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Casimir-like tunnelling-induced electronic forces

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Abstract

We study the quantum forces that act between two nearby conductors due to electronic tunnelling. We derive an expression for these forces by calculating the flux of momentum arising from the overlap of evanescent electronic fields. Our result is written in terms of the electronic reflection amplitudes of the conductors and it has the same structure as Lifshitz's formula for the electromagnetically mediated Casimir forces. We evaluate the tunnelling force between two semiinfinite conductors and between two thin films separated by an insulating gap. We discuss some applications of our results.

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1. Introduction

The increased accuracy of experimental studies [1–5] of the Casimir force [6] between conducting bodies has opened the possibility of exploring new ideas related to the understanding and control of quantum vacuum fluctuations. Research projects on Casimir torques [7], or the possible applications of the Casimir forces in the development of micro and nano-electromechanical devices are now under way [8–10]. Understanding Casimir forces [11] has become fundamental in the investigation of additional long-range forces [12] and deviations [13] of Newton's gravitational law at micrometre distances [14, 15], related to the search for extra dimensions in spacetime [16]. Recent experiments employing atomic force microscopes have taken advantage of the isoelectronic/isotopic [17] effect to explore gravity corrections at distances as small as 1–4 nm [18], so that understanding all the forces acting at ultrashort distances has acquired a paramount importance.

The usual Casimir effect may be understood as a force due to the quantum nature of the electromagnetic radiation. In this paper, we study another source of quantum forces, namely,

the tunnel effect. Particles that tunnel across a barrier separating two materials transport momentum and therefore produce forces. Since quantum tunnelling arises from evanescent electronic fields, this force has similarities to the contributions of evanescent electromagnetic waves to the standard Casimir force.

In this paper, we concentrate our attention on conduction electrons in conductors, i.e., on massive non-relativistic Fermions. We derive the tunnelling force by calculating the flux of momentum between two regions delimited by an arbitrary potential $V(x)$. We express the momentum flux in terms of Green's function of the system, which we evaluate by means of a scattering method involving amplitude reflection coefficients [19, 20]. This method yields an expression for the tunnelling force with a structure that is essentially identical to Lifshitz's formula [21] and which has not been uncovered by previous related calculations [22, 23]. We first perform the calculation for a one-dimensional system. We then extend the calculation to the three-dimensional case. Finally, we evaluate the tunnelling force for a configuration consisting of two semiinfinite or two thin metallic slabs separated by a thin insulating gap and we discuss some applications of our results. Our calculations are performed for model conductors in which free, independent electrons are confined by simple potential barriers. Our neglect of crystalline structure and many-body interactions might render our results quantitatively inaccurate, especially at distances comparable to an atomic size, though we believe they should be qualitatively correct. Our calculation shows that although electronic originated forces are due to the interchange of massive real Fermions instead of massless virtual Bosons, they may be calculated in a way that parallels closely the calculation of the usual Casimir force in terms of reflection amplitudes.

2. One-dimensional systems

The dynamical equation for the wavefunctions of an electronic system may be derived from a Lagrangian density [24],

$$\mathcal{L} = \frac{\hbar^2}{2m}|\psi_{,z}|^2 + V|\psi|^2 + \frac{\mathrm{i}\hbar}{2}(\psi\psi^*_{,t} - \psi^*\psi_{,t}) \tag{1}$$

for which Euler–Lagrange's equations yield Schrödinger's equation,

$$\partial_t \frac{\partial\mathcal{L}}{\partial(\psi^*_{,t})} + \partial_z \frac{\partial\mathcal{L}}{\partial(\psi^*_{,z})} - \frac{\partial\mathcal{L}}{\partial\psi^*} = \mathrm{i}\hbar\psi_{,t} + \frac{\hbar^2}{2m}\psi_{,z,z} - V\psi = 0. \tag{2}$$

The field carries mechanical properties such as a momentum flux [25]:

$$T^z_z = \frac{\partial\mathcal{L}}{\partial\psi^*_{,z}}\psi^*_{,z} + \frac{\partial\mathcal{L}}{\partial\psi_{,z}}\psi_{,z} - \mathcal{L} = \frac{\hbar^2}{2m}|\psi_{,z}|^2 - V|\psi|^2 - \frac{\mathrm{i}\hbar}{2}(\psi\psi^*_{,t} - \psi^*\psi_{,t}). \tag{3}$$

Consider now an eigenstate ψ_n of the Schrödinger Hamiltonian $\hat{H} = -(\hbar^2/2m)\partial_z^2 + \hat{V}$ corresponding to an energy E_n. From equation (3), its contribution to the momentum flux is

$$T^z_z = \frac{\hbar^2}{2m}|\partial_z\psi_n|^2 + (E_n - V)|\psi_n|^2. \tag{4}$$

Within a region $\mathcal{V}$ in which $V(z)$ may be taken as a constant, we can write $E_n - V = \hbar^2 k_n^2/2m$, i.e., the kinetic energy of particles with wavenumber k within $\mathcal{V}$. We now sum the contributions (4) over all the occupied orbitals,

$$T^z_z(z) = \frac{\hbar^2}{2m}\sum_n \int \mathrm{d}E\,\delta(E - E_n)\,f(E)[k^2|\psi_n(z)|^2 + |\partial_z\psi_n(z)|^2], \tag{5}$$

where $f(E_n)$ is the occupation number of orbital n, given in equilibrium by the Fermi–Dirac distribution function, and $k^2 = 2m(E - V)/\hbar^2$. The energy integration and Dirac's δ allow us to write T_z^z in terms of the Green's function of the system,

$$G_E(z, z') = \langle z|(E - \hat{H})^{-1}|z'\rangle = \sum_n \frac{\psi_n(z)\psi_n^*(z')}{E - E_n}, \tag{6}$$

employing the relation $\mathrm{Im}(E^+ - E_n)^{-1} = -\pi\delta(E - E_n)$, where $E^+ = E + \mathrm{i}\eta$ with E and $\eta \to 0^+$ real. Substituting this latter relation in (5) and employing (6) we obtain

$$T_z^z(z) = -\frac{\hbar^2}{2\pi m}\,\mathrm{Im}\int \mathrm{d}E[k^2 G_{E^+}(z, z') + \partial_z\partial_{z'}G_{E^+}(z, z')]_{z'\to z} f(E). \tag{7}$$

Notice that equation (7) may be interpreted as

$$T_z^z(z) = \int \mathrm{d}E\rho_E^{ef} f(E)(\hbar k)\left(\frac{\hbar k}{m}\right), \tag{8}$$

where $\pm\hbar k$ is the momentum of a particle which moves with velocity $\pm\hbar k/m$, thus contributing the amount $(\hbar k)\hbar k/m$ to the momentum flux, and

$$\rho_E^{ef}(z) = -\frac{1}{2\pi}\,\mathrm{Im}\left[G_{E^+}(z, z') + \frac{1}{k^2}\partial_z\partial_{z'}G_{E^+}(z, z')\right]_{z'\to z} \tag{9}$$

plays the role of an effective local density of states.

We now assume that $\mathcal{V}$ has a width L and is bounded on both sides by arbitrary potentials, and we evaluate Green's function following a scattering approach [19, 20]. Within $\mathcal{V}$, the solution of $(E - \hat{H})G_E(z, z') = \delta(z - z')$ may be written as $G_E(z, z') = (2m/\hbar^2)\psi_{\mathrm{L}}(z_L)\psi_{\mathrm{R}}(z_R)/W$, where ψ_{L} and ψ_{R} are the two solutions of the Schrödinger-like homogeneous equation $(E - \hat{H})\psi = 0$ that satisfy the boundary conditions on the left and the right side of the system respectively, $W = \psi_{\mathrm{L}}\psi_{\mathrm{R},z} - \psi_{\mathrm{L},z}\psi_{\mathrm{R}}$ is their Wronskian, and z_L and z_R are the smallest and the largest among z and z'. We write $\psi_{\mathrm{L}}(z) = \mathrm{e}^{-\mathrm{i}kz_L} + r_1\,\mathrm{e}^{\mathrm{i}kz_L}$ and $\psi_{\mathrm{R}}(z) = \mathrm{e}^{\mathrm{i}k(z_R-L)} + r_2\,\mathrm{e}^{-\mathrm{i}k(z_R-L)}$, where r_1 and r_2 are the reflection amplitudes for particles impinging on the left and right boundaries of $\mathcal{V}$, which we assume at $z = 0$ and $z = L$, and we obtain

