega_p$. The main issue arose in the local description of the dielectric model is that it depends only on the frequency of the incident photon and has no restriction on its momentum $k$. Resumming these high momentum contributions to the zero-point energy thus would be not physical and reliable whether the results diverge or not. From a fundamental point of view, this means a more realistic modelling of the surface boundary that includes the short distances phenomenon, such as electron tunneling and nonlocal effects, need to be constructed and employed. Similar problems can be found when calculating the Casimir energies for the objects or surface structures with small length, $a \ll 1/\omega_p$, scale [4, 5] where the high momentum contributions dominate the interaction.

As a system’s length scale decreases, its optical response becomes more and more sensitive to the electronic structure near surface boundaries. The inhomogeneity in the surface charge distribution gives rise to the spatial dispersion in its permittivity. This nonlocal (wave-vector dependence) effect to the nano-optics and Casimir
interaction has been studied by a number of authors using different approaches including: the phenomenological methods [6–8], random-phase approximation [9, 10], and computational self-consistent jellium model [11–13]. They examined the nonlocal effects at relative large separations, $a \gg 1/\omega_p$, and found the corrections are almost negligible ($\sim 1\%$). In this study, we address the related but somewhat different issue. We investigate the effects of spatial dispersion and electron tunneling at smaller distances $a \ll 1/\omega_p$. Emphasis will be placed on the UV behavior of the Casimir/vdW interaction as $a \rightarrow 0$.

At short ranges, the most relevant photons possess energies and momentum much higher than the binding energies of the electrons in metallic materials. In this energy scale the plasmonic systems behave more like an electron gas rather than bulk materials. As a result, the usual description of Casimir/vdW interaction employing the model of electromagnetic scattering with macroscopic media does not hold and one should consider the more fundamental approach of electron-photon scattering from the first principle of QED. The idea of deriving Casimir interaction from the point of this free-charge model has been studied using both statistical and quantum mechanical approaches [14–17]. The model prevents the divergence in calculating the Casimir energy as $a \rightarrow 0$ and suggests an effective cutoff distance in the order of atomic dimensions ($\sim 1\, \text{Å}$). This can be understood since the average distance, $r_s$, between the valence electrons in the dielectric is about this length scale. The spatial dispersion of the charges therefore sets an upper bound to the momentum transfers $k \sim 1/r_s$ for the electron-photon scattering. Similar conclusion can also be obtained by using the thermodynamic requirements [18]. In our model, we will demonstrate that this cutoff scale relates to the Fermi wave-vector, $k_F$, in the metallic system.

In this paper, we present a simple but comprehensive approach to analytically investigate the asymptotic behavior of the Casimir interaction between two metallic planes based on the free-electron jellium model. The article is organized as follows. In section 2 we obtain the quantum-mechanical expression for the Casimir energy in terms of fluctuating charge-charge interaction without imposing any macroscopic permittivity models. In section 3 we show that the usual Lifshitz’s result with local dielectric function can be recovered by employing the bulk charge density function of the materials. We also show that the UV divergence at zero distance can be traced to the unphysical contributions from the reflection coefficient of TM modes in the high momentum regime. In section 4 the near-surface charge density distributions corresponding to a finite potential well are derived to capture the nonlocal and tunneling effects. We renormalize the theory by subtracting the single-body contribution originating from the symmetric (S) mode of the density function. The result is then free from divergence at zero distance and sets an upper bound to the zero-point interaction in this model. Section 5 presents our results for gold plates and compares them to the Lifshitz’s theory.

2. Formulation of the problem

We begin by considering the regular configuration of two semi-infinite metallic planes 1 and 2 separated by vacuum, $\varepsilon_0 = \mu_0 = 1^1$, of distance $a$ shown in figure 1. We focus our attention on the Casimir/vdW interaction in the nonretarded regime where the nonlocal and tunneling effects are significant. The system can be described by a non-relativistic Hamiltonian written as

$^1$ We set $\hbar = c = 1$ and adopt Heaviside-Lorentz units for electromagnetic quantities, $\varepsilon_0 = \mu_0 = 1$ and $\varepsilon^2/4\pi \sim 1/137$. 

