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Self-energy of an electron in a gap between two metals and near a metallic slab

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Using the formalism of Manson and Ritchie, we have calculated the self-energy of an electron located in the gap between two similar metals and near a metallic slab. The electron is described in terms of a plane-wave basis set. Numerical work indicates that for gap separations $\gtrsim 4$ Å, quantal corrections to the classical image potential are not large in the case of a zero-momentum electron.

The study of the self-energy of a charged particle located in a gap between two metals or near a metallic slab is of great interest in order to understand a number of experimental techniques frequently used in surface physics. The charge-slab interaction plays an important role in the analysis of thin films by means of particle-beam spectroscopies.[1-6] As another example, the image potential experienced by a tunneling electron is of paramount importance in determining the I-V response of a junction.[7,8] This problem has recently received a great deal of attention in connection with the scanning tunneling microscope.[9,10]

We present here a theoretical analysis of the interaction between a charged particle and the polarization modes of both a metallic slab and a metal-metal gap. We benefit from the similarity between these two physical systems by employing a common approach. We are particularly interested in studying the recoil effects associated with the charge's finite mass. This physical effect has so far been neglected in the literature, and we think it is of interest to estimate its importance in the total potential experienced by an electron. Manson and Ritchie[11] have proposed a projected local self-energy formalism that accounts for the particle's recoil accompanying the virtual excitation of polarization modes. Along the same line, Mahanty, Pathak, and Paranjape,[12] using the Manson-Ritchie approach, have recently studied the combined effects of recoil and plasmon dispersion in the charge–metal-surface interaction, and Sols and Ritchie[13] have extended this method to calculate the self-energy of a charge near an interface. To calculate the effective polarization potential experienced by a charge near a slab or in a gap, we must first know the dispersion relation of the surfacelike plasmons and their coupling to a charge. Since we are concerned with particles exterior to the metal, we will not consider the bulk polarization.

We idealize our physical system by considering two media described by dielectric functions $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$. We assume that medium 1 fills the space defined by $|z|>a$ and medium 2 lies in the region $|z|<a$, where $d=2a$ is the width of either the gap or the slab. If we take a local dielectric function for the metal's response, the metallic slab will correspond to the case $\epsilon_1(\omega)=1$ and $\epsilon_2(\omega)=1-\omega_p^2/\omega^2$, and a gap between two metals will be described by the reversed case.

The frequencies of the plasma oscillations which satisfy the matching condition are given implicitly by the dispersion relation[7]

$$\frac{\epsilon_1(\omega)-\epsilon_2(\omega)}{\epsilon_1(\omega)+\epsilon_2(\omega)}=\alpha e^{2Qa} , \tag{1}$$

where α can take the values 1 (symmetric mode) or -1 (antisymmetric mode), and Q is the modulus of the surface-plasmon wave vector. The frequencies satisfying Eq. (1) are

$$\omega_{Q\alpha}=\omega_s(1+\sigma\alpha e^{-2Qa})^{1/2} , \tag{2}$$

where $\omega_s=\omega_p/\sqrt{2}$ and $\sigma=1$ (-1) for a slab (gap).

If we assume the two media to be described by dielectric functions

$$\epsilon_i(\omega)=1-\sum_j \frac{\Omega_{ij}^2}{\omega^2-\omega_{ij}^2},\quad i=1,2 , \tag{3}$$

where index j is summed over the effective oscillators of medium i, then it can be shown that the interaction between a charge and the boundary modes is given by the Hamiltonian

$$\hat{V}=\sum_{\mathbf{Q},\alpha}\Gamma_{Q\alpha}g_{Q\alpha}(z)e^{i\mathbf{Q}\cdot\boldsymbol{\rho}}(a_{\mathbf{Q}\alpha}+a^{\dagger}_{-\mathbf{Q}\alpha}) , \tag{4a}$$

$$g_{Q\alpha}(z)=\begin{cases}(1+\alpha e^{2Qa})e^{Qz}, & z<-a\\ e^{Qz}+\alpha e^{-Qz}, & -a<z<a\\ \alpha(1+\alpha e^{2Qa})e^{-Qz}, & z>a\end{cases} , \tag{4b}$$

$$\Gamma_{Q\alpha}^2=\frac{\pi e^2\hbar\,\omega_{Q\alpha}}{AQ}\lambda_{Q\alpha} , \tag{4c}$$

$$\lambda_{Q\alpha}=2\left[\sum_{i,j}\frac{\Omega_{ij}^2\omega_{Q\alpha}^2}{(\omega_{ij}^2-\omega_{Q\alpha}^2)^2}F_{Q\alpha}^{(i)}\right]^{-1} , \tag{4d}$$

$$F_{Q\alpha}^{(1)}=2(e^{Qa}+\alpha e^{-Qa})^2;\quad F_{Q\alpha}^{(2)}=4\sinh(2Qa) , \tag{4e}$$

where $\mathbf{r}=(\boldsymbol{\rho},z)$ is the vector position of the charge, A is the interface area, and $a^{\dagger}_{\mathbf{Q}\alpha}$ and $a_{\mathbf{Q}\alpha}$ are the creation and annihilation operators of the surfacelike plasmons. It may be noted that Eq. (4) can also be applied to the case where one or both media are insulators. In the particular cases of a metallic slab or a metal-metal gap, the coupling parameter $\lambda_{Q\alpha}$ becomes

$$\lambda_{Q\alpha}=\frac{1}{2(e^{2Qa}+\alpha)} . \tag{5}$$

Thus the electric potential created by a boundary plasmon of momentum $\hbar\mathbf{Q}$ and parity α is the same in either the gap or the slab. Differences in the interaction energy with a charge will come from the value of σ in the plasmon dispersion relation (2). The charge-slab interaction given by Eq. (4) is equivalent to the Hamiltonian used by previous authors.[4,5]

From the second-order energy shift, we can define the following projected self-energy:[11,13]

$$\Sigma(\mathbf{r}) = -\sum_{\mathbf{k},n} \frac{\psi_k(\mathbf{r})}{\psi_0(\mathbf{r})} \frac{\langle 0|\hat{V}|n\rangle\langle n\psi_k|\hat{V}|0\psi_0\rangle}{\varepsilon_k-\varepsilon_0+\hbar\omega_{n0}-i\eta} , \quad (6)$$

where $|0\rangle$ and $|\psi_0\rangle$ are the eigenvectors corresponding to the initial states of the medium and the particle, respectively; $|n\rangle$ and $|\psi_k\rangle$ are those of the intermediate states; $\psi_k(\mathbf{r})=\langle\mathbf{r}|\psi_k\rangle$; ε_k and ε_0 are the eigenenergies of the particle's motion; $\hbar\omega_{n0}$ is the excitation energy of the nth eigenstate of the medium; $\hat{V}$ is the particle-solid interaction; and $\eta\rightarrow 0+$.

If a plane-wave basis set is chosen for the unperturbed motion of the particle, and expressions (2), (4), and (5) are introduced in Eq. (6), the self-energy of a charge with velocity $\mathbf{V}=\hbar(\mathbf{K}_0,k_0)/m$ interacting with the surfacelike plasmons of a gap or a slab is given by

$$\Sigma(z) = -\frac{e^2}{(4\pi)^2}\sum_\alpha \int d^2Q \int dk \frac{e^{-ikz}(e^{ika}+\alpha e^{-ika})}{k^2+Q^2} \frac{e^{-Qa}}{1+\alpha e^{-2Qa}} \frac{P_{Q\alpha}^2 g_{Q\alpha}(z)}{k^2+Q^2+k_0k+\mathbf{K}_0\cdot\mathbf{Q}+P_{Q\alpha}-i\eta} , \quad (7)$$

where $P_{Q\alpha}=(2m\omega_{Q\alpha}/\hbar)^{1/2}$ is the momentum associated with the recoil of the particle.