$$G_E(z, z') = \frac{2m}{\hbar^2}\frac{(\mathrm{e}^{-\mathrm{i}kz_L} + r_1\,\mathrm{e}^{\mathrm{i}kz_L})(\mathrm{e}^{\mathrm{i}k(z_R-L)} + r_2\,\mathrm{e}^{-\mathrm{i}k(z_R-L)})}{2\mathrm{i}k\,\mathrm{e}^{-\mathrm{i}kL}(1 - r_1r_2\,\mathrm{e}^{2\mathrm{i}kL})}, \tag{10}$$

which together with equation (7) yields the momentum flowing within $\mathcal{V}$,

$$T_z^z = \frac{1}{\pi}\,\mathrm{Re}\int \mathrm{d}E\,k\frac{1 + r_1r_2\,\mathrm{e}^{2\mathrm{i}kL}}{1 - r_1r_2\,\mathrm{e}^{2\mathrm{i}kL}} f(E) = \frac{\hbar^2}{\pi m}\,\mathrm{Re}\int \mathrm{d}k\,k^2\frac{1 + r_1r_2\,\mathrm{e}^{2\mathrm{i}kL}}{1 - r_1r_2\,\mathrm{e}^{2\mathrm{i}kL}} f(E), \tag{11}$$

where we used $E = \hbar^2k^2/2m + V$. As expected in an equilibrium situation, T_z^z is independent of z within $\mathcal{V}$.

3. Three-dimensional systems

The generalization of the results derived above to the three-dimensional case is straightforward for systems which are translationally invariant along a symmetry plane, say xy. In that case, the parallel wave vector $\vec{Q} = (Q_x, Q_y)$ is a conserved quantity, and for each $\vec{Q}$ the problem is identical to the 1D case. Thus, we only have to sum equation (11) over the allowed wavevectors,

$$\mathcal{T}_z^z = \frac{\hbar^2}{4\pi^3 m}\,\mathrm{Re}\int \mathrm{d}^2Q\int \mathrm{d}k\,k^2\frac{1 + r_1r_2\,\mathrm{e}^{2\mathrm{i}kL}}{1 - r_1r_2\,\mathrm{e}^{2\mathrm{i}kL}} f(E), \tag{12}$$

where we introduced the number $\mathcal{A}d^2Q/(2\pi)^2$ of wavevectors within a region d^2Q of reciprocal space by applying Born–von Karman boundary conditions in a system with total area $\mathcal{A} \to \infty$, and we introduced the momentum flux *density* $\mathcal{T}_z^z = T_z^z/\mathcal{A}$. Note that $-\mathcal{T}_z^z$ coincides with the zz component of the stress tensor as defined in elasticity theory.

We remark that the structure of equation (12) is essentially identical to Lifshitz's formula and the procedure followed resembles closely the scattering approach [19, 20] to the Casimir effect. The main differences are that the electromagnetic field has two independent transverse polarizations whose contributions would have to be summed over, and that the speed of light is a constant c, while the speed of electrons is proportional to the wavevector, i.e., the dispersion relation between electrons and photons is different, and consequently, there is an extra power of $\hbar$ in equation (12). Another difference is that $f(E)$ is a Fermi–Dirac instead of a Bose–Einstein distribution and that the zero-point contribution is missing, as virtual pair production would be irrelevant for the low energy applications we study below.

