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AN EVALUATION OF TOTAL SELF ENERGY FOR A MOVING CHARGE AS A FUNCTION OF DISTANCE FOR THE METAL INSULATOR INTERFACE

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Abstract: In this paper, we have evaluated the real part of the self energy of a moving charge near a metal insulator interface like Al – LiF, Al-KCl and Al-NaCl. We have taken the polarization interaction due to Plasmon's, optical phonon and excitons. Our result indicates that the real part of self energy as a function of Z-decreases for Z< 0 and increases for Z > 0.

Keywords: Optical ultraviolet region, surface Plasmon's, polarization mode, structure less dielectric constant, eigenfrequencies, exciton field, polarization interaction.

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INTRODUCTION

In this paper we have presented the method of evaluation of real part of self energy due to metal-insulator surface for moving charge. This has been possible by obtaining an interaction Hamiltonian of charge 'e' with the electrostatic field created by the interface modes. Here, one analyse the properties of the polarization modes which are localized at the interface. The fact that the exciton and Plasmon energies are usually comparable because both lie in the optical ultraviolet region. These facts have forced to consider the electromagnetic coupling between these two different free surface modes. The response of the insulator in front of the metal plasmons can be described by a structureless dielectric constant. Within a local response model, one obtains a simple expressions for the eigenfrequencies of the strongly mixed interface modes as well as for their coupling Hamiltonian to an external charge[1-10]. The slow surface optical phonons have been found to be strongly screened by the fast surface plasmons and thus to contribute negligibly to the charge self energy. When fictitiously assuming that the exciton field is much faster than the Plasmon field, one has obtained expansions for the frequencies and coupling parameters which plays the role of dielectric constant. It has been noticed that a very good result can be obtained from the assumption of very fast exciton field[11]. Since the polarization contribution is only part of the total potential experienced by an electron, one adds a step function in the calculation of that part of the total self energy of the charge Re $\Sigma_t(z)$. This makes the resulting profile look closer to the actual total potential and the results can be modified by the inclusion of more reliable response modes[12].

MATERIALS AND METHODS:

One studies the polarization modes of a metal-insulator interface and their contribution to the self energy of a charge. One assumes a sharp boundary between the two media. Let the interface be at z = 0 the metal in z<0 and the insulator in z>0. The metal and insulator is described by the following dielectric functions.

$$\varepsilon_1(\omega) = 1 - \Omega_p^2/\omega^2 \qquad (1)$$

$$\varepsilon_2(\omega) = 1 - \frac{\Omega_e^2}{\omega^2 - \omega_e^2} - \frac{\Omega_1^2}{\omega^2 - \omega_t^2} \qquad (2)$$

Where Ω_p is the bulk Plasmon frequency of the metal $\Omega_e^2 = 4\pi\eta\alpha_0\omega_e^2$ where η is the atomic density and α_0 is the static atomic polarizability and $\Omega_t^2 = \omega_1^2 - \omega_t^2$ where ω_e is the longitudinal optical phonon frequency and ω_t is the transverse optical phonon frequency ω_e is the electronic excitation frequency. Use of equation (1) for the metal is equivalent to use of Hamiltonian (4) and (5) for the interaction with a changed particle. The validity of equation (2) to describe the response of a dielectric.

At the interface between the media described by dielectric function $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, the eigenmodes must satisfy the equation[13].

$$\varepsilon_1(\omega) + \varepsilon_2(\omega) = 0 \qquad (3)$$

Introducing (1) and (2) in (3) one finds and algebric equation with three solutions for ω^2. Taking advantage of the fact that $\omega_t << \Omega_p$ and $\omega_t << \Omega_e$, one finds the following three solutions.

$$\omega_1 = \omega_{-,}\ \omega_2 = \omega_+ \text{ and } \omega_3 = \omega_\varepsilon \qquad (4)$$

$$\omega_\pm^2 = \frac{1}{4}\left[\left(\Omega_p^2 + 2\omega_e^2 + \Omega_e^2\right) \pm \frac{1}{4}\left(\Omega_p^2 + 2\omega_e^2 + \Omega_p^2\right)^2 - 8\omega_e^2\Omega_p^2\right]^{\frac{1}{2}} \qquad (5)$$

Corrections to the expression given in (4) and (5) go like $(\omega_t/\Omega_p)^2 \sim 10^{-4}$. Thus the approximation $\omega_t/\Omega_p = 0$ can be considered exact for many practical purposes. Now one consider the limit.

$$\Omega_p^2/2 << \omega_e^2 + \Omega_e^2/2 \qquad (6)$$

In such cases, expression for the frequencies of the mixed modes reduce to very simple forces. The approximation (6) will not be acceptable in most real materials but is useful for qualitative in sight. When taken the limit in (6).

