(B) NON-POLAR OPTICAL PHONON SCATTERING - INTRAVALLEY

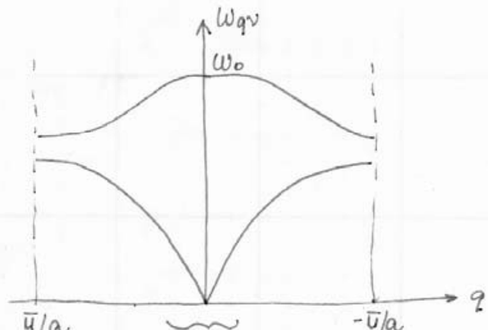
- Unlike the case of acoustic phonons, long wavelength optical displacement affects the electronic energy directly. Thus, the electron-phonon interaction Hamiltonian takes the form:

$$H_{ep} = \vec{D}_o \cdot \vec{u}$$

where $\vec{D}_o$ is the optical deformation potential constant and $\vec{u}$ represents the relative displacement of the two atoms within the unit cell. The units of D_o are eV/cm. The coupling constant $C_{q\nu}$ in the expression for the matrix element is $C_{q\nu} = D_o$, which leads to:

$$|M_{fi}|^2 = \frac{\hbar D_o^2}{2\rho V \omega_{q\nu}} \left(n_{q\nu} + \frac{1}{2} \mp \frac{1}{2}\right) \delta(\vec{k} \pm \vec{q} - \vec{k}') \quad \text{for normal processes}$$

- For long-wavelength phonons near the center of the Brillouin zone, the dispersion curve is very flat and one can assume that $\omega_{q\nu} = \omega_o = \text{const}$



phonons involved in intravalley scattering processes

Therefore, q_{min} and q_{max}, are calculated by solving:

$$\frac{q}{2k} \overset{\text{abs.}}{\underset{\text{em.}}{\pm}} \cos\theta \mp \frac{m^*\omega_o}{\hbar k q} = 0 \implies q^2 \pm 2kq\cos\theta \mp \frac{2m^*\omega_o}{\hbar} = 0$$

The solutions of this quadratic equation are:

$$q_{1/2} = \mp \frac{2k\cos\theta}{2} \pm \frac{1}{2}\sqrt{4k^2\cos^2\theta \pm \frac{8m^*\omega_o}{\hbar}}$$

$$= \mp k\cos\theta \pm \sqrt{k^2\cos^2\theta \pm \frac{2m^*\omega_o}{\hbar}} = \mp k\cos\theta \pm k\sqrt{\cos^2\theta \pm \frac{2m^*\hbar\omega_o}{\hbar^2 k^2}}$$

$$q_{1/2} = k\left[\mp\cos\theta \pm \sqrt{\cos^2\theta \pm \frac{\hbar\omega_o}{E_K}}\right]$$

(a) Absorption process: $q_{1/2} = k\left[-\cos\theta \pm \sqrt{\cos^2\theta + \frac{\hbar\omega_0}{E_K}}\right]$

- $\theta = \pi \Rightarrow q^{ab}_{max} = k\left[\sqrt{1 + \frac{\hbar\omega_0}{E_K}} + 1\right]$
- $\theta = 0 \Rightarrow q^{ab}_{min} = k\left[\sqrt{1 + \frac{\hbar\omega_0}{E_K}} - 1\right]$

Therefore, only valid solutions are obtained when:

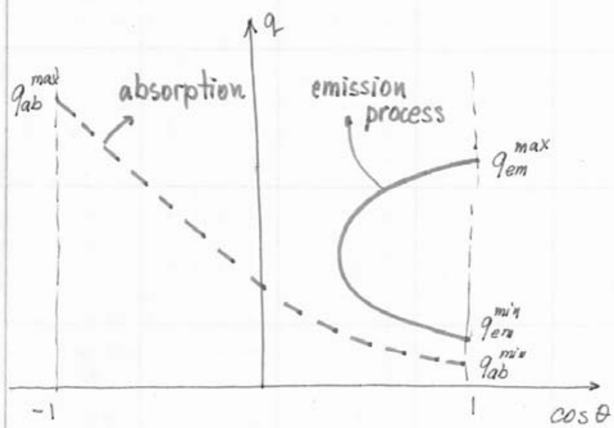
$$q = k\left[\sqrt{\cos^2\theta + \frac{\hbar\omega_0}{E_K}} - \cos\theta\right]$$

(b) Emission process $q_{1/2} = k\left[\cos\theta \pm \sqrt{\cos^2\theta - \frac{\hbar\omega_0}{E_K}}\right]$

- $\theta = \pi \Rightarrow q_{1/2} = k\left[-1 \pm \sqrt{1 - \frac{\hbar\omega_0}{E_K}}\right] < 0 \Rightarrow$ none of the two roots is a valid solution since $q<0$ in both cases.
- $\theta = 0 \Rightarrow q_{1/2} = k\left[1 \pm \sqrt{1 - \hbar\omega_0/E_K}\right] \Rightarrow q^{ab}_{min} = k\left[1 - \sqrt{1 - \hbar\omega_0/E_K}\right]$

$$q^{em}_{max} = k\left[1 + \sqrt{1 - \hbar\omega_0/E_K}\right]$$

The variation of the phonon wavevector involved in the momentum and energy conservation process with $\cos\theta$ is shown below.



- Once we have calculated the maximum and minimum wavevectors q_{min} and q_{max}, the evaluation of the scattering rate is obtained by direct application of the previously derived expression:

$$|M(\vec{k},\vec{q})|^2 = \frac{\hbar D_0^2}{2\rho V\omega_0}\left(n_0 + \frac{1}{2} \mp \frac{1}{2}\right)$$

i.e.

$$\frac{1}{\tau(k)} = \frac{m^* V}{2\pi\hbar^3 k}\int_{q_{min}^{ab}}^{q_{max}^{ab}} q\,|M(k,q)|^2_{ab}\,dq + \frac{m^* V}{2\pi\hbar^3 k}\int_{q_{min}^{em}}^{q_{max}^{em}} q\,|M(k,q)|^2_{em}\,dq$$

$$= \frac{m^* V}{2\pi\hbar^3 k}\,\frac{\hbar D_0^2}{2\rho V\omega_0}\,\frac{1}{2}\Big[N_0\underbrace{(q_{max,ab}^2 - q_{min,ab}^2)} + (N_0+1)\underbrace{(q_{max,em}^2 - q_{min,em}^2)}\Big]$$

involve terms of the form

$$(a+b)^2 - (a-b)^2 =$$
$$= \cancel{a^2} + 2ab + \cancel{b^2} - \cancel{a^2} + 2ab - \cancel{b^2} