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AN EVALUATION OF SELF ENERGY OF AN ELECTRON IN A GAP BETWEEN TWO METAL AND NEAR A METALLIC SLAB.

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Abstract: In this paper, we have evaluated the self energy of an electron located in the gap between two similar metals and near a metallic slab. Our theoretical result indicates that the self energy of an electron increases as a function of distance 'd' for $r_s = 2$ to 6, where r_s is a dimensionless parameter. The self energy of an electron located at the surface of metallic slab decreases with distance 'd'. We have observed that the quantum effects due to barrier height of the potential experienced by an electron between two metals are important for $d > 4 \text{ \AA}$.

Keywords: Scanning tunneling microscope, virtual excitation of polarization modes, surface like polarization, bulk polarization,, image potential, Thomas-Fermi length.

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INTRODUCTION

The study of the self-energy of a charged particle located in a gap between two metals or near a metallic slab is great interest in order to understand a number of experimental techniques frequently used in surface physics. Incharge-slab interaction plays an important role in the studies of thin films by means of particle-beam spectroscopy¹⁻⁶. As another example, the image potential expressed by a tunneling electron is of paramount importance in determining the I-V response of a junction^{7,8}. A problem has recently received a great deal of attention in connection with the scanning tunneling microscope^{9, 10}. The present paper is, a theoretical analysis of the interaction between a charged particle and the polarization modes of between a metallic slab and a metal-metal gap. One benefit at the similarity between these two physical systems by applying a common approach. One is particularly interested in studying the recoil effects which has so far been located with finite mass. This physical effect has so far been located in the literature, and one think it is of interest to made its importance in the total potential experienced by an electron. Manson and Ritchie¹¹ have proposed a reduced local self-energy formalism that accounts for the side's recoil accompanying the virtual excitation of polarization modes. Along the same line, Mahanty¹², Pathak, Paranjape, using the Manson-Ritchie approach, have studied the combined effects of recoil and Plasmon dispersion in the charge-metal-surface interaction. Sols and Ritchie¹³ have extended this method to locate the self-energy of a charge near an interface. To locate the effective polarization potential experienced a charge near a slab or in a gap, one must first know the dispersion relation of the surface like plasmons and their coupling to a charge. Since one is concerned with particular to the metal, one will not consider the bulk polarization.

MATERIALS AND METHODS :

One idealize the physical system by considering two media described by dielectric functions $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$. Assume that medium 1 fills the space defined by $z>a$ and medium 2 lies in the region $|z|<a$ where 'za' is the width of either the gap or the slab. If one takes the metal 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 reduced by the reversed case. The frequencies of the plasma oscillations which satisfy the matching condition are given implicitly by the dispersion relation⁷

$$\frac{\epsilon_1(\omega) - \epsilon_2(\omega)}{\epsilon_1(\omega) + \epsilon_2(\omega)} = \infty e^{-2Qa} \quad (1)$$

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

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

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.

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

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.

$$\hat{V} \sum_{Q,a} \Gamma_{Q\alpha g_{Q\alpha}}(z) e^{iQ \cdot \mathbf{p}} (a_{Q\alpha} + a_{Q\alpha}^+) \quad (4a)$$

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

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

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

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

where $\mathbf{r} = (\rho, z)$ is the vector position of the charge, A is the interface area, and $a_{Q\alpha}^+$ and $a_{Q\alpha}$ are the creation and annihilation operators of the surface like plasmons. It may be noted that

Eq. (4) can also be applied to be 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 $\lambda_{Q\infty}$ becomes

$$\lambda_{Q\infty} = \frac{1}{2(e^{2Q\infty} + \infty)} \quad (5)$$

Thus the electric potential created by a boundary Plasmon of momentum $\hbar Q$ and parity ∞ 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. The charge-slab interaction given by Eq. (4) is equivalent to the Hamiltonian used by various authors.^{4,5}