The unperturbed Hamiltonian, $H_0$, consists of two parts $H_0 = H_0^0 + H_0^{EM}$. $H_0^{EM}$ describes the energy of the electromagnetic field in vacuum while $H_0^0$ represents the electron kinetic energy and all the electrostatic interactions between the electron-electron, ion-ion, and electron-ion within each slabs. For the simplest jellium model, these electrostatic interactions compensate each other and the metallic slabs can be approximated by non-interacting electron gases confined in some potential barrier. We modeled the potential boundaries, $\vec{\varphi}$, by the finite potential wells shown in figure 1. The perturbed potential $V$, in equation (1), is the correlated electromagnetic interaction between the free-electron gases within dielectrics $I$ and $II$, which in Coulomb gauge $\nabla \cdot \vec{A} = 0$ can be written as

$$V = \sum_i \left\{ -\frac{e}{m_i} \vec{A}_i \cdot \vec{p}_i + \frac{e^2}{2m_i} \vec{A}_i^2 \right\}$$

where $e$, $m_i$, and $\vec{p}_i$ are respectively the charge, mass, canonical momentum of the electron, and $\vec{A}$ is the vector potential. This interaction represents the multiple-loop scattering between disjoint objects and gives rise to the Casimir energies of the system. The model presented in figure 1 is an approximation in the sense that it simulates the electrostatic boundary potential in terms of the square-like potential wells $\vec{\varphi}$. For more rigorous calculation [19], this boundary potential and the corresponding surface charge distribution should be acquired self-consistently since they depend on each other. Nevertheless, this model should give a reasonably qualitative description as it is able to capture the dispersion and tunneling effects near the surfaces. Moreover, contrary to other computational approaches such as density functional theory, it allows analytic investigation of the nonlocal and tunneling effects to the Casimir/vdW interaction at short distances, $a \ll \omega_p$ as the electron density function, $n_e^0(z_j)$, $\nu = 1, 2$, can be obtained analytically. The Casimir energy of this configuration is thus defined as the shift of the zero-point energy due to the fluctuating charge-charge interaction between $n_e^0(z_1)$ and $n_e^0(z_2)$. Taking $H_0$ as the unperturbed Hamiltonian, the change of the zero-point energy, $V = V^0 + V^{ph} = \sum_i \left\{ -\frac{e}{m_i} \vec{A}_i \cdot \vec{p}_i \right\} + \sum_i \left\{ \frac{e^2}{2m_i} \vec{A}_i^2 \right\}$, can be evaluated perturbatively in the form of Dyson expansion of S-matrix,

$$S = 1 + \sum_{n=1}^{\infty} \left( -\frac{i}{n!} \right) \int ... \int dx_3 ... dx_n T \{ V(\vec{x}_1) ... V(\vec{x}_n) \}.$$  

where $T$ is the time ordering operator, $V^0 = \sum_i \left\{ -\frac{e}{m_i} \vec{A}_i \cdot \vec{p}_i \right\}$, and $V^{ph} = \sum_i \left\{ \frac{e^2}{2m_i} \vec{A}_i^2 \right\}$.

The first order contribution of equation (3) comes from the interaction proportional to $\vec{A}^2$ while $\vec{A} \cdot \vec{p}$ contributes to the second order. We here are interested in the regime where the frequency, $\omega \sim 1/a$, of the most contributed photon is much larger than the plasma frequency $\omega_p$ of the electron but very small compared to the electron rest energy $mc^2$. In this scale, the Kramers-Heisenberg polarization contribution, $V^p$, makes a relatively small contribution [20] to the electron-photon scattering. We will thus focus on the shift of the ground state energy due to the point scattering of the electromagnetic field, $V^{ph}$, and neglect the dynamic effect of the electrons $V^s$. The quantization of the electromagnetic field in the absence of net charges and currents can be achieved by replacing the vector potential $\vec{A}(\vec{x}, t)$ with the time-dependent operator confined to a volume $V$ in free space

$$\vec{A}(\vec{x}, t) = \sum_k \sum_{n=0}^{\infty} \left( \frac{1}{2V\omega_0} \right)^{1/2} e_{\nu}(k)[a_{\nu}(k)e^{i(k\vec{x}-\omega_0t)} + a_{\nu}^+(k)e^{-i(k\vec{x}-\omega_0t)}],$$

