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Collision Integral For The Interaction Of Electrons With Long Wavelength LO Phonons In Spatially Inhomogeneous Medium.

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Abstract : We have evaluated the total mechanical energy of the long wavelength longitudinal optical (LO) phonons. Then we have calculated the transition probability for the interaction of electrons with long wavelength longitudinal optical (LO)phonons in the spatially inhomogeneous medium. For the evaluation of transition probability we have calculated the advanced Green's function and hence the retarded Green's function. finally we have used the transition probability to find the expression for the collision integral for the interaction of electrons with long wavelength LO phonons in spatially inhomogeneous medium.

Key words : Phonons, Green's function, transition probability, collision integral.

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1. Introduction :

There are various types of electron-phonon interaction[1], such as interaction of the electrons with longitudinal optical (LO) phonons known as Fröhlich interaction, deformation potential interaction, interaction of the electrons with optical phonons due to deformation of the lattice which is important only in the non-ionic crystals where the Fröelich interaction is not present, and interaction of the electrons with acoustic phonons due to piezoelectric fields which is often weaker than the deformation-potential interaction. We have to mainly consider only the interaction of long wavelength LO phonons with electrons.

2. Energy of LO phonon

In case of ionic crystals, the optical phonons produce a dipolar field when the oppositely charged ions oscillate as a whole with respect to each other [2]. This dipolar field polarizes the electrons and leads to the coupling of electrons and phonons. Consider a biatomic ionic crystal, under the optical vibrations, the centre of mass of the cell remains at rest, and the atoms of the cell oscillate in antiphase. Here we have made the approximation that the displacements $\mathbf{u}_{\mathbf{n}s}$ (where elementary crystal cell is numbered by the integer vector **n** and the index s is the number of atoms in the cell) from the equilibrium position of the ions, do not depend on **n**, and the vibrations are described by the two variables $\mathbf{u}_+$ and $\mathbf{u}_-$ corresponding to the two ions having atomic masses m_+ and m_- and effective charges +e and –e respectively. Now as the centre of mass of the cell remains at rest, and the atoms of the cell oscillate in antiphase $m_+ \mathbf{u}_+ + m_- \mathbf{u}_- = 0$ therefore both $\mathbf{u}_+$ and $\mathbf{u}_-$ may be expressed in terms of the relative ionic displacement $\mathbf{u} = \mathbf{u}_+ - \mathbf{u}_-$ so there is only one independent variable **u** . In such vibrations each elementary cell will have a dipole moment e.**u** , and a significant contribution to the interatomic forces comes from the long range dipole-dipole interaction. The short-range part of the force is proportional to the relative shift **u** , and the long-range part is given by e·**E.** The longitudinal field **E** induces the polarization (N/V)α**E,** where α is the polarizability of the cell and N/V is the number of cells per unit volume. Therefore total polarization is **P** = (N/V)[e.**u** + α**E**] .
when the polarization induced by longitudinal modes is expressed in terms of the effective dielectric constant ε^* we get

$$\mathbf{P} = \sqrt{\frac{\omega_{LO}^2}{4\pi\varepsilon^*}}\,.\,\mathbf{W} \qquad \text{……….(i)}$$

The potential energy of interaction of electrons with the field induced by long wavelength optical phonons is obtained from the poisson equation

$$\nabla\left(\frac{U}{e}\right) = \mathbf{4\pi P} \,. \qquad \text{.........(ii)}$$

Only longitudinal optical(LO) phonons produce the long range electric field. The mechanical energy of the long wavelength longitudinal optical vibration in an ionic biatomic crystal is given by the expression[3]

$$\mathcal{E}_{LO} = \int_{(v)} d\mathbf{r} \; (\omega_{LO}^2 \, .\mathbf{W} + \dot{\mathbf{W}}^2) \qquad \text{..........(iii)}$$

Where $\mathbf{W} = (Nm/V)^{1/2}\,\mathbf{u}$, and m is the reduced mass given by the expression $m = (m_+ m_-)/(m_+ + m_-)$.

Therefore using (ii), (iii) and (iv) we can write,

$$\mathcal{E}_{LO} = 2\pi \int_{(v)} d\mathbf{r} \;\; \varepsilon^* (\dot{\mathbf{P}}^2 \omega_{LO}^{-2} + \mathbf{P}^2) \qquad \text{.........(iv)}$$

$$\mathcal{E}_{LO} = \frac{1}{8\pi e^2} \int_{(v)} d\mathbf{r} \;\; \varepsilon^* [(\nabla\dot{U})^2 \omega_{LO}^{-2} + (\nabla U)^2] \qquad \text{..........(v)}$$

In case of inhomogeneous medium the dielectric constant $\varepsilon^* = \varepsilon^*(\mathbf{r})$ and the longitudinal optical phonon frequency $\omega_{LO} = \omega_{LO}(\mathbf{r})$.