$$\varepsilon_\infty = 1 + \Omega_e^2/\omega_e^2$$

Then this will play the role of the dielectric constant which is of the used to describe the response of the insulator in the optical region of the spectrum[14-17]. The approximation (6) with transform equations (4) and (5) into

$$\omega_1^2 = \Omega_p^2/(\varepsilon_\infty + 1)$$
$$\omega_2^2 = \frac{1}{2}(\varepsilon_\infty + 1)\omega_e^2$$
$$\omega_3^2 = \omega_t^2 \qquad (7)$$

Clearly ω_1 corresponds to a surface Plasmon whose natural frequency $\left(\Omega_p/\sqrt{2}\right)$ has been shifted by the presence of the semi-infinite dielectric medium. ω_2 correspond to the free surface excitons which has not been altered by the slow surface plasmons. Both in (5) and (7), ω_3 is the vibrational frequency of the strongly screened surface phonons and is essentially different from ω_{s_0} where

$$\omega_{s_0}^2 = \left(\frac{\varepsilon_0 + 1}{\varepsilon_\infty + 1}\right)\omega_t^2$$

These conclusions have been confirmed by the calculations of the coupling of these modes to an external charge, because of this similarity one change the notation from equations (5) to (7) to

$$\omega_{ip} = \omega_1, \qquad \omega_{ie} = \omega_2, \qquad \omega_{i0} = \omega_3 \qquad (8)$$

where the subscript i stand for interface. The subscripts p, e and 0 for Plasmon, exciton and optical phonon respectively. Interface models are supposed to be in general of a mixed nature LiF two semi-infinite media i = 1, 2 be described by bulk dielectric functions.

$$\varepsilon_i(\omega) = 1 - \sum_j \frac{\Omega_{ij}^2}{\omega^1 - \omega_{ij}^2}.i = 1,2 \qquad (9)$$

Index J is summed over all.

The correlation self-energy for a charge moving in a medium whose only excitation is a dispersionless Plasmon of frequency ω_p is given by

$$\Sigma_b(\infty) = S(Q_p, 0) = -\frac{e^2\omega_p}{2\pi^2}\int \frac{d^3q}{q^2}\left(\omega_p + \frac{q^2}{2m} - q.\upsilon - i\eta\right) \quad (10)$$

It must be remembered that $\Sigma_s(0) = S(Q_s, 0)$ and thus the discussion applies entirely to the surface self-energy right at the interface.

The integral (10) can be calculated in several ways. One can use cylindrical coordinates. It is more straightforward to calculate first the angular variable in spherical polar coordinates. For the real part, we have.

$$\mathrm{Re}\,\Sigma_b(\infty) = -\frac{e^2\omega_p}{2\pi\upsilon}\int_0^\infty \frac{dq}{q}\,\mathrm{In}\left|\frac{1+q/2m\upsilon+\omega_p/q\upsilon}{1-q/2m\upsilon-\omega_p/q\upsilon}\right| \quad (11)$$

Eq. (11) can be written :

$$\mathrm{Re}\,\Sigma_b(\infty) = -\frac{e^2\omega_p}{2\pi\upsilon}\int_0^\infty \frac{dq}{q}\,\mathrm{In}\left|\frac{q+q_1}{q-q_1}\right| - \frac{e^2\omega_p}{2\pi\upsilon}\int_0^\infty \frac{dq}{q}\,\mathrm{In}\left|\frac{q+q_2}{q-q_2}\right| \quad (12)$$

Where $q_1 = m\upsilon - (m^2\upsilon^2 - 2m\omega_p/h)^{1/2},\ q_2 = m\upsilon + (m^2\upsilon^2 - 2m\omega_p/h)^{1/2}$ (13)

Both integrals in eq. (13) give the same result :

$$q_1 = \omega_p/\upsilon,\ q_2 \square\ 2m\upsilon \quad (14)$$

$$\int_0^\infty \frac{dx}{x}\,\mathrm{In}\left|\frac{1+x}{1-x}\right| = \frac{\pi^2}{2} \quad (15)$$

Thus

$$\mathrm{Re}\,\Sigma_b(\infty) = -\frac{\pi e^2\omega_p}{4\upsilon} \quad (14)$$

No matter what the value m is, as long as we are above the threshold. However, if we had assumed that the particle was classical $(m=\infty)$, the term $q^2/2m << q\upsilon$ for all q is a slowly convergent integral like (13). This makes the limit $m \to \infty$ not well defined.