where $e_{\nu}(k)$ is the polarization vector, and the annihilation $a_{\nu}$ and creation $a_{\nu}^+$ operators satisfy the commutation relations, $[a_{\nu}, a_{\nu}^+] = [a_{\nu}^+, a_{\nu}^+] = 0$ and $[a_{\nu}, a_{\nu}^+] = \delta_{\nu\nu}$. The system is assumed to be in the composite state $|\rho\rangle$ with the electron in state $|0\rangle$ and the electromagnetic field in its vacuum state $|0\rangle$ where $a_{\nu}|0\rangle = 0$. In this model, we consider the scenario of electron-photon scattering in free space since the medium is not subject to any macroscopic dielectric models. The scattering intensity is purely determined by the density distribution of the charges. In this sense, there is no sharp interface causing an abrupt change in system’s dielectric properties. Instead, the effective dielectric response varies gradually corresponding to the changes in the electron density distribution near the surface. This leads to a more realistic boundary condition especially for the objects with small length scale. The charge density function, on the other hand, incorporates the knowledge of surface electronic structure, therefore, the effects of spatial dispersion and electron tunneling are included. We will show that this microscopic approach relieves the divergences at short distances, in the meantime, the bulk optic response can also be recovered in the low energy, large wavelength, limit.

The leading correction to the zero-point energy is given by the first order perturbation in equation (3) that is the quadratic term $\vec{A}^2$ in the vector potential $E^{(1)}_c = \langle 0 | \frac{e^2}{2m} \vec{A}^2 | n_e^0 \rangle$, where $n_e^0$ is the electron density operator corresponding to the potential wells as in figure 1. From the macroscopic points of view, this one-point correlated contribution and all the similar higher order tadpole corrections normally can be dropped since they are not considered as the correlated interaction between disjoint objects and are independent of the separation.
Nevertheless, due to the tunneling effect near the surface, the contributions could be physical and \( a \)-dependent at short distances. It represents the parts of energies to rearrange the charge density configuration, \( n^e_2 \), due to the change in separation \( a \). It is purely a quantum mechanical effect as it depends on the distribution of the tunneling density ‘tail’ outside of the surface boundary. However, for the purpose of the discussion presented here, we will drop this single-body contribution and focus on the correlated-interaction between two disjoint dielectrics for the comparison with the Lifshitz’s model.

The second order interaction of equation (3) arises from the two-points correlated scattering between two dielectrics, \( z_1 > 0 \) and \( z_2 < 0 \). The Casimir energy density thus can be calculated as

\[
E_c^{(2)} = \frac{1}{iT \bar{A}} \left\{ \frac{(-i)^2}{2!} \int d^4x_1 \int d^4x_2 \mathbf{T} \left( n^i_1 V^p (x_1) n^e_2 V^p (x_2) \right) \right\},
\]

(5)

where \( \bar{A} \) is the plane’s surface area and \( T \) is the time. Using the quantized vector potential, \( \mathbf{A}(x, t) \), in equations (4), (5) can be evaluated at the poles of the photon propagators located at the second and fourth quadrant by performing an Euclidean rotation and switching to imaginary frequency \( \omega \rightarrow i \zeta \)

\[
E_c^{(2)} = \frac{-1}{2} \sum_{a, a'} \int_{-\infty}^{\infty} \frac{d\zeta}{2\pi} \int \frac{d \mathbf{k}_1}{(2\pi)^2} (e_{\alpha}(\mathbf{k}_1) \cdot e_{\alpha}(\mathbf{k}_2))^2 \int_{-\infty}^{\infty} dz_2 \int_{-\infty}^{0} dz_1 e^{-2i\zeta(z_2 - z_1)} \left( \frac{e^2n^i_1(z_2)}{m} \right)^2 \left( \frac{e^2n^e_2(z_2)}{m} \right)^2
\]

(6)

where \( \zeta = \sqrt{\zeta^2 + k_1^2} \). The product of the polarization vectors at the pole values, \( \mathbf{k}_1 = (k_1, i\sqrt{\zeta^2 + k_1^2}) \) and \( \mathbf{k}_2 = (k_2, -i\sqrt{\zeta^2 + k_2^2}) \), defines the TE and TM modes, \( O_{TE} \) and \( O_{TM} \),

\[
\sum_{\alpha, \alpha'} (e_{\alpha}(\mathbf{k}_1) \cdot e_{\alpha}(\mathbf{k}_2))^2 = 1 + \frac{(\mathbf{k}_1 \cdot \mathbf{k}_2)^2}{k_1^2 k_2^2} = 1 + \left( \frac{2\zeta^2}{\zeta^2} - 1 \right)^2 = O_{TE} + O_{TM}
\]