In the low-velocity limit, $\mathbf{V}\rightarrow 0$, the self-energy (7) can be neatly separated into a classical and a quantum recoil contribution:

$$\Sigma(z)=\Sigma_c(z)+\Sigma_r(z) . \quad (8)$$

The classical term is

$$\Sigma_c(z)=\begin{cases} -\dfrac{e^2}{8a}\left[2\psi(1)-\psi\left(\dfrac{1}{2}+\dfrac{z}{2a}\right)-\psi\left(\dfrac{1}{2}-\dfrac{z}{2a}\right)\right], \; z<a , & (9a) \\ -\dfrac{e^2}{4(z-a)}, \; z>a , & (9b) \end{cases}$$

where $\psi(x)=d\ln\Gamma(x)/dx$ is the digamma function. Since Σ_c is symmetric about the plane $z=0$ we give only the expression for $z>0$. Equation (9a) gives the classical image potential experienced by a charge between two semi-infinite metals and can be obtained by summing the infinite series resulting from the interaction of the external charge with the effective image charges on both metals.[14] Analogously, Eq. (9b) gives the classical image potential seen by a charge near a metallic slab. It is interesting to note that such potential only depends on the distance between the charge and the boundary of the slab, and not on the slab width. In particular, it coincides with the classical image potential between a charge and a semi-infinite metal. This is what should be expected from a classical approach to the electrodynamical boundary problem where the implicit assumption is made that the width of the slab is much greater than the Thomas-Fermi length of the metal. It is in a region of such width near the metal surface where the induced charge density giving rise to the image charge is localized. These two cases further confirm that the classical method of image charges is equivalent to the use of a local dielectric function for the metal interacting with a classical particle at rest.

Due to the difference in the dispersion relations of the gap and the slab plasmons, the recoil term of the boundary-plasmon contribution to the self-energy will be given by different expressions in each case. For a particle near a slab $(z>a)$, we obtain

$$\Sigma_r(z)=\frac{e^2}{2}\sum_\alpha\int_0^\infty \frac{dQ}{1+\alpha e^{-2Qa}}\frac{Q}{S}e^{-(S+Q)a} \times\{\cosh[(S+Q)z]+\alpha\cosh[(S-Q)z]\} , \quad (10a)$$

and for a particle in the gap $(z<a)$

$$\Sigma_r(z)=\frac{e^2}{4}\sum_\alpha\int_0^\infty dQ\, e^{-Q(z-a)}\frac{Q}{S} \times\{e^{-S(z-a)}+\alpha e^{-S(z+a)}\} , \quad (10b)$$

where, in both equations,

$$S^2=Q^2+P_{Q\alpha}^2=Q^2+\frac{2m}{\hbar}\omega_{Q\alpha} . \quad (10c)$$

It may be noted that, when $S=Q$ is taken, Eqs. (10) become identical to Eqs. (9).

The self-energy [(8)-(10)], when evaluated at points $z=0$ and $z=a$, adopts simple analytical expressions in the limits $Q_sa\ll 1$ and $Q_sa\gg 1$. For a very narrow gap, we obtain

$$\Sigma(0)=\Sigma(a)=-\frac{e^2Q_b}{2}, \; Q_sa\ll 1 , \quad (11)$$

where $Q_b=(2m\omega_p/\hbar)^{1/2}$, while for a wide gap,

$$\Sigma(0)=-\frac{e^2\ln 2}{2a}\left[1-\frac{2}{\ln 2}\frac{e^{-Q_sa}}{Q_sa}\right], \; Q_sa\gg 1 , \quad (12a)$$

$$\Sigma(a)=-\frac{e^2Q_s}{2}, \; Q_sa\gg 1 . \quad (12b)$$

The limit (11) shows that the self-energy for a charge between two metals that are very close to one another tends to a uniform value equal to the bulk saturation value of a charge within the metal.[12,13] In the opposite limit of a very wide gap between two metals, the self-energy of the middle of the gap tends to the classical value $-e^2\ln 2/d$,

