Journal of Chemical, Biological and Physical Sciences

An International Peer Review E-3 Journal of Sciences

*Available online at*www.jcbsc.org

Ssection C: Physical Sciences

CODEN (USA): JCBPAT Research Article

A Theoretical Evaluation of Total Self Energy for a Static Charge near an Insulator-Vacuum Surface

Mundrika Mistry[1] and L. K. Mishra

[1]Department of Physics, D. N. College, Masaurhi, Patna (Bihar)

Department of Physics, Magadh University, Bodh-Gaya-824234(Bihar)

Received: 20 March 2014**; Revised:** 05 April 2014; **Accepted**: 10 April 2014

Abstract: The total self-energy for a static charge of mass m= 1 near an insulator-vacuum surface has been evaluated .The contribution to the total self-energy comes from exciton and optical phonon excitations. We have shown that the contribution to the exciton field for a distance close to the surface dominates over the optical phonons. Our theoretically evaluated results are of good agreement with the other theoretical workers.

Keywords: Self-energy for a static charge, Insulator-Vacuum surface, polarizable medium, second order perturbation theory, time dependent interaction Hamiltonian, effective particle-medium interaction energy

INTRODUCTION

The self-energy approach has proven to be a powerful technique to deal with interaction of charged particle with polarizable medium.. The self-energy is a complex quantity whose real part is the effective particle-medium interaction energy whose imaginary part gives the rate at which excitations are induced in the medium. The self-energy can be introduced different ways[1-4]. The most rigorous approach is that of many body theory, where the self-energy is defined as the shift in the poles of the propagator. The real part gives an effective potential which in general is non-local and energy dependent. For particles, whose motion is described classically a phenomenological definition of the self-energy can be introduced. If the response of the medium is described by classical electrodynamics, the real part is defined as one half the electrostatic potential experienced by the particle and the imaginary part is obtained from the dissipated power[5]. If the medium is described by quantum field theory as a system with many degrees of freedom, then the real part is defined as one half the expectation value of the time dependent interaction Hamiltonian and the imaginary part is obtained from the transition rate[6]. The factor (1/2) which is required in the definition of the real part of the self-energy for a classical particle interacting with a polarizable physical system is a characteristic feature of the linear response approximation to polarization interactions. The factor (1/2) appears naturally when a full quantum-mechanical treatment is applied. Monson and Ritchie[7] have proposed a prescription to calculate a projected self-energy that takes into account the quantum nature of the particle's motion. The starting point is the energy shift as calculated by an ordinary second order perturbation theory. This is equivalent to use the linearly response approximation for the medium. Such approximation is widely used in the study of particle motion in condensed matter and is known to keep most of the essential physics. Recently[6], we have evaluated the real and imaginary part of the surface contribution to the charge self-energy as a function metal-vacuum surface for different values of parameter $u\left(=k_0/Q_s\right)$ where k_0 is the wave vector of the particle and $Q_s=\sqrt{\dfrac{2m\omega_s}{\hbar}}$ m is the particle mass and $\hbar\omega_s$ is the surface Plasmon of the metal concerned. We have adopted Soles and Ritchie[9] formalism in our evaluation. The metal surfaces were Al, Na and K whose $\hbar\omega_s$ has been measured experimentally. Our analysis indicates that below the threshold $\left(k_0<Q_s\right)$ a small symmetric oscillations of $\Sigma_s(z)$ start to appear whereas above threshold on each side of z oscillations began to differentiate. In the positive side of z oscillations $\Sigma_s(z)$ are lengthening whereas in the negative side they are shortening. We have used for values of $v(=k_0/Q_s)$ in our calculations namely 0.9, 0.995, 1.005 and 1.1. For high $k_0(v=1.1)$ there is a rapid oscillation in the negative side and in the positive side oscillations are something like exp $(\mathrm{i}\omega_s z/\mathrm{u})$ where u is the particle velocity and u is finite. This type of signature is well pronounced in the case of Al metal vacuum surface whereas in the case of Na and K metal surface these oscillations are seen even for $k_0<Q_s$.

In this paper, we have estimated the total self-energy, for a static charge of mass m =1 near an insulator vacuum surface. The contribution to the total self-energy comes from exciton and optical phonon contribution. The insulators are LiF, NaCl and KCl. Our theoretical results indicate that $\Sigma_t(z)$ in both these insulators increase and decrease as a function of z between the value of z = -10 auto +1 au.