(7)

3. Bulk dielectric response

The \( z_1 \) and \( z_2 \) integrations of equation (6) depend on the density distribution, \( n^e_2(z_2) \), of the free electron in \( z \) direction. In the limit where the separations are much larger than the Fermi wavelength, \( a \gg \lambda_F \), of the dielectric, the tunneling effect is negligible. The free electron distribution, \( n^e_2(z_2) \), in this case can be represented by the step function indicating the boundaries of the planes at \( z_{\min} = a/2 \) and \( z_{\max} = -a/2 \),

\[
n^e_1(z_1) = n_0 (z_1 - a/2) \quad \text{and} \quad n^e_2(z_2) = n_0 (z_2 - a/2)
\]

(8)

where \( n_0 = \frac{\rho_n}{m} \) is the bulk electron density which only depends on the Fermi wave-vector, \( \mathbf{k}_f \), at zero temperature. We can then derive the Casimir energy by using the density function of equations (8) in (6)

\[
E_c^{(2)} = \frac{-1}{2} \int_{-\infty}^{\infty} \frac{d\zeta}{2\pi} \int \frac{d \mathbf{k}_1}{(2\pi)^2} (n^e_1 z_1 \cdot n^e_2 z_2)^2 e^{-2i\zeta}
\]

(9)

where \( r^p = TE, TM \), represents the reflection coefficients. It is given by summing all the multiple-scattering events within each dielectric,

\[
r^p_T = \sum_{n=1}^{\infty} (R^p_T n) = \frac{\omega^2 p}{4\zeta^2 + \omega^2 p} \quad \text{and} \quad r^p_T = \sum_{n=1}^{\infty} (R^p_T n) = \frac{\omega^2 p}{2\zeta^2 + \omega^2 p} \left( 1 - \frac{\zeta^2}{2\zeta^2} \right)
\]

where \( R^p_T = -\frac{\omega^2 p}{4\zeta^2}, R^p_T = -\frac{\omega^2 p}{4\zeta^2} \left( 2\zeta^2 + \omega^2 p \right)^{-1} = 1 \), \( n = 1, 2, \) and \( \omega p_1 \equiv \frac{m e^2}{\zeta}, \omega p_2 \equiv \frac{m e^2}{\zeta} \)

(10)

Equation (9) can be recognized as the lowest order in the loop expansion of the zero-point energy correlating two plates. The higher order corrections can be obtained by using equation (3) and can be summed in terms of the logarithm expansion for small \( r^p \),

\[
E_c = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\zeta}{2\pi} \int \frac{d \mathbf{k}_1}{(2\pi)^2} \left[ \ln(1 - r^p_T^2 z_2 e^{-2i\zeta}) + \ln(1 - r^p_T^2 z_2 e^{-2i\zeta}) \right]
\]

(11)
We now compare the results, equation (11), with the well-known Lifshitz’s expression for two parallel planes

\[
E_i = \frac{1}{2} \int_{-\infty}^{\infty} dq \int \frac{dk}{(2\pi)^2} \left[ \ln(1 - \gamma_{1,1}^{\text{TE}} e^{-2i\nu}) + \ln(1 - \gamma_{1,1}^{\text{TM}} e^{-2i\nu}) \right]
\]

where \( \gamma_{1,1}^{\text{TE}} = \frac{\kappa - \kappa_{iv}}{\kappa + \kappa_{iv}} \) and \( \gamma_{1,1}^{\text{TM}} = \frac{\varepsilon_{iv} \kappa - \kappa_{iv}}{\varepsilon_{iv} \kappa + \kappa_{iv}} \) with \( \kappa_{sv} = \sqrt{\varepsilon_{sv} \kappa^2 + k_{1,1}^2} \).

