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On the interaction of electrons with electromagnetically active excitations in bulk polar semiconductors

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Abstract. The interaction of electrons with LO phonons, plasmons and coupled LO-phonon/plasmons is described. A simple unifying theory describing long-wavelength excitations in bulk polar semiconductors is developed using results from crystal optics. Predictions pertaining to hot electron relaxation via the emission of coupled modes are shown to be in excellent agreement with recent key investigations.

The interaction of electrons with the electromagnetic fields associated with the elementary excitations of a polar semiconductor is of crucial importance for electron energy relaxation [1, 2]. In particular, longitudinal optical (LO) phonons, plasmons and coupled LO-phonon/plasmons are known to be important in limiting device performance at high fields [3–5]. In this paper, we develop a simple unifying method, utilizing general results from crystal optics, to obtain the interaction Hamiltonian for general electromagnetically active modes interacting with electrons. In particular, it is shown that the simple long-wavelength approximations, which have the advantage of yielding analytic results, agree very well with recent investigations concerning the relaxation of electron energy via the emission of coupled LO-phonon/plasmon modes.

Our approach views the fields associated with the modes as simply electromagnetic waves propagating through the polar material which is characterized by a frequency-dependent dielectric function $\epsilon(\omega)$ (we ignore damping and spatial dispersion). From general considerations, the details of which may be found in the works by Landau and Lifshitz [6] and Agranovich and Ginzburg [7], the field Hamiltonian is

$$H_{\mathrm{f}} = \tfrac{1}{2}\epsilon_0 \int \left\{ \frac{\partial[\omega\epsilon(\omega)]}{\partial\omega} E^2 + c^2 B^2 \right\} \mathrm{d}^3 r \qquad (1)$$

in which $\boldsymbol{E}$ is the electric field, $\boldsymbol{B}$ the magnetic field, ϵ_0 the permittivity of free space and c the velocity of light in vacuo. This Hamiltonian, together with Maxwell's equations in the absence of free charges completely determine the electromagnetic fields.

We now restrict the investigation to the most important class of excitations which interact with electrons in bulk materials, namely the longitudinal modes defined by

$$\epsilon(\omega) = 0. \qquad (2)$$

In general there will be more than a single frequency satisfying (2); we label these by ω_j. Due to Faraday's law of induction, longitudinal modes are characterized by a vanishing magnetic field. We now express the electric field in the quantized form

$$\hat{E}_j(\boldsymbol{r}) = \int \mathrm{d}^3 q\,(\boldsymbol{E}_{0j}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} a_j(\boldsymbol{q}) + \mathrm{HC}). \tag{3}$$

Here $a_j(\boldsymbol{q})$ is a Boson operator satisfying the usual commutator relationships. The field amplitudes $\boldsymbol{E}_{0j}$ are obtained by substituting (3) into (1) and expressing the Hamiltonian in the canonical form.

$$\tfrac{1}{2}\epsilon_0 \int \mathrm{d}^3 r \left\{ \omega_j \left(\frac{\partial\epsilon(\omega)}{\partial\omega}\right)_{\omega=\omega_j} \right\} \hat{E}_j^2(\boldsymbol{r}) = \int \mathrm{d}^3 q\, \hbar\omega_j [a_j^{\dagger}(q) a_j(q) + \tfrac{1}{2}]. \tag{4}$$

It is then straightforward to show that

$$\boldsymbol{E}_{0j} = \left[\frac{\hbar}{(2\pi)^3\epsilon_0} \left(\frac{\partial\epsilon(\omega)}{\partial\omega}\right)^{-1}_{\omega=\omega_j} \right]^{1/2} \hat{\boldsymbol{q}} \tag{5}$$

where $\hat{\boldsymbol{q}}$ is the unit vector in the $\boldsymbol{q}$-direction since for longitudinal modes the electric field and wavevector are parallel. The electrons couple to these Coulomb modes via their electrostatic potentials with the interaction Hamiltonian given by

$$\hat{H}_j^{(\mathrm{int})}(\boldsymbol{r}) = -e\hat{\Phi}_j(\boldsymbol{r}) \tag{6}$$

where the potential operator $\hat{\Phi}_j(\boldsymbol{r})$ is related to $\hat{E}_j(\boldsymbol{r})$ through

$$\hat{E}_j(\boldsymbol{r}) = -\nabla\hat{\Phi}_j(\boldsymbol{r}). \tag{7}$$

The interaction Hamiltonian can be expressed as

$$\hat{H}_j^{(\mathrm{int})}(\boldsymbol{r}) = \int \mathrm{d}^3 q\, \{C_j(q)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} a_j(q) + \mathrm{HC}\} \tag{8}$$

with

$$C_j(q) = -\frac{\mathrm{i}}{|q|} \left[\frac{e^2\hbar}{(2\pi)^3\epsilon_0} \left(\frac{\partial\epsilon(\omega)}{\partial\omega}\right)^{-1}_{\omega=\omega_j} \right]^{1/2} \tag{9}$$

the coupling parameter. We have finally arrived at a concise, general expression for the interaction Hamiltonian for which we now consider specific examples.