It was general belief that the optical phonon contribution is smaller and converges much more slowly as $z\to\infty$ than its exciton counterpart. But from our theoretical results, it indicates that $\Sigma_t(z)$ is of same trend although the values are slightly higher of KCl and NaCl in comparison to LiF values. One can say that in an insulator for an electron at rest, the effective cutoff due to electron's recoil is much more important that the stemming from the medium response. The contribution of the exciton field to that image potential at the distances close to the surface dominates the contribution from the optical phonons[10-12].

Mathematical formulae used in the evaluation: First, we discuss the self-energy induced by the bulk Plasmon modes. The coupling of a charged particle with the bulk modes of a semi-infinite medium may be written in terms of the Hamiltonian.

$$V_{eh}Q(Z)\sum_{Q}\sum_{p>0}X_q\exp(i.Q.q)$$

$$\sin(pz)(bq + \overset{+}{\underline{b}}q) \tag{1}$$

Where $q = (Q, p), b\overset{+}{q}, bq$, are the creation and annihilation operators of the bulk modes, $\overline{r} = (\overline{p}, z)$ is any point for charged particle.

$$\lambda_q^2 = \frac{4\pi e^2 \hbar \omega_b}{q^2 V} \lambda_b \tag{2}$$

Here $\lambda_b = 1$ for the plasmons, $\lambda_b = \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)$ for the optical phonons, $\lambda_b = \left(1 - \frac{1}{\varepsilon_\infty}\right)$ for the excitons and ω_b is the frequency of the bulk modes has been assumed dispersion less. If the unperturbed motion of the electron is supposed to be described by plane waves then after some calculations one can write.

$$\Sigma_b(z) = Q(z)\lambda_b\left[S(Q_b, 0) - S(Q_b, z)\right] \tag{3}$$

Where

$Q_b = (2m_b\omega_b/\hbar)^{1/2}$ And

$$S(Q_b, z) = -\frac{e^2 Q_b^2}{(2\pi)^2}\int a^2 Q \int dk$$

$$\frac{\exp(-Q/z)}{Q^2 + k^2} \frac{\exp(ikz)}{Q^2 + k^2 + 2k_0 k + 2k_0.Q + Q_b^2 - i\eta} \tag{4}$$

Where $u = \hbar(k_0, k_0)/m$ is the velocity of the particle and $\hbar(Q, k)$ is the momentum transfer to the medium $\eta \to O^+$. Equation (3) accounts for some well-known properties of the bulk energy. In the case of metal plasmons, for while $\lambda_s = \lambda_b = 1$ equation (3) shows that the contribution of the surface and the bulk to the static classical electric field (both mode frequency independent) exactly cancel in the metal. This is not the case for an insulator for which $\lambda_s \neq \lambda_b$.

Another important consequence of equation (3) is that the saturation value for the bulk self-energy is

$$\Sigma_b(\infty) = \lambda_b S(Q_b, 0) \tag{5}$$

The surface self-energy at z=0 applies identically for $\Sigma_b(\infty)$. One can in particular derive the stopping power of the medium for a charged particle from equation (5). In order to give an expression for stopping power, one introduces a cutoff q_c in the wave vector of the Plasmon cutoff would allow for unphysically large momentum transfers.

The following results are obtained[13-14].

$$\frac{dE}{dz} = -\frac{e^2\omega_b^2}{u^2} \ln\left(\frac{q_{max}}{q_{min}}\right) \tag{5a}$$

$$q_{min} = k_0 - (k_0^2 - Q_b^2)^{1/2} \tag{5b}$$

$$q_{max} = \min\left[q_c, k_0 + (k_0^2 - Q_b^2)^{1/2}\right] \tag{5c}$$

Suitable choices for the wave vector cutoff q_c are the limit of the Brillouin zone in the case of optical phonons. $q_c / k_F = (1 + \omega_b / E_F)^{1/2} - 1$ for the plasma oscillation of an electron gas[13] $q_c = r_0^{-1}$ where r_0 is the radius of the deepest atomic orbital involved in the excitation. When the cutoff plays no role equation (6) gives the stopping power which corresponds to the self-energy $S(Q_b, 0)$.