Equations (11) and (12) have the same expression with slightly different reflection coefficients \( r_{sv}^\text{TE} \) and \( r_{sv}^\text{TM} \). We here employ the plasma model \( \varepsilon_{iv} = 1 + \omega_{p,sv}^2 / \kappa^2 \) for the dielectric permittivity in Fresnel reflection coefficients \( r_{sv} \) in equation (12) and neglect the finite conductivity effects. \( r_{sv}^\text{TE} \) and \( r_{sv}^\text{TM} \) in this case approach to the same high-momentum limit, \( \kappa \to \infty \), as

\[
r_{sv}^\text{TE} \to r_{sv}^\text{TE} \to \frac{-\omega_{p,sv}^2}{4\kappa^2} \text{ and } r_{sv}^\text{TM} \to r_{sv}^\text{TM} \to \frac{-\omega_{p,sv}^2}{2\kappa^2 + \omega_{p,sv}^2}.
\]

This indicates equation (11) recovers Lifshitz’s results equation (12) at short distances shown as the inset of figure 3. One can show that in this limit the Casimir force is proportional to \( 1/a^3 \) [21]

\[
F_i = -\frac{H}{6\pi a^3} \quad \text{and} \quad H = \frac{3}{8\pi} \int_0^\infty d\zeta \int_{-\infty}^{\infty} y^2 dy \left( (\gamma_{1,1}^{\text{TM}})^2 e^y - 1 \right)^{-1}
\]

where \( y = 2\kappa \) and \( H \) is the Hamaker constant. It is clear from equation (13) that the divergence at zero distance arises due to lacking effective UV cutoff in the transverse momentum \( k_{1,1} \) to the reflection coefficient of TM modes. The result that \( \gamma_{1,1}^{\text{TM}} \) remains as a constant for arbitrary high momentum, \( k_{1,1} \to \infty \), is not physical due to the fact that the external photons can only couple to the electronic excitation up to the fermi energy. The scattering intensity therefore should be largely suppressed as \( k_{1,1} \gg k_f \). We will see this cutoff momentum will automatically emerge from the dispersion of the electron density near surface boundaries.

4. Nonlocal and tunneling effects

As the separation decreases, the main contributions to the Casimir energy arise from the photons with short wavelength \( \lambda \sim a \sim \lambda_f \). In this limit, the optical response is sensitive to the electron density distributions near the surface boundaries. We here compute the density function, \( n_s(z) \), from the electron wave-functions satisfying the semi-infinite potential wells \( \Phi(z) \)

\[
\left\{ \frac{P^2}{2m} + \Phi(z) \right\} \psi_n = \epsilon_n \psi_n
\]

with

\[
\Phi(z) = \begin{cases} \bar{\psi}, & \bar{a} > z > -\frac{\bar{a}}{2} \\ 0, & \frac{\bar{a}}{2} > L > z > \frac{\bar{a}}{2} & \text{and} & -\frac{\bar{a}}{2} > z > -L - \frac{\bar{a}}{2} \\ \infty, & z > \frac{\bar{a}}{2} + L, & \text{and} & z < -L - \frac{\bar{a}}{2} \end{cases}
\]

The wave-functions in region I, II, and III of figure 1 are written as

\[
\psi_{n,I} = B_s \sin \left( q_{n1}^I \frac{z - L - \frac{a}{2}}{2} \right), \quad \psi_{n,II} = B_s \sin \left( q_{n1}^I \frac{z + L + \frac{a}{2}}{2} \right), \quad \text{and} \quad \psi_{n,III} = C_s e^{\sigma_{n1}^I z} + e^{-\sigma_{n1}^I z}
\]

where \( q_{n1}^I = (q_{n1}^s, q_{n1}^a) \) is the electron momentum, \( \sigma_{n1}^I = \sqrt{2m\bar{\psi} - q_{n1}^s^2} \) and \( \sigma = s, a \) as represents the symmetric (S) and antisymmetric (AS) modes. The continuity and differentiable of the wave-functions at the boundary, \( z = \pm a/2 \), define the eigenfunctions for \( \psi_n^I \) and \( \psi_{n1}^I \):

\[
F_{1}(q_{n1}^I) = \tan(q_{n1}^I L) + \frac{q_{n1}^a}{\sigma_{n1}^I} \coth(q_{n1}^I \frac{a}{2}) = 0 \quad \text{and} \quad \frac{F_{1}(q_{n1}^I) + q_{n1}^a}{\sigma_{n1}^I} \tanh(q_{n1}^I \frac{a}{2}) = 0
\]