3.Calculation of retarded Green’s function

Using the equation (v), we can write the equation for Green’s function[4] corresponding to the Lagrange equation of motion for U as follows,

$$[\,(\omega - i0)^2 \, \nabla \frac{\varepsilon^*}{\omega_{LO}^2} \nabla - \nabla\varepsilon^* \nabla] \;\; g_\omega^A(\mathbf{r},\mathbf{r'}) = 4\pi e^2 \,\delta\,(\mathbf{r} - \mathbf{r'}) \qquad \text{.........(vi)}$$

The equation for the retarded Green’s function differs from this equation by the factor $(\omega + i0)$ in place of $(\omega - i0)$. These functions are expressed through each other as[3] $g_\omega^R(\mathbf{r},\mathbf{r}') = g_\omega^{A*}(\mathbf{r},\mathbf{r'})$.

We are going to define the spatial in-homogeneity in such a way that the spatial in-homogeneity is along the z-axis only and the medium is homogeneous along x-axis and y-axis. i.e. the total mechanical energy for the long wavelength longitudinal optical phonon $\mathcal{E}_{LO}$ will depend on the z- coordinate only. Now to simplify the problem we define

$$\left[\frac{\varepsilon^*(\mathbf{r})}{\omega_{LO}(\mathbf{r})}\right] = \left[\frac{\varepsilon^*(z)}{\omega_{LO}(z)}\right] = \left[\frac{\varepsilon_1^*}{\omega_{LO\,1}}\right] \quad \text{for} \quad z > 0 \qquad \text{..........(vii)}$$

$$\left[\frac{\varepsilon^*(\mathbf{r})}{\omega_{LO}(\mathbf{r})}\right] = \left[\frac{\varepsilon^*(z)}{\omega_{LO}(z)}\right] = \left[\frac{\varepsilon_2^*}{\omega_{LO\,2}}\right] \quad \text{for} \quad z < 0 \qquad \text{..........(viii)}$$

and $\left[\frac{\varepsilon^*(\mathbf{r})}{\omega_{LO}(\mathbf{r})}\right]$ changes abruptly at $z = 0$.

Where ε_1^* , ε_2^* , $\omega_{LO\,1}$ and $\omega_{LO\,2}$ are constants.

Equation (vi) can be solved using the boundary conditions (vii) and (viii).

To find the transition probability $K_\omega(q \mid z, z')$, first of all we shall evaluate the advanced Green's function and hence the retarded Green's function using the equations (vi) , (vii) and (viii).

The advanced Green's function can be written in the (q,z) representation as $g_\omega^A(q \mid z, z')$. After simplifying the equation (vi) we get

$$\left[\frac{\partial^2}{\partial z^2} - q^2\right] g_\omega^A(q \mid z, z') = \frac{4\pi e^2 \omega_{LO\,1}^2\, \delta(\mathbf{r}-\mathbf{r}')}{\varepsilon_1^*[(\omega - i0)^2 - \omega_{LO\,1}^2]} \quad \text{for} \quad z > 0 \qquad \text{...........(ix)}$$

$$\left[\frac{\partial^2}{\partial z^2} - q^2\right] g_\omega^A(q \mid z, z') = \frac{4\pi e^2 \omega_{LO\,2}^2\, \delta(\mathbf{r}-\mathbf{r}')}{\varepsilon_2^*[(\omega - i0)^2 - \omega_{LO\,2}^2]} \quad \text{for} \quad z < 0 \qquad \text{..........(x)}$$

Now we solve the equation (ix) and (x) under the circumstances that

(a) $\lim_{z\to\pm\infty} g_\omega^A(q \mid z, z') = \text{finite}.$

(b) $g_\omega^A(q \mid z, z')$ is continuous at $z = 0$.

(c) $\varepsilon^{*}[\frac{(\omega-i0)^2}{\omega_{LO}^2}-1]\,.\,\frac{\partial}{\partial z}\,g_{\omega}^{A}(q\mid z,z')$ is continuous at z = 0.

After solving the equation (ix) we get

$$g_{\omega}^{A}(q\mid z,z') = \frac{2\pi e^2\omega_{LO1}^2}{q\varepsilon_1^{*}[(\omega-i0)^2-\omega_{LO1}^2]}\left(e^{-q|z-z'|}+\frac{\xi_{+}-\xi_{-}}{\xi_{+}+\xi_{-}}\;e^{-q|z|-|z'|}\right)$$

for $z > 0$ ……(xi)

and after solving the equation (x) we get

$$g_{\omega}^{A}(q\mid z,z') = \frac{2\pi e^2\omega_{LO2}^2}{q\varepsilon_2^{*}[(\omega-i0)^2-\omega_{LO2}^2]}\left(e^{-q|z-z'|}-\frac{\xi_{+}-\xi_{-}}{\xi_{+}+\xi_{-}}\;e^{-q|z|-|z'|}\right)$$

for $z < 0$ …….(xii)