Case (i) LO *phonons.* To describe the interaction of electrons with LO phonons the appropriate dielectric function is

$$\epsilon(\omega) = \epsilon_\infty \left(\frac{\omega^2 - \omega_{\mathrm{L}}^2}{\omega^2 - \omega_{\mathrm{T}}^2} \right). \tag{10}$$

In this equation ω_{L} and ω_{T} are the longitudinal and transverse optical phonon frequencies with ϵ_∞ the high frequency dielectric constant. Substitution of equation (10) into (9) and making use of the Lyddane–Sachs–Teller relationship gives

$$C(q) = \frac{-\mathrm{i}}{4|q|} \left\{ \frac{e^2\hbar\omega_{\mathrm{L}}}{\pi^3\epsilon_0} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) \right\}^{1/2} \tag{11}$$

which is the usual Fröhlich coupling parameter (see e.g. [2]).

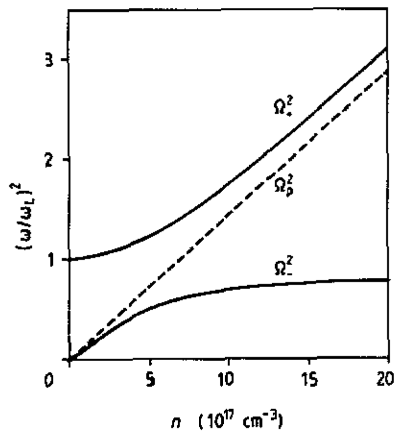

Figure 1. Coupled mode frequencies as a function of carrier concentration.

Case (ii) plasmons. To describe the plasma modes we use the simple long-wavelength expression for the dielectric function namely

$$\epsilon(\omega) = \epsilon_\infty \left(1 - \frac{\omega_p^2}{\omega^2}\right) \tag{12}$$

where ω_p is the plasma frequency given by

$$\omega_p^2 = \frac{ne^2}{m^* \epsilon_\infty \epsilon_0} \tag{13}$$

with n the carrier concentration and m^* the effective mass. In this case the coupling parameter is found to be

$$C(q) = \frac{-i}{4|q|} \left[\frac{e^2 \hbar \omega_p}{\pi^3 \epsilon_0 \epsilon_\infty}\right]^{1/2} \tag{14}$$

when the plasmon dielectric function is substituted into the general expression. The plasmon coupling parameter can also be obtained by replacing ω_L by ω_p in (11) and letting the static dielectric constant, ϵ_s, tend to infinity (i.e. $\omega_T \to 0$).

Case (iii) coupled LO-phonon/plasmons. It is well known that if ω_p is close to ω_L then pronounced coupling between the LO phonons and the plasmons occurs. The dielectric function appropriate for this coupled mode regime is [8]

$$\epsilon(\omega) = \epsilon_\infty \left(\frac{\omega^2 - \omega_L^2}{\omega^2 - \omega_T^2} - \frac{\omega_p^2}{\omega^2}\right). \tag{15}$$

Again we ignore the dispersion of the modes and concentrate on the long-wavelength limit for which (15) is appropriate. For the coupled mode case there are two solutions to equation (2) given by

$$\omega_\pm^2 = \tfrac{1}{2}[(\omega_L^2 + \omega_p^2) \pm \{(\omega_L^2 + \omega_p^2)^2 - 4\omega_p^2\omega_T^2\}^{1/2}]. \tag{16}$$

It is straightforward to show that at low carrier concentration $\omega_+ \simeq \omega_L$ with $\omega_- \sim \omega_p(\epsilon_\infty/\epsilon_s)^{1/2}$. At high densities $\omega_+ \simeq \omega_p$ and $\omega_- \simeq \omega_T$ the latter illustrating that the LO-phonon is screened and hence oscillates at the transverse optical frequency [2]. Figure 1 illustrates the variation of these modes with carrier concentration.

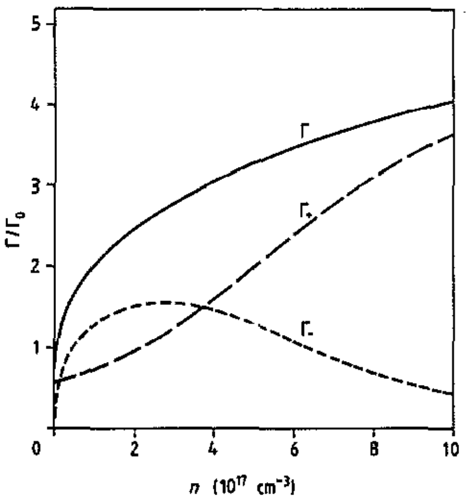

Figure 2. Total emission rate $\Gamma(=\Gamma_+ + \Gamma_-)$ as a function of carrier concentration for fixed $x = 7.7$.