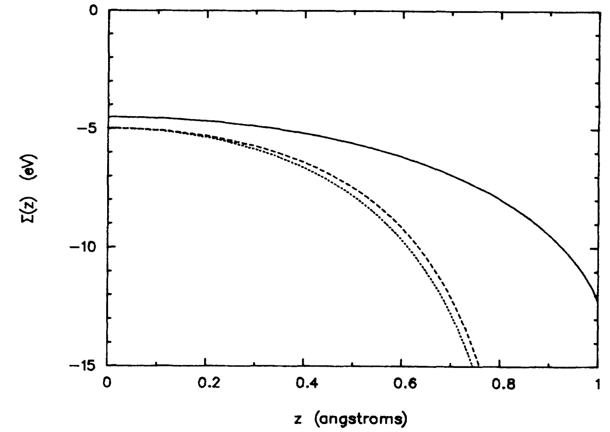

FIG. 1. Self-energy of an electron between two metals separated by $d=2$ Å, plotted as a function of the distance from the center of the gap. Solid line shows the quantum self-energy as calculated from Eqs. (8), (9a), and (10a) of the text. Dashed line shows the classical image potential obtained by the image charge method [see Eq. (9a) in the text]. Dotted line represents the image potential used in Ref. 9. For both metals $r_s=2.07$ has been taken to represent Al.

with exponential recoil corrections. As should be expected, in the same limit, the self-energy (12b) at the metal surface ($z=a$) tends to the free-surface value.[11-13]

For a very thin slab, it can be shown that $\Sigma(a)\simeq 0$. In the opposite limit of a very thick slab, $\Sigma(a)$ tends to the free-surface value (12b).

In Fig. 1 we plot the self-energy of an electron between two metals separated by $d=2$ Å, as calculated from Eq. (9a) (classical) and Eqs. (8)–(10) (total quantum). The approximate classical image potential proposed by Binnig *et al.*[9] is also shown. For the recoil contribution we have taken $r_s=2.07$ to represent Al. Clearly, the presence of recoil reduces everywhere the effective potential and makes it saturate to a finite value at the surface.

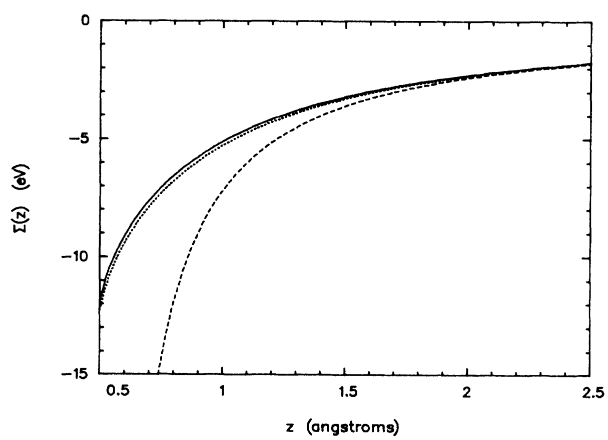

FIG. 2. Self-energy of an electron near an Al slab, plotted as a function of the distance from the center of the slab. The solid line shows the quantum self-energy as calculated from Eqs. (8), (9b), and (10b) of the text, and the dashed line represents the classical image potential [Eq. (9b) of the text]. The dotted line shows the quantum self-energy of an electron near a semi-infinite medium whose surface is located at $z=a$. Thickness has been taken $d=2a=1$ Å for the finite width effects to be shown.

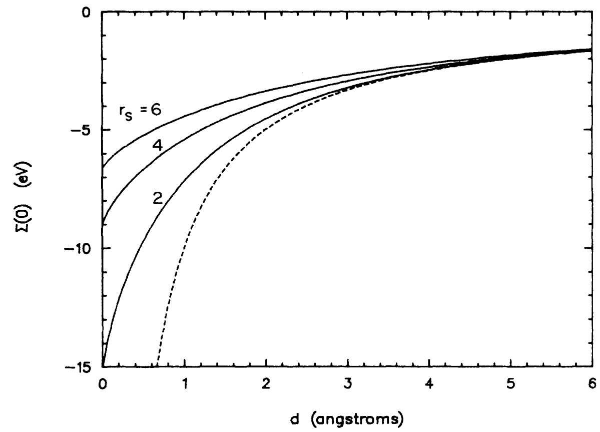

FIG. 3. Self-energy of an electron in the middle of a gap between two metals, plotted as a function of the metal-metal distance d, for various metal electronic densities $r_s=2$, 4, and 6 (solid lines). The dashed line shows the classical result $-e^2\ln 2/d$.