In the limit of semi-infinite plates \( L \to \infty \), the wave-function coefficients reduce to

\[
B_s = B_{sa} = \frac{\Gamma}{L}, \quad C_s = \frac{\Gamma}{L \cosh(q_{n1}^a \frac{a}{2})}, \quad \text{and} \quad C_{a} = -\frac{\Gamma}{L \sinh(q_{n1}^a \frac{a}{2})}
\]
with the normalization condition
\[
\sum_{\sigma} \left\{ \int_{-a/2}^{a/2} |\psi_{n,\sigma}^0(z)|^2 dz + \int_{-a/2}^{0} |\psi_{n,\sigma}^0(z)|^2 dz \right\} = \frac{1}{2} \quad (20)
\]
The electron density function can then be calculated by taking the square of the wave-functions in equation (17) and summing over all the eigenmodes, \( q_{n,\sigma}^0 \), up to the Fermi level \( k_f \). Here we focus on the region \( z < 0 \)
\[
n_s^0(z < 0) = g \sum_{\sigma=\uparrow,\downarrow} \sum_{q_{n,\sigma}^0} \left\{ |\psi_{n,\uparrow,\sigma}^0(z)|^2 \left[ -z - \frac{a}{2} \right] + |\psi_{n,\downarrow,\sigma}^0(z)|^2 \left[ \theta(-z) - \theta(-z - \frac{a}{2}) \right] \right\}
\]
\[
\times \int d^2q_z \frac{e^{i\vec{q}_z \cdot \vec{r}}}{(2\pi)^2} \delta(k_f^2 - q_z^2)
\]
where \( g = 2 \) is the number of spin states. The summation over the eigenvalues of \( q_{n,\sigma}^0 \) can be evaluated by performing a contour integral, \( C \), enclosing all the poles of the factor function \( G_\sigma(q_{n,\sigma}^0) \), in complex plane where
\[
G_\sigma(q_{n,\sigma}^0) = \frac{E_\sigma(q_{n,\sigma}^0)}{E_0(q_{n,\sigma}^0)} \quad \text{and} \quad \sum_{q_{n,\sigma}^0} \to \oint_C \frac{dq_{n,\sigma}^0}{2\pi i} G_\sigma(q_{n,\sigma}^0)
\]
Using the relation in equation (22), the density function, \( n_s(z) \), for the S and AS modes are calculated and displayed in figure 2 for \( a = 0.5/k_f \).

We then try to obtain the Casimir interaction of the configuration with the electron density distribution in equation (21). Since we are interested only in the Casimir energy that arises from the presence of the two planes and not from the interaction of the single object and the electromagnetic field in general, we should renormalize our results by subtracting the corresponding single-body contribution. In our case, we should remove the contributions from the S mode as its density is continuous and finite at \( z = 0 \). This contribution represents the part of energy to completely break a single dielectric due to the tunneling electrons. The subtraction ensures the interaction only result from the disjointed bodies. We will see that this renormalization automatically removes all the divergences in our calculation and leads to a finite Casimir energy even at distance \( a = 0 \).

We follow equation (6) and obtain the leading order contribution to the Casimir energy with only the AS mode electron density distribution.
\[
E^{(2)}_c \propto \lambda = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\zeta}{2\pi} \int d\mathbf{k}_1 \left[ R_1^{TE} R_2^{TE} + R_1^{TM} R_2^{TM} \right] e^{-2i\zeta}
\]

---

**Figure 2.** Electron density function normalized by the bulk density, \( n_s = \frac{n_s^0}{n_b} \), for gold with \( k_f = 12 \text{ nm}^{-1} \) at zero temperature. The dashed lines indicate the surface boundaries where \( a = 0.5/k_f \). The red and blue lines represent antisymmetric (AS) and symmetric (S) modes of the density function. The total density, AS + S, is given by the black line.
The single-scattering coefficients, $\mathcal{R}_\nu^P$, are given as:

$$
\mathcal{R}_\nu^TE = \frac{\omega_{pv}^2}{4\kappa^2} \quad \text{and} \quad \mathcal{R}_\nu^{TM} = -\frac{\omega_{pv}^2}{4\kappa^2}\left(\frac{2\kappa^2}{\zeta^2} - 1\right)
$$

(24)

where the effective plasma frequency in this case has the form

$$
\omega_{pv}^2 = \frac{e^2}{m\pi^2} \int_0^{k_p} d\zeta \frac{q_e^2(q_e^2 - k_p^2)(q_e^2 + \chi^2)}{(q_e^2 + \chi^2)\chi^2\omega_{pv}^2} \left[\chi\cosh(\kappa\zeta) + \kappa\sinh(\kappa\zeta)\right]^2
$$