The coupling parameter is given, after substituting equation (15) into equation (9), by

$$C_\pm(q) = \frac{-\mathrm{i}}{4|q|}\left[\frac{e^2\hbar\omega_{\mathrm{L}}\Omega_\pm}{\pi^3\epsilon_0\epsilon_{\mathrm{s}}F_\pm}\right]^{1/2} \tag{17}$$

where

$$F_\pm = \Omega_\pm^2\left[\frac{1-\Omega_{\mathrm{T}}^2}{(\Omega_\pm^2-\Omega_{\mathrm{T}}^2)^2}\right] + \frac{\Omega_{\mathrm{p}}^2}{\Omega_\pm^2} \tag{18}$$

and all the frequencies are in units of ω_{L} (e.g. $\Omega_\pm = \omega_\pm/\omega_{\mathrm{L}}$). It is a simple exercise to obtain the previous coupling parameters from equation (17). We take the analysis further by considering the electron relaxation rate which is given by Fermi's golden rule (assuming that only emission processes are allowed).

$$\Gamma_\pm = \frac{2\pi}{\hbar}\int\int \mathrm{d}^3K_{\mathrm{f}}\,\mathrm{d}^3q|\langle K_{\mathrm{f}},\{q\}|\hat{H}_\pm^{(\mathrm{int})}|K_{\mathrm{i}},\{0\}\rangle|^2\delta(E_{\mathrm{i}}-E_{\mathrm{f}}-\hbar\omega_\pm). \tag{19}$$

Here the electron states are simply plane waves

$$|K\rangle = \frac{1}{(2\pi)^{3/2}}\mathrm{e}^{\mathrm{i}K\cdot r} \tag{20}$$

with energy

$$E = \frac{\hbar^2K^2}{2m^*}. \tag{21}$$

In equation (19) i and f refer to the initial and final states. The integrations involved in determining the rate are straightforward and we find

$$\Gamma_\pm = \Gamma_0\left(\frac{\epsilon_{\mathrm{s}}}{\epsilon_{\mathrm{s}}-\epsilon_\infty}\right)\frac{\Omega_\pm}{F_\pm x^{1/2}}[\ln\{x^{1/2}+(x-\Omega_\pm)^{1/2}\} - \tfrac{1}{2}\ln\Omega_\pm] \tag{22}$$

with $x = E_i/\hbar\omega_L$ and Γ_0 is the typical scattering rate with bare LO phonons expressible as

$$\Gamma_0 = \frac{e^2}{4\pi\epsilon_0\hbar}\left(\frac{2m^*\omega_L}{\hbar}\right)^{1/2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right) \tag{23}$$

which has a value of approximately 8.7×10^{12} s^{-1} for GaAs.

Recent experiments by Peterson and Lyon [9, 10] have demonstrated electron energy relaxation via these coupled modes. Figure 2 depicts the variation in the rates as a function of carrier concentration for fixed $x = 7.7$ which correspond to their experimental value. It is seen that at low concentrations Γ_+ is close to the bare LO-phonon rate whilst Γ_- is small. As the carrier concentration increases, Γ_- rapidly increases before dropping below Γ_+ above a concentration of around 4×10^{17} cm^{-3}. We may now compare our results with those reported by Peterson and Lyon. The total rate at a carrier concentration of 7×10^{17} cm^{-3} is 3.62 Γ_0 which is 2.6 times that for a concentration of 3×10^{16} cm^{-3} (where the contribution to the total rate of Γ_- is still important). This is in excellent accord with the results reported by Peterson and Lyon. The scattering time obtained is 32 fs again in agreement with the results of [10] where 35 fs is quoted. These successful comparisons indicate that the long-wavelength modes ($q \simeq 0$) are mainly responsible for electron energy relaxation. The reason for this is as follows. The theory presented here completely ignores the damping of the modes. This is an oversimplification especially for modes which lie within the single particle continuum where Landau damping may make the concept of a well defined mode meaningless. Nevertheless, in the experiments of Peterson and Lyon the initial electron energy is high ($x = 7.7$) and hence the wavevectors of the scattered coupled modes can be very small compared with the Fermi wavevector and thus lie outside the single particle regime. The coupling parameters favour just these modes. For the initial electron energy and carrier concentrations considered here it seems that these well defined modes are largely responsible for relaxing the carrier energy.

In conclusion we have shown how the interaction of an electron with the electromagnetic waves produced by dipole active excitations may be described in a simple unified manner. We have assumed that the dielectric function is wavevector independent, although this was shown not to be too much of a handicap as successful comparison was achieved with recent results. A wavevector-dependent dielectric function may be readily incorporated within this formulation. The interaction of electrons with the polariton modes has not been included here as they do not interact strongly with electrons in bulk systems [11]†. The formalism described in this work has also been extended to excitations in lower dimensional systems [12] in which surface polariton waves are important.

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† It should be noted that the authors in this work used an incomplete Hamiltonian for the free fields. Their quantitative results that the electromagnetic field associated with polaritons scatter electrons weakly in the bulk should still hold.

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