From the second-order energy shift, we can define the following projected self-energy

$$\Sigma(\mathbf{r}) = - \sum_{\mathbf{k}, \mathbf{n}} \frac{\Psi_{\mathbf{k}}(\mathbf{r}) \langle 0 | \hat{V} | \mathbf{n} \rangle \langle \mathbf{n} \Psi_{\mathbf{k}} | \hat{V} | 0 \Psi_0 \rangle}{\Psi_0(\mathbf{r}) \epsilon_{\mathbf{k}} - \epsilon_0 + \hbar \omega_{\mathbf{n}0} - i\eta} \quad (6)$$

$$\begin{aligned} \Sigma(z) = & - \frac{e^2}{(4\pi)^2} \sum_a \int d^2 Q \int dk \frac{e^{-ikz} (e^{ik\infty} + \infty e^{-ik\infty})}{k^2 + Q^2} \\ & \times \frac{e^{-Q\infty}}{1 + \infty e^{-eQ\infty}} \frac{P_{Q\infty}^2 g_{Q\infty}(z)}{k^2 + Q^2 + k_0 k + k_0 \cdot Q + P_{Q\infty} - i\eta} \end{aligned} \quad (7)$$

Where $P_{Q\infty} = (2m\omega Q \infty / \hbar)^{1/2}$ is the momentum associated with the recoil of the particle. In the low-velocity limit, $V \rightarrow 0$, the self-energy can be nearly separated into a classical and a quantum recoil contribution :

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

The classical term is

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

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 (7, 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. 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 electro dynamical 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 ($z>a$), one obtains

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

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 and $\Psi_k(r) = \langle r | \Psi_k \rangle$; ϵ_k and ϵ_0 are the eigenenergies of particle's motion; $\hbar\omega_{n0}$ is the excitation energy of a 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), (3) are introduced in Eq. (4) the self-energy of a charge velocity $\bar{V} = \hbar(\bar{K}_0, k_0) / m$ interacting with the surface plasmons of a gap or a slab is given by equation (7) and for a particle in the gap ($z<a$) is given by

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

where, in both equation,

$$S^2 = Q^2 + P_{Q\infty}^2 = Q^2 + \frac{2m}{\hbar} \omega_{Q\infty} \quad (11)$$

It may be noted that, when $S = Q$ is taken, equation (7) come identical to equation (9).

The self-energy (7.8-7.10), when evaluated as per $z=0$ and $z=a$, adopts simple analytical expressions limits $Q_s a \ll 1$ and $Q_s a \gg 1$. For a very narrow gap one obtains

$$\Sigma(0) = \Sigma(a) = -\frac{e^2 Q_b}{2}, Q_s a \ll 1, \quad (12)$$

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

$$\Sigma(0) = -\frac{e^2 \ln 2}{2a} \left(1 - \frac{2}{\ln 2} \frac{e^{-Q_s a}}{Q_s a} \right), Q_s a \gg 1,$$

$$\Sigma(0) = -\frac{e^2 Q_s}{2}, Q_s a \gg 1 \quad (13)$$

The limit (11) shows that the self-energy for a charge between two metals that are very close to one another to a uniform value equal to the bulk saturation value charge within the metal. In the opposite limits very wide gap between two metals, the self-energy of middle of the gap tends to the classical value.

RESULTS AND DISCUSSION :