Which is given by

$$S(Q_b,0) = \begin{cases} -\dfrac{e^2\omega_b}{u}\sin^{-1}(r), |k_0| < Q_b \\ -\dfrac{e^2\omega_b}{u}(\pi/2 + i\cosh^{-1}(r), |k_0|) > Q_b \end{cases} \tag{6}$$

$$\nu = |k_0| Q_b$$

Now $q_{min} < q_c$ is required for the stopping power to be non-zero. Since $q_{min} \cong \omega_b / u$ for high momenta, this accounts is a simple way for the absence of losses to plasmons when slow massive particles move in the metals.

From equations (5) and (6) the effective mass m^* of the charged particle is obtained without cutoff.

$$m^* = \frac{m}{1 - \propto_b / b} \tag{7}$$

Where

$$\propto_b = \lambda_b e^2 Q_b / 2\hbar\omega_b \tag{8}$$

$= \lambda_b (e^2/\hbar)\left(m/2\hbar\omega_b\right)^{1/2}$ is dimensionless coupling constant between the charge and the bulk mode. For an electron interacting with the optical phonons of an insulator equation (8) gives the well-known formulae for the polaron effective mass obtained from perturbation treatment[15].

The total self-energy of the solid surface is given by

$$\Sigma_t(z) = \Sigma_s(z) + \Sigma_b(z) \tag{9}$$

Where

$$\Sigma_s(z) = \lambda_s S(Q_s, z)$$

And

$$S(Q_s, z) = -\frac{e^2 Q_s^2}{(2\pi)^2}\int d^2\vec{Q}\int dk \frac{e^{-Q|z|}}{Q^2+k^2} \times \frac{e^{ikz}}{Q^2+k^2 = 2k_0 k + 2k_0.Q + Q_s^2 - i\eta} \tag{10}$$

$\lambda_s = 1$ For metal surface Plasmon.

Now one proceeds to study the total self-energy for a charge near an insulator surface. The long wavelength response of an insulator can be approximated by the schematic dielectric function.

$$\varepsilon(\omega) = 1 - \frac{\Omega_e^2}{(\omega^2 - \omega_e^2)} - \frac{\Omega_t^2}{(\omega^2 - \omega_t^2)} \tag{11}$$

Where ω_t is the frequency of the transverse optical phonons and $\hbar\omega_e$ is an effective excitation energy of electronic transitions. Now, $\Omega_e^2 = 4\pi n \propto_0^2 \omega_0^2$ where n is the atomic density and $\propto_0$ is the static atomic polarizability. $\Omega_t^2 = (\omega_l^2 - \omega_t^2)$ Where ω_l is the longitudinal optical phonon frequency.

If ε_0 is the static dielectric constant and ε_∞ is the dielectric constant for frequencies $\omega_t \le \omega \le \omega_e$ the following relations hold

$$\varepsilon_0 = 1 + \frac{\Omega_e^2}{\omega_e^2} + \frac{\Omega_t^2}{\omega_t^2} \tag{12a}$$

$$\varepsilon_\infty = 1 + \Omega_e^2 / \omega_e^2 \tag{12b}$$

A medium described by equation (11) supports two different bulk modes together with their two surface counterparts. One follows Mahan[16] in referring to the higher frequency mode as the exciton while lower frequency on corresponds to the optical phenomenon. The frequencies of those modes[16] are

$$\left.\begin{aligned} \omega_{b0}^2 &= \frac{\varepsilon_0}{\varepsilon_\infty}\omega_t^2 \\ \omega_{be}^2 &= \varepsilon_\infty \omega_e^2 \end{aligned}\right\} \tag{13a}$$

$$\left.\begin{aligned}\omega_{s0}^2 &= \frac{\varepsilon_0+1}{\varepsilon_0-1}\omega_t^2\\ \omega_{se}^2 &= \frac{\varepsilon_\infty+1}{2}\omega_e^2\end{aligned}\right\} \tag{13b}$$

Where subscripts b and s stand for bulk and surface respectively and O and e optical phonon and exciton. The corresponding constants appear in Hamiltonian (1) are given below

$$\hat{V}_{es} = \sum_Q \Gamma_Q \exp(iQ.P)\exp(-Q|z|)(a_Q + \underline{a}_Q^+) \tag{14}$$

Where a_Q^+ and a_Q are the creation and annihilation operators for surface excitation with momentum Q parallel to the surface.

$$\lambda_{b0} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}, \lambda_{be} = 1 - \frac{1}{\varepsilon_\infty} \tag{15a}$$

$$\lambda_{s0} = \frac{\varepsilon_0-1}{\varepsilon_0+1} - \frac{\varepsilon_\infty-1}{\varepsilon_\infty+1}$$

$$\lambda_{se} = \frac{\varepsilon_\infty-1}{\varepsilon_\infty+1}$$

Since the dielectric function (11) is wave number independent, it is only strictly valid in the long wavelength limit. The separation between electron and ionic polarizability is not entirely correct. The fact can be partially accounted for by introducing effective charges in the displacement contribution. The modeling of the excitonic responses by a single atomic oscillator would be appropriate for a noble gas solid (without the optical phonon contribution), but for an ionic solid the polarizability of both anions and cations should be induced.