(25)

The effective plasma frequency, $\omega_{pv}$, in equation (25) incorporates all the information of the electronic structure, including electron tunneling, near the solid surface. The inhomogeneity in the charge density distribution gives rise to the dispersion effects in objects’ dielectric properties. This nonlocal response provides an additional, other than frequency $\zeta$, suppression to the reflection coefficients in the transverse momentum $k_\perp$, as a result, relieves the UV-divergences at short distances. On the other hand, one can recover the bulk plasma frequency and optical response at large distance by taking the long wavelength limit, $\kappa \sim 1/\lambda \to 0$, of equation (25) as

$$
\omega_{pv}^2 \xrightarrow{\kappa\to0} \frac{e^2k_p^3}{3\pi^2m} = \omega_{pv,0}^2 \quad \text{and} \quad \mathcal{R}_\nu^P \xrightarrow{\kappa\to0} \mathcal{R}_\nu^P.
$$

(26)

We obtain the reflection coefficients by including all the multiple scattering within each dielectrics

$$
\mathcal{R}_\nu^TE = \sum_{n=0}^\infty \frac{\omega_{pv}^2}{4\kappa^2 + \omega_{pv}^2} \quad \text{and} \quad \mathcal{R}_\nu^{TM} = -\sum_{n=0}^\infty \frac{\omega_{pv}^2}{4\kappa^2 + \omega_{pv}^2}(1 - \frac{\zeta^2}{2\kappa^2})
$$

and recover the logarithm by summing all the higher order terms in perturbation equation (3)

$$
\mathcal{E}_0 = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\zeta}{2\pi} \int_0^{k_f} \frac{d\zeta}{(2\pi)^2} \ln(1 - \mathcal{R}_\nu^TE e^{-2\zeta^2}) + \ln(1 - \mathcal{R}_\nu^{TM} e^{-2\zeta^2})
$$

(27)

5. Results and discussion

We now examine the nonlocal and tunneling effects on Casimir energies at short distances, $a \ll 1/\omega_{pv}$ by comparing equation (27) and the Lifshitz’s formula with plasma model given by [22]

$$
\mathcal{E}_{0,\lambda \to 0} = -\frac{1}{(2\pi)^2} \frac{\omega_{pv}^2}{a^2} \int_0^\infty dy \int_0^\infty dx \frac{x^2}{(2y^2 + 1)^2 e^{2x} - 1}
$$

(28)

We evaluate the Casimir energies for gold with parameters $\omega_{pv} = 9$ eV and $\lambda_f = 2\pi/k_f = 0.52$ nm. The potential barrier, $\varphi$, in figure 1 represents the energy gap for an electron to escape from the solid surface at zero temperature. It is modeled by the sum of electron work function and Fermi energy of materials, $\varphi = 10.9$ eV for gold. In figure 3, we can see that two results converge at large distances and start to deviate when the separations approach to the fermi wavelength $\lambda_f$. The results of equation (28) are much larger at short distances and diverge with $1/a^2$ as $a \to 0$. We remark that in the local dielectric model the electronic density is constant up to the abruptly truncated surface and the reflection coefficient remains unchanged for large momentum transfer as shown in equation (13). This boundary condition is not realistic since the electronic excitation should be largely suppressed above Fermi level even at zero distance. The minimum wavelength of the scattered photon in a free-electron gas is restricted by the average distance, $r_\alpha$, between two electrons. In this sense, the Fermi wave-vector, $k_f \sim 1/r_\alpha$, serves as the UV cutoff for the photon momenta, $k$, through the density function equation (21). Similar UV problems may occur when calculating the Casimir energies for small length scales such as edges, tips, and surface roughness where the high-momentum contributions are enhanced by the surface’s profile and dominate the interaction. On the other hand in the free-electron jellium model, the results given by equation (27) are much smaller and approach to a finite and sensible, $\mathcal{E}_{0,0} \sim -1.27$ eV for gold, limit as $a \to 0$. The energy at zero distance, $\mathcal{E}_{0,0}$, can be found by expanding equation (27) for small $a/\lambda_f < 1$

$$
\mathcal{E}_{0,\lambda \leq \lambda_f} \sim \mathcal{E}_{0,0} + \mathcal{E}_{0,1} + ... = \frac{1}{(2\pi)^4} \sqrt{\frac{e^2k_f^2}{4\pi m}} + 0.065(\varphi m \omega_{pv}) \frac{a^3}{\lambda_f^3} + ...
$$