In Fig. 2, both the classical and the quantum self-energies of a charge near an Al slab are represented. The quantum self-energy of a charge near a semi-infinite medium[11-13] is also plotted for comparison. Finite thickness corrections are very small even for a slab of thickness $d=1$ Å.

Figure 3 shows the value of the self-energy at the middle of the gap as a function of the gap width d for several metallic densities. The classical value $-e^2\ln 2/d$ is also shown. Recoil effects become negligible for $d\gtrsim 4$ Å, de-

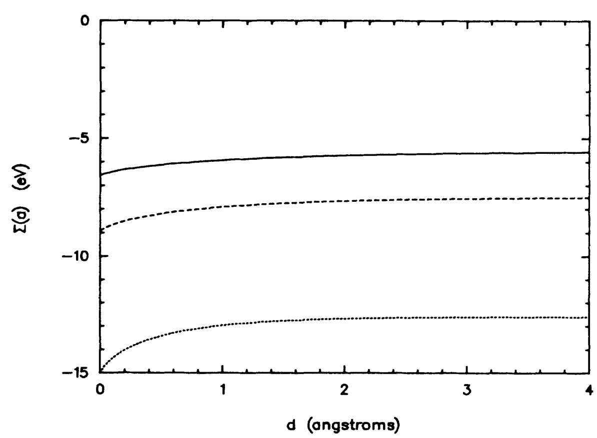

FIG. 4. Self-energy of an electron located at one metal surface ($z=a$), as a function of the metal-metal gap width $d=2a$, for various metal electronic densities: $r_s=2$ (dotted line), 4 (dashed line), and 6 (solid line).

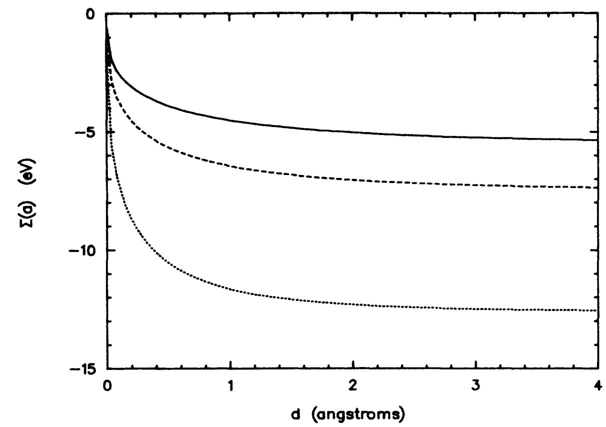

FIG. 5. Self-energy of an electron located at the surface of a metallic slab ($z = a$), as a function of the slab width $d = 2a$. The metal electronic densities are $r_s = 2$ (dotted line), 4 (dashed line), and 6 (solid line).

pending on the density: The lower the density, the larger the range where recoil corrections are important.

In Fig. 4, we plot the self-energy right at the surface as a function of the gap width. $\Sigma(a)$ saturates rather quickly to the free-surface limit, since the surface-surface coupling effects are not very important at one extreme of the gap.

Figure 5 shows the self-energy at the edge of a slab, as a function of the slab thickness. As in the case of the gap, the self-energy at the surface soon saturates to the limit of infinite thickness. This should be expected from the fact that the recoil distances are not very large in the metallic range: Typically, $0.5\ \text{Å} \lesssim Q_s^{-1} \lesssim 1.3\ \text{Å}$.

In conclusion, we have calculated the self-energy experienced by an electron near a metallic slab and between two metal surfaces. We have studied the role played by the particle's recoil accompanying the virtual excitation of plasmons. For the interaction Hamiltonian between a charge and the slab or gap surfacelike modes, we have given expressions that can account for the presence of insulators. We have shown that quantal effects in the barrier height of the potential experienced by an electron between two metals are important for $d \lesssim 4$ Å. For an electron at the edge of both a gap and a slab, finite width corrections are negligible for physical systems of interest.

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