The total self-energy for a charge at an insulator surface computed in straight forward manner. Both the bulk and the surface self-energy have separate contribution form the excitons and optical Plasmon's.

The qualitative trends are the same as those of the self-energy at the metal surface. Difference comes from the coupling and the energy scale. We have static limit far from and right at the interface.

$$\Sigma_t(z \to -\infty) \cong -\frac{e^2(\varepsilon_0-1)}{4|z|(\varepsilon_0+1)} \tag{16a}$$

$$\Sigma_t(0) = -\frac{1}{2}e^2(\lambda_{so}Q_{so} + \lambda_{se}Q_{se}) \tag{16b}$$

$$\Sigma_t(z \to \infty) = -\frac{1}{2}e^2(\lambda_{so}Q_{so} + \lambda_{se}Q_{se}) + \frac{e^2}{4z\varepsilon_0}\frac{(\varepsilon_0 - 1)}{(\varepsilon_0 + 1)} \quad (16c)$$

Equation (16a) and the second term in equation (16c) are the well-known expressions for the classical image potential outside and inside an insulator respectively. The optical phonon contribution to the bulk saturation term corresponds to the body energy of the bulk polaran[13,14].

DISCUSSION OF RESULTS

In this paper, we have evaluated the total self-energy (excition plus optical phonon contribution) for a static charge of mass m =1 near an insulator vacuum surface. The evaluation has been carried out as function of distance z only. The insulators of our investigations are LiF, NaCl and KCl respectively. We have taken the experimental values of $\hbar\omega_t, \hbar\omega_e \in (\infty)$ amd $\varepsilon(0)$ in our calculations. Our theoretical results for total self-energy $\Sigma_t(z)$ in case of LiF-vacuum interface indicates that there is a two well defined peak of $\Sigma_t(z)$ both in the positive value of z = 0^4 and z = 8.0. In case of NaCl-vacuum surface the value of $\Sigma_t(z)$ have three well defined peak one at z = -3 a.u., z = 5 a.u. and z = 8 a.u. Similarly in the case of KCl – vacuum surface, our theoretical values indicates that there is only one peak of $\Sigma_t(z)$ as z = 6 a.u. between the value of z = -10 a.u. to +10 a.u. From these calculations it is clear that the results are same for these insulators indicating that the exciton and phonon contribution are exactly the same nature in these insulators[17-20]. There is some recent results[21-28] which also shows the similar behavior.

Table-1: Total self-energy (exciton plus optical phonon contribution) for a static charge of mass m = 1 near a LiF = vacuum surface. Following parameters have been used in the calculation.

Z(a.u.)	$\Sigma_t(z)$a.u.
-6	-0.055
-5	-0.065
-4	-0.070
-3	-0.075
-2	-0.082
-1	-0.093
0	-0.162
1	-0.234
2	-0.278
3	-0.342
4	-0.318
5	-0.306
6	-0.292
8	-0.216
10	-0.253

$\hbar\omega_t = 38\text{MeV}$; $\hbar\omega_e = 16.8\text{eV}$; $\varepsilon_\infty = 1.92$; $\varepsilon_0 = 8.9$; **LiF – Vacuum Surface**

Table-2: Total self-energy (exciton plus optical phonon contribution) for a static charge of mass m = 1 near a KCl= vacuum surface. Following parameters have been used in the calculation.

Z(a.u.)	$\Sigma_t(z)$a.u.
-10	-0.126
-8	-0.144
-6	-0.173
-4	-0.216
-2	-0.138
-0	-0.088
2	-0.052
4	-0.036
6	-0.075
8	-0.129
10	-0.216

$\hbar\omega_t = 17.61\text{MeV}$; $\hbar\omega_e = 8.4\text{eV}$; $\varepsilon_\infty = 2.1$; $\varepsilon(0) = 4.85$; **KCl – Vacuum Surface**

Table-3: Total self-energy (exciton plus optical phonon contribution) for a static charge of mass m = 1 near a NaCl= vacuum surface. Following parameters have been used in the calculation.