Where we have defined the parameters ξ_{+} and ξ_{-} as

$$\xi_{+} = \varepsilon_1^{*}[\frac{(\omega-i0)^2}{\omega_{LO\,1}^2}-1] \quad \text{and} \quad \xi_{-} = \varepsilon_2^{*}[\frac{(\omega-i0)^2}{\omega_{LO\,2}^2}-1]$$

Therefore from equations (xi) and (xii) we can find $g_{\omega}^{R}(q\mid z,z')$ using the relation $g_{\omega}^{R}(q\mid z,z') = g_{\omega}^{A*}(q\mid z,z')$

4. Transition probability

The transition probability[5],[6] from the electron state Ψ_z for the electron with momentum **p** to the state $\Psi_{z'}$ with momentum **p′** due to the interaction of an electron with long wavelength LO phonon is given by

(i) For the emission process

$$W(\mathbf{p},\mathbf{p}') = \frac{1}{L^2}\int d\omega\; K_{\omega}[(p-p')/\hbar].\,[N(\omega)+1].\,\delta(\varepsilon_p-\varepsilon_{p'}-\hbar\omega) \quad ….(xiii)$$

(ii) For the absorption process

$$W(\mathbf{p}', \mathbf{p}) = \frac{1}{L^2} \int d\omega\, K_\omega[(p - p') / \hbar].\; N(\omega) \,.\, \delta(\varepsilon_p - \varepsilon_{p'} - \hbar\omega) \qquad \text{.......(xiv)}$$

Where $N(\omega) = [\exp(\hbar\omega/kT) - 1]^{-1}$ is planck distribution function. k is Boltzmann's constant, and L^2 is the normalized area in the x-y plane.

and $$K_\omega(q) = \int dz \int dz' \mid \Psi_z \mid^2 . \mid \Psi_{z'} \mid^2 .\, K_\omega(q \mid z, z') \;. \qquad \text{......(xv)}$$

To find $K_\omega(q)$ in the above integral, we consider a rectangular potential well in the hard-wall model[6] , with $\Psi_z = \sqrt{2/d}\cos[\pi(z - z_0)/d]$, where z_0 is the distance of the centre of the well from the surface.

And the function $K_\omega(q \mid z, z')$ is given by the equation[3]

$$K_\omega(q \mid z, z') = i[g_\omega^R(q \mid z, z') - g_\omega^A(q \mid z, z')]$$

$$= -2.\ \text{Imaginary part of}\ g_\omega^R(q \mid z, z') \qquad \text{.......(xvi)}$$

Hence we can write from equation (xv) and (xvi)

$$K_\omega(q) = \int dz \int dz' \mid \Psi_z \mid^2 . \mid \Psi_{z'} \mid^2 .\, K_\omega(q \mid z, z')$$

$$= -2. \int dz \int dz' . \mid \sqrt{2/d}\cos[\pi(z - z_0)/d] \mid^2 .$$

$$\mid \sqrt{2/d}\cos[\pi(z' - z_0)/d] \mid^2 . \mathrm{Im} g_\omega^R(q \mid z, z')$$

$$= -\frac{8}{d^2} \int dz \int dz' . \mid \cos[\pi(z - z_0)/d] \mid^2 .$$

$$\mid \cos[\pi(z' - z_0)/d] \mid^2 . \mathrm{Im} g_\omega^R(q \mid z, z') \qquad \text{......(xvii)}$$

From (xiii), (xiv) and (xvii) we can write

$$W(\mathbf{p}, \mathbf{p}') = W(\mathbf{p}', \mathbf{p}).\ \exp[(\varepsilon_p - \varepsilon_{p'})/kT] \qquad \text{.......(xviii)}$$

Finally we get the collision integral[6] corresponding to the kinetic equation for the electrons interacting with long wavelength LO phonons in spatially inhomogeneous medium as follows

$$J_{e,\,\text{LO phonon}} = \sum_{\mathbf{p}} [W(\mathbf{p}', \mathbf{p}).\, f_{\mathbf{rp}'t}\,(1 - f_{\mathbf{rp}t}) - W(\mathbf{p}, \mathbf{p}').\, f_{\mathbf{rp}t}(1 - f_{\mathbf{rp}'t})]$$

……….(xix)

Where $f_{\mathbf{rp}t}$ is Wigner distribution function of electrons for the case of weakly inhomogeneous system.

5. Conclusion

From the equation (xix) for the collision integral it is obvious that, as a special case if we assume Fermi distribution function in place of Wigner distribution function we will get the zero value (as it should be) for the collision integral. The equation (xix) may also be used to find the quantum kinetic equation[7] for the electrons interacting with long wavelength LO phonons in a spatially non-homogeneous medium.

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