The discrepancy would be removed if: (i) a cutoff were introduced in the q integral, (ii) an exponentially decaying factor were introduced, as in the surface self-energy, or (iii) Plasmon dispersion were taken into account. The result would be uniquely given by eq. (14) in the limit of high velocities, as can be argued from general considerations.

Let two semi-infinite media i = 1, 2 be described by bulk dielectric function:

$$\varepsilon_i(\omega) = 1 - \sum_j \frac{\Omega_{ij}^2}{\omega^2 - \omega_0^2}, i = 1,2 \qquad (15)$$

Index j is summned over all effective oscillators contributing to the response. Let ω_α be the frequencies satisfying the matching condition

$$\varepsilon_1(\omega_\alpha) + \varepsilon_2(\omega_\alpha) = 0 \qquad (16)$$

One assumes that the dielectric response has its origin in the polarizability of a set of microscopic oscillators such that the polarization vector is given by

$$\bar{P}_i = \sum_j n_y e_y \bar{k}_y \qquad (17)$$

Given by the definition of the dielectric constant where n_y is the density of oscillations of type j in medium i, e_y is their effective charge and $\overrightarrow{hy}$ in the dipole moment of the oscillator.

The equation of motion for a single oscillator will be

$$m_y(\bar{k}_y + \omega_y^2 \bar{k}_y) = lyE_2 \qquad (18)$$

Where $\bar{E}_i$ is the electric field in medium i. If the medium vibrates with frequency ω then equation (18) becomes.

$$m_{ij}(\omega_{ij} - \Omega^2) = l_{ij}\vec{E}_0 \tag{19}$$

$$P_1 = \frac{\varepsilon_1(\omega) - 1}{4\pi} E_i \tag{20}$$

(18) and (20) lead to the dielectric function (18), provided that

$$\Omega_{ij}^2 = 4\pi n_{ij} e_{ij}^2 / m_{ij} \tag{21}$$

General solutions for the electrostatic potential at an interface will be

$$\phi(r,t) = \sum_{Q.\alpha} \phi Q\alpha(t) \exp(iQ,\rho) \exp(-Q|z|) \tag{22}$$

Where α is summed over all possible interface modes. Since $\bar{E} = -\nabla\phi$ eqs. (21) and (22) lead to the general expression for the ocillators displacement.

$$u_{ij} = \sum_{Q.\alpha} \frac{e_{ij}/m_{ij}}{\omega_\alpha^2 - \omega_{ij}^2} [iQ, -Q\,sgn(z)] \phi_{Q\alpha}(t) \exp(iQ.\rho) \exp(-Q|z|) \tag{23}$$

The mechanical energy stored in the vibrating oscillators will be

$$W_M = \frac{1}{2} \sum_{ij} dV_i n_{ij} m_{ij} (u_{ij}^2 + \omega_{ij}^2 u_{ij}^2) \tag{24}$$

Where dV_i is the volume element in medium i.

The energy in the fields will be

$$W_F = \frac{1}{8\pi} \int dV E^2 \tag{25}$$

If the magnetic field energy is neglected.

From eqn. (23) and (25) the total energy for the particles plus the field, $W = W_M + W_{F+}$ is given by

$$W = \sum_{Q} C_{Q\alpha}(|\phi^2_{Q\alpha}|^2 + \omega^2_{\alpha}|\phi^2_{Q\alpha}|^2) \quad (26)$$

$$C_{Q\alpha} = \frac{AQ}{16\pi\omega_{\alpha}}\frac{d}{\omega_{\alpha}}(\varepsilon_1 + \varepsilon_2), \quad (27)$$

Where A is the total interface area. To obtain eqs. (26, 27) one has exploited the fact that the ω_{α} satisfy condition (26).

One now introduces the new variables $a_{Q\alpha}$; such that

$$\phi_{Q\alpha} = (D_{Q\alpha}/2\omega_{\alpha})(a_{Q\alpha} + a^*_{-Q\alpha}) \quad (28)$$

$$\phi_{Q\alpha} = -\frac{1}{2}iD_{Q\alpha}(a_{Q\alpha} + a^*_{-Q\alpha}) \quad (29)$$

Where $D_{Q\alpha}$ is a suitable constant,

The total energy W can now be written

$$\omega = \frac{1}{2}\sum_{Q.\alpha} C_{Q\alpha}D^2_{Q\alpha}(a_{Q\alpha}a^*_{Q\alpha} + a^*_{Q\alpha}a_{Q\alpha}) \quad (30)$$

If the a's are now interpreted as boson operators, i.e., $a^*_{Q\alpha} \rightarrow a^+_{Q\alpha}$ (an operator), and assuming

$$D^2_{Q\alpha} = \hbar\omega_a / C_{Q\alpha} \quad (31)$$

One has finally

$$W = \sum_{Q\alpha} \hbar\omega_{\alpha}\left(a^*_{Q\alpha}a_{Q\alpha} + \frac{1}{2}\right) \quad (32)$$