(29)

This leading order term, $\mathcal{E}_{0,0}$, sets the upper bound to the maximum Casimir energy in this model. The value of $\mathcal{E}_{0,0}$ is determined by the Fermi wave-vector $k_f$ and independent of the boundary parameter $\varphi$. One can also see
that $E^{(0)}_c$ diverges as $\omega_p \rightarrow \infty$ in the metal limit. This can be understood since the $k_f$ serves as the momentum cutoff to the reflection coefficient $r_k$ through equation (25). Taking $\omega_p \rightarrow \infty$ equivalently removes this UV cutoff by sending $k_f \rightarrow \infty$. It allows photon to interact with materials for arbitrarily large momentum, small wavelength, which is not physical. Another result can be seen from equation (29) is that the next-to-leading order term, $E^{(1)}_c$, is proportional to $a^3$. This implies that the Casimir pressure vanishes at $a = 0$ and the whole system balances as it merges into a single electron gas.

In summary, we have proposed an analytic approach to incorporate the nonlocal and tunneling effects on Casimir/vdW interaction based on the free-electron jellium model. The model yields a finite result at zero separation and reproduce Lifshitz’s formula with bulk dielectric model in the long-wavelength limit. The near-surface charge distribution is found to be essential for a qualitatively correct description at small distances. We hope our approach can be extended to calculate the Casimir interaction for the system with arbitrary geometry at the sub-wavelength scale.

6. Acknowledgments

Hua-Yao Wu dedicates this work to the memory of his mentor Dr. Martin Schaden who passed away in July 2016. The present paper is the succeeding study of the previous works with Martin. He would also like to thank Dr. K.V. Shajesh for his stimulating discussion and collaborative assistance.

ORCID iDs

Hua-Yao Wu @ https://orcid.org/0000-0001-6078-3105

References

[1] Casimir H B G 1948 Kon. Ned. Akad. Wetensch. Proc. 51 793
[2] Lifshitz E 1956 Zh. Eksp. Teor. Fiz. 29 94
[3] Schwinger J, DeRaad L L and Milton K 1978 Annals of Phys. 115 1
[4] Wu H Y and Schaden M 2014 Phys. Rev. D 89 105003
[5] Wu H Y and Schaden M 2012 Phys. Rev. D 85 045008
[6] Esquivel R, Villarreal C and Mochan W L 2003 Phys. Rev. A 68 052103
[7] Esquivel R and Svetovoy V B 2004 Phys. Rev. A 69 062102
[8] Esteban R, Borisov A G, Nordlander P and Aizpurua J 2012 Nature Commun. 3 825
[9] Bostrom M and Sernelius B E 2000 Phys. Rev. Lett. 84 4757
[10] Sernelius B E 2005 Phys. Rev. B 71 235114
[11] Contreras-Reyes A M and Mochan W L 2005 Phys. Rev. A 72 034102
[12] Esquivel-Sirvent R, Villarreal C, Mochan W L, Contreras-Reyes A M and Svetovoy V B 2006 J. Phys. A: Math. Gen. 39 6323
[13] Despoja V, Sunjic M and Marusic I 2011 Phys. Rev. B 83 165421
[14] Jancoveci B and Samaj I 2004 J. Stat. Mech. 2004 P08006
[15] Buenzli P R and Martin P A 2008 Phys. Rev. E 77 011114
[16] Hoye J S and Brevik I 2009 Phys. Rev. E 80 011104
[17] Hoye J S and Brevik I 2017 Phys. Rev. A 95 052127
[18] White Lee R 2010 J. Colloid Interface Sci 343 338
[19] Woods L M, Dalvit D A R, Tkatchenko A, Rodriguez-Lopez P, Rodriguez A W and Podgornik R 2016 Rev. Mod. Phys. 88 045003
[20] Sakurai J J 1967 Advanced Quantum Mechanics (Reading, MA: Addison-Wesley)
[21] Bordag M, Klimchitskaya G, Mohideen U and Mostepanenko V 2009 Advances in the Casimir Effect (Oxford: Oxford University Press)
[22] Kampen N G V, Nijboer B R A and Schram K 1968 Phys. Lett. A 26 307