Z(a.u.)	$\Sigma_t(z)$a.u.
-8	-0.092
-7	-0.086
-6	-0.074
-5	-0.061
-4	-0.053
-3	-0.044
-2	-0.068
-1	-0.084
0	-0.124
1	-0.136
2	-0.148
3	-0.203
4	-0.214
5	-0.146
6	-0.118
7	-0.098
8	-0.054
10	-0.078

$\hbar\omega_t = 20.33\text{MeV}$; $\hbar\omega_e = 13.6\text{eV}$; $\varepsilon_\infty = 2.25$; $\varepsilon(0) = 5.9$; **NaCl – Vacuum Surface**

CONCLUSION

In this paper, total self-energy for a static charge of mass m = 1 near an insulator- vacuum surface has been estimated. The contribution to the total self-energy comes from both exciton and optical phonons. However, it is seen that the exciton contribution dominates over the optical phonons close to the surface.

REFERENCES

1. R. H. Ritchie, *Phys. Rev.,* 1957, 106**,** 874.
2. N. Takimoto, *Phys. Rev.,* 1966, 146**,** 366.
3. R. H. Ritchie, *Surface Sci.,* 1973, **34**, 1.
4. S. Munnix, and M. Scheits, *Phys. Rev.,* 1985, **B32,** 4192.
5. F. Flores, and F. Garcia Molinear, *J. Phys.* C., 1979, **12,** 907.
6. P.M. Echenique, R. H. Ritchie, M. Barbercon, and J.C. Inkson, *Phys Rev.,* 1981, **B23,** 6486.
7. J.R. Manson, and R.H., Ritchie, *Phys. Rev.,* 1981, **B24,** 4867.
8. K. P. Sinha, P. K. Verma, and L.K. Mishra, *Acta Ciencia Indica,* 2002, XXII**,** 207.
9. F. Soles, and R.H. Ritchie, *Phys. Rev.,* 1987, B35**,** 9314.
10. F. Soles, and R.H. Ritchie, *Solid State Common*, 1982, **63,** 248.
11. P de Andres, P.M. Echenque and F. Soles, *Phys., Rev.* 1987, **B35,** 4529.
12. F. Cuinea, J. Sanchez-Dehesa and F.Flores*, J. Phys.,* 1983, **16,** 6499.
13. R. H. Ritchie, *Phys., Rev.,* 1959, **114,** 644.
14. J. J. Quinn, *Phys. Rev.* 1962, **126,** 1453.
15. D. Pines, In polarons and excitons Eds. C.G. Kuper and G.D. Whitefield, *Plenum,* New York, 1963.
16. G. D. Mahan, *Phys. Rev.,* 1972, **B5,** 739.
17. C. Tejedor, F. Flores and E. Lovis, *J. Phys.,* 1997, **C20,** 2163.
18. R Ruppin, *Surface Sci.,* 1998, **129,** 286.
19. R. A.Young, *Solid State Common,* 1991, **65,** 263.
20. J. Sak, *Phys. Rev.,* 1996, **B62,** 1234.
21. S. Takanashi, K. Kawasaki and P. Toknre, Applied Physics Lett. (APL) 2001, **79**, 1324
22. I. Zutc , J. Fabion and S.D. Surve, Rev. Mod. Phys. 2004, **76,** 323
23. K. Uchida, S. Takanashi, K. Haril, J. Zeda and E. Saitoh, Nature, 2008, **455,** 778
24. A. Krejel, F. Sauli, L. Bartojel and P. Kopietz, Eur. Phys. J. 2009, **B71**, 59
25. J.C. Slonczlwski, Phys. Rev. 2010, **B82**, 054403
26. B. Lezk, H. Ulrich, F. Garbs and M. Munzlnbery, Phys. Report, 2011, **507** 107
27. C.E.W. Banch, E. Saitosh and B.J. Van Weel, Nature Mater, 2012, **11**, 391
28. L. Zhang, J. Ren, J.S. Wang and B.Li, Phys. Rev. 2013, **B87**, 144101

***Corresponding author: Mundrika Mistry;** Department of Physics, D. N. College, Masaurhi, Patna (Bihar)