The interaction energy of a charge e with the electrostatic field created by the interface modes will be given by the Hamiltonian :

$$\bar{V} = e\phi(r) = \sum_{Q.\alpha} \Gamma_{Q\alpha} \exp(iQ.\rho) \exp(-Q|z|)(a_{Q\alpha} + a^{+}_{-Q\alpha}) \quad (33)$$

$$\Gamma^2_{Q\alpha} = \frac{\pi e^2 h\omega_\alpha}{AQ}\lambda_\alpha \quad (34)$$

$$\lambda_\alpha = 4\left(\omega_\alpha \frac{d}{d\omega_\alpha}(\varepsilon_1 + \varepsilon_2\right)^{-1} \quad (35)$$

RESULTS AND DISCUSSION:

In this paper, we have evaluated the real part of the self energy of a moving charge near a metal, insulator interface system. The metal insulator interface of the system chosen are Al-LiF, Al-KCl and Al-NaCl. These calculations have been performed by aking the velocity $u = u_F = 0.93$ au and m = 1. The Re $\Sigma(z)$ have been calculated as a function of z and the results for the above three systems have been given in table T_1, T_2 and T_3 respectively. The calculations have been performed by equations (1) and (2) in the light of equation (6). Our results indicate that the real part of the self energy due to moving charge near a metal insulator interface as a function of z decreases for z<0 and have a maximum negative values for z = 0 after that they increases for z>0. The negative values at z = 0 increases as one goes from Al/LiF to Al/NaCl interface. In the self energy calculations, we have taken the polarization interaction due to plasmons, optical phonons and excitons. Besides these, there are other physical effects which contribute to the total effective potential. To describe the motion of an electron between the conduction bands of a metal and an insulator, one suggests the simple rule that a step function be added such that the difference between the bulk saturation terms equals the difference between the bottom of the conduction bands as obtained from experimental data. The calculations of the total charge self energy near metal and insulator surface shown the role played by the different dynamical parameters like particle velocity etc. The particle velocity determines the overall value of the self-energy while momentum controls the small oscillations on the incident side and the range of convergence to semi classical limit. Due to the small value of the optical phonon frequency, the recoil of the particle has furned out to play a very important role near an insulator surface[14-17]. Recoil effects cannot be neglected upto distances of the order of $20\,\mathring{A}$ from the surface where one recovers the classical image potential. Another important conclusions concerning an insulator surface is the strong space dependence

of the electronic contribution to the charge self energy. This implies that the study of surface polaron must properly be included for the coupling of the electron to the localized electronic excitations in the insulator[18-20]. There is some recent calculation[21-28] on the metal insulator interface which also reveal the similar facts.

Table 1 : Evaluation of real part of the self-energy due to charge moving with velocity u for Al/LiF (metal insulator) surface modes $u = u_F = 0.93$ au, m =1

$Z(A^\circ)$	$Re\Sigma(z)eV$
-8	0.0534
-6	0.0405
-4	0.0058
-2	-0.2756
0	-16.273
2	-5.339
4	-2.674
6	0.0392
8	**0.0586**

Table 2: Real part of self energy due to Al/KCl (metal-insulator) surface modes for a charge moving with velocity $u = u_F = 0.93$ au, and m =1; $u = u_F = 0.93$ au, m =1

$Z(A^\circ)$	$Re\Sigma(z)eV$
-10	**0.0683**
-8	**0.0435**
-6	**0.0178**
-4	**-0.0534**
-2	**-0.6759**

0	-18.536
2	-8.027
4	-1.786
6	0.0138
8	0.0569
10	0.0758

Table 3: Real part of self energy due to Al/NaCl (metal-insulator) surface modes for a charge moving with velocity $u = u_F = 0.93$ au, and m =1; $u = u_F = 0.93$ au, m =1

$Z(A^\circ)$	$\mathrm{Re}\,\Sigma(z)eV$
-12	0.0742
-10	0.0510
-8	0.0267
-6	0.0089
-4	-0.3596
-2	-10.1267
0	-21.813
2	-8.532
4	-2.867
6	-0.1544
8	0.0435
10	0.0658
12	0.0789

CONCLUSIONS:

In this paper, we have presented a method of evaluation of real part of self energy due to metal-insulator interface due to moving charge. On insulator surface a strong space dependence of the electronic contribution to self energy of charge has been noticed. This work will help to study the coupling of the electron to the localized electronic excitations in the insulator.

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