In this paper, we have studied and evaluated the self-energy of an electron in a gap between two metal and near a metallic slab. Using the formalism of Manson and Ritchie, we have evaluated the self-energy of an electron located in the gap between two similar metals and near a metallic slab. The results are shown in Table, T_1, T_2 and T_3 representing. In Table T_1 we

have evaluated the self energy of an electron $\Sigma(0)$ in eV in the middle of a gap between two metals as a function of the metal-metal distance of for various metal electronic densities $r_s = 2, 4$ and 6 . From our theoretical result it appears that the self energy an electron $\Sigma(0)$, increases as a function of distance d for all the three metallic densities $r_s=2$ to 6 . In an another calculation, we have calculated the self energy of an electron located at one metal surface ($z=0$) as a function of the metal-metal gap width $d=2a$ for $r_s=2$ to 6 . These results indicate that $\Sigma(a)$ eV in larger for $r_s=6$ and smaller for $r_s=2$. In the results of Table T₃ the self energy of an electron located at the surface of metallic slab $\Sigma(a)$ as a function of slab width $2a$ for $r_s=2$ to 6 have been determined. Here $\Sigma(a)$ decreases with distance d . The decrease is larger for $r_s = 6$ and lower for $r_s=2$.

Table 1 : Result of self energy of an electron in the middle of a gap between two metals as a function of the metal-metal distance d for $r_s=2, 4$ and 6 .

$d(\text{Å}^0)$	$\Sigma(0)\text{eV}$		
	$r_s=2$	$r_s=4$	$r_s=6$
0	-15.2	-8.7	-6.2
0.5	-12.6	-6.2	-4.7
1.0	-8.4	-4.8	-4.3
1.5	-7.8	-4.7	-4.0
2.0	-6.2	-4.4	-3.8
2.5	-6.0	-4.3	-3.6
3.0	-5.8	-4.2	-3.4
3.5	-5.4	-4.1	-3.2
4.0	-5.0	-3.9	-3.0
4.5	-4.8	-3.8	-3.0
5.0	-4.6	-3.7	-2.6
5.5	-4.5	-3.6	-2.4
6.0	-4.3	-3.6	-2.0

Table 2 : Result of self energy of an electron location at one metal surface ($z=0$) as a function of metal-metal gap width $d=2a$ for various electron densities $r_s=2, 4$ and 6 .

$d(A^0)$	$\Sigma(0)eV$		
	$r_s=2$	$r_s=4$	$r_s=6$
0	-15.6	-8.6	-6.8
0.5	-14.2	-8.4	-6.4
1.0	-14.0	-8.2	-6.0
1.5	-13.8	-8.0	-5.8
2.0	-13.6	-7.8	-5.6
2.5	-13.4	-7.6	-5.4
3.0	-13.5	-7.4	-5.2
3.5	-13.2	-7.2	-5.0
4.0	-13.0	-7.0	-5.0

Table 3 : Result of self energy of an electron located at the surface of a metallic slab ($z=0$) as a function of slab width $d=2a$ for $r_s=2, 4$ and 6 .

$d(A^0)$	$\Sigma(0)eV$		
	$r_s=2$	$r_s=4$	$r_s=6$
0	-3.2	-2.0	-1.6
0.5	-5.4	-3.5	-2.2
1.0	-8.6	-5.8	-3.6
1.5	-12.6	-8.6	-4.8
2.0	-12.8	-11.8	-5.9
2.5	-13.6	-13.4	-6.2
3.0	-13.9	-14.0	-8.6
3.5	-14.2	-14.5	-9.8
4.0	-15.0	-15.6	-12.9

In these works, our theoretical results indicates about the role played by the particle recoil accompanying the virtual excitations of the Plasmon. For the interaction Hamiltonian between a change and the slab or gap surface like modes, one can account the expressions for the presence of insulators. It has been shown that quantum effects in the barrier height of the

potential experienced by an electron between two metals are important for $d > 4 \text{ \AA}$. For an electrons all the use both a gap and a slab finite width currents are negligible.¹⁵⁻²⁰

There are some recent calculation²¹⁻²⁸ for the self energy of electron near the metal-vacuum interface.

CONCLUSION :

In this paper, self energy of an electron located in the gap between two similar metals and near a metallic slab has been evaluated. It has been seen that self energy of electron increases as a function of distance for $r_s = 2$ to 6. However, the self-energy of electron located at the surface of metallic slab decreases with distance 'd'.

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