As r_1 and r_2 are independent of Q for scalar fields, the first integral in equation (12) may be performed immediately. At zero temperature we obtain

$$\mathcal{T}_z^z = \frac{1}{\pi^2}\,\mathrm{Re}\int \mathrm{d}k \left(K_\mathrm{F} - \frac{\hbar^2}{2m}k^2\right) k^2 \frac{1 + r_1 r_2\,\mathrm{e}^{2\mathrm{i}kL}}{1 - r_1 r_2\,\mathrm{e}^{2\mathrm{i}kL}}, \tag{13}$$

where the integration region includes all states below the Fermi level, whose kinetic energy within $\mathcal{V}$ is K_F, and for which we took $f(E) = 2$, including the spin degeneracy.

4. Applications

4.1. One semiinfinite metal

Within the bulk of a semiinfinite metal the electrons are reflected by the surface potential barrier on one side, while there is no barrier on the other side. Thus, the pressure p with which the electrons push the surface of the metal may be obtained by setting $r_1 = 0$ in equation (13). The result is simply

$$p = \mathcal{T}_z^z = \frac{1}{\pi^2}\int_0^{k_\mathrm{F}} \mathrm{d}k \left(E_\mathrm{F} - \frac{\hbar^2k^2}{2m}\right) k^2 = \frac{2}{5}nE_\mathrm{F}, \tag{14}$$

where $\hbar k_\mathrm{F}$ is the Fermi momentum, $E_\mathrm{F} = K_\mathrm{F}$ (within the metal) is the Fermi energy, and $n = k_\mathrm{F}^3/3\pi^2$ is the electronic density. As could have been expected, this result coincides with the well-known pressure of a degenerate fermion gas [26].

4.2. Two semiinfinite metals

We consider now two identical semiinfinite metals separated by vacuum. The force $F/\mathcal{A}$ per unit area between both metals may be obtained from the momentum flux (13) within the vacuum region, where the wavefunction of all the occupied states are evanescent, and it may be written as

$$\frac{F}{\mathcal{A}} = -2\,\mathrm{Im}\frac{\hbar^2}{2m\pi^2}\int_{\kappa_0}^{\kappa_F} \mathrm{d}\kappa\left(\kappa_F^2 - \kappa^2\right)\kappa^2\frac{1}{\zeta - 1}, \tag{15}$$

where $\zeta^{-1} = r^2\,\mathrm{e}^{-2\kappa L}$, and we wrote the wavenumber $k = \mathrm{i}\kappa$ in terms of the decay constant κ. The integration limits in (15) are the decay constants for electrons at the bottom of the conduction band, $\kappa_0 = \sqrt{[2m(W + E_\mathrm{F})/\hbar^2]}$, and at the Fermi level $\kappa_F = \sqrt{(2mW/\hbar^2)}$, while $W = -K_\mathrm{F}$ (within vacuum) > 0 is the work function, and $r = r_1 = r_2$ is the complex reflection amplitude corresponding to evanescent wavefunctions that *propagate* (i.e., decay) through vacuum towards a surface and are reflected back. Assuming that the potential

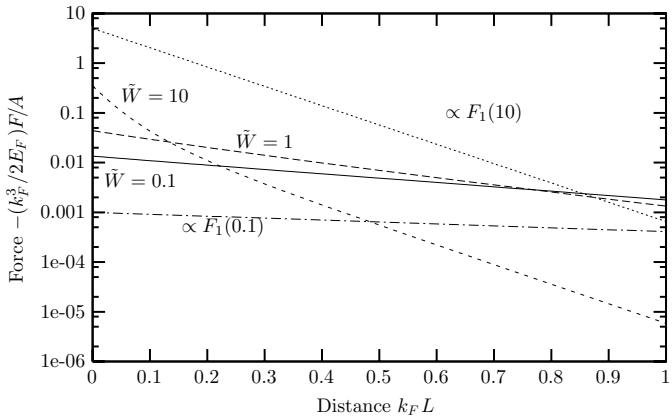

Figure 1. Force per unit area between two semiinfinite metals as a function of their separation L for different values 0.1, 1, 10 of the dimensionless work function $\tilde{W} = W/2E_F$. Also shown schematically is the contribution $e^{-2\kappa_F L} \propto F_1$ expected for one electron at the Fermi surface in the cases $\tilde{W} = 0.1, 10$.

$V(z)$ is constant within the metals and within vacuum, and that it changes abruptly at the vacuum–metal interface by an amount $W + E_F$, the reflection amplitude may be calculated as $r = (i\kappa - k_M)/(i\kappa + k_M)$, where $k_M = \sqrt{[2m(W + E_F)/\hbar^2 - \kappa^2]}$ is the wavenumber within the metal of the state corresponding to κ. We have verified that the 1D counterpart of equation (15), obtained from (11) instead of (12) is consistent with equation (5.24) of [22] for the case of square potential barriers. However, its simple structure was not identified previously, as the momentum flux and scattering coefficients were calculated within the metals and not in the vacuum gap between them.

In figure 1 we plot the force per unit area as a function of distance for different values of the workfunction W. The force is attractive, seems to decay exponentially for *large* separations and attains a finite value at zero separation. For large W the force is larger at small separation and smaller at large separations as the energy decays very fast towards that of two isolated semiinfinite metals. As could have been expected, the smaller the work function, the larger the spatial range of the force. We might expect the decay to be dominated by those electrons closest to the Fermi energy whose contribution becomes proportional to $e^{-2\kappa_F L}$. Figure 1 includes two curves illustrating this behaviour for the cases of large and small W. The actual decay of the force is slightly faster, more so for small W. This is due to the fact that not only the contribution of each electron decays with increasing distance, but also the number of electrons that contribute effectively to the force. Furthermore, the phase space available right at the Fermi energy is null, due to the prefactor $\kappa_F^2 - \kappa^2$ in equation (15), so the contributing electrons have a slightly larger decay constant (i.e., smaller range) than those at the Fermi level. This prefactor is absent in 1D calculations [22, 23].

In figure 2 we show the force for several distances as a function of W. For finite separation distances the force is small for large W, for which the surfaces do not interact, and it is also small for small W, for which the electrons tunnel easily regardless of the separation. Thus, the magnitude of the force is largest at some intermediate value of W which increases as L decreases. At contact, $L = 0$, there is no such extreme anymore and we obtain a linear behaviour,

$$\frac{F(0)}{\mathcal{A}} = -\frac{k_F^3}{\pi^2}\left(\frac{E_F}{5} + \frac{W}{3}\right), \tag{16}$$

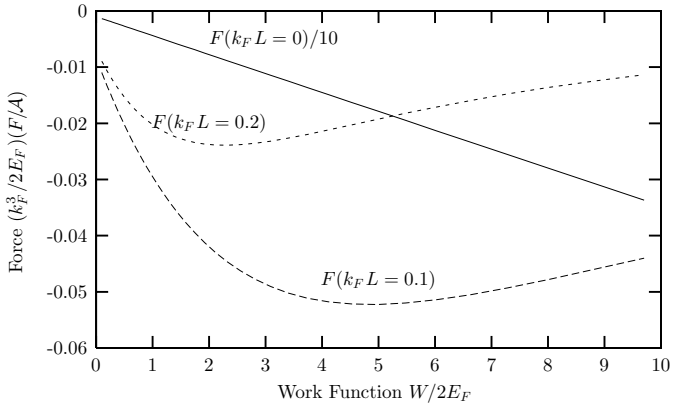

Figure 2. Force between two metals as a function of the work function for several values of the separation $\tilde{L} = 0, 0.1, 0.2$ in units of k_{F}^{-1}.

as can be shown by integrating equation (15) analytically. $F(0)$ is the force that would be required in order to break an infinite metal into two semiinfinite ones. Substitution of typical values into equation (16) yields $F(0)/\mathcal{A} \sim 100$ GPa, several orders of magnitude larger than the ultimate breaking strength of real materials, as our model fails to account for dislocations whose motion within the metal would relax the stress, and for the growth of fractures which are actually responsible for the failure of real metals. Real metals break gradually, not simultaneously over the whole separation surface. Nevertheless, integrating equation (15) over L we have obtained an analytical estimate of the surface energy of metals in terms only of their Fermi energy and their work function. This turns out to be surprisingly accurate [27] given our simplifying assumptions, namely, our use of an independent free particle model, neglecting the crystalline structure, the electronic charge and many-body corrections, as well as our use of a square potential barrier at the surface. For example, we obtain a surface tension of $\gamma \approx 1223$ erg cm^{-2} for Ag, 8% larger than measured in the liquid state [28]. The discrepancy for other metals is typically larger; about 30–50%.

5. Thin films

Equation (15) may be employed to calculate the force between more complicated systems simply by introducing the appropriate value of the reflection amplitude. For example, in figure 3 we display the force between two free standing very thin metallic films as a function of distance for a fixed Fermi energy, or more properly, a fixed electrochemical potential. Note that for very thin films the force is identically zero, as there are no states at all below the Fermi energy and therefore there are no available electrons to tunnel between the films. For wider films the force is finite at small separations but becomes zero after a finite separation. As the width is further increased, the force approaches that corresponding to semiinfinite metals, although not monotonously; it actually oscillates between larger and smaller values. This behaviour may be understood by considering the finite size effect on the levels of the individual films and the interaction of levels within both films, yielding alternating bonding and antibonding states which may be occupied only when they lie below the Fermi level.

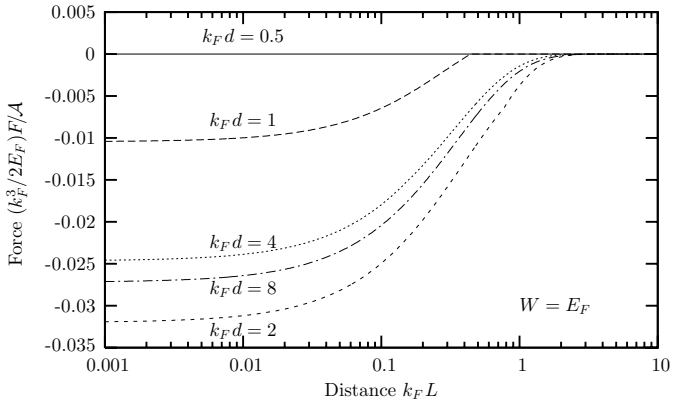

Figure 3. Force between two films of widths $\tilde{d} = 0.5, 1, 2, 4, 8$ (in units of k_{F}^{-1}) as a function of the distance L between them. We took $W = E_{\mathrm{F}}$.

6. Conclusions

By calculating the mechanical properties carried by the electronic wavefunctions, we have shown that the interchange of electrons between conductors produces a force that may be calculated in terms of the electronic reflection amplitudes using formulae that are very closely related to the Lifshitz formula for the usual Casimir force. We illustrated our formalism by calculating the electronic pressure within a conductor and the force between semiinfinite conductors and between thin films at very small distances, of the order of the Fermi wavelength. These distances are extremely small, beyond the expected limit of validity of the usual Casimir effect. Thus, we expect our results to be important to study the forces that act, for example, between the tip and the substrate of a scanning tunnelling microscope (STM) or an atomic force microscope [29, 30]. Related calculations in 1D have been employed to quantify the quantum position and momentum uncertainties of the STM [22, 23] and to study the statistics of electromechanical fluctuations in low-dimensional conductors [31]. We discussed how our results may be employed to calculate the surface energy of conductors without having to subtract total energies. Other applications which are currently under study include the calculation of the force between impurities embedded within three- and one-dimensional conductors. Our current calculations were performed only for free, independent electron conductors. However, the main ingredients of our calculation are the reflection amplitudes as a function of energy and parallel momentum and the electronic dispersion relation, so we believe that within a quasi-particle approach, introducing Bloch's momentum, and using the appropriate band structures, our scattering approach might be generalized to more realistic systems. We hope that the similarities we exhibited between the calculation of electronic forces and of the Casimir effect may stimulate the Casimir community to employ their expertise to further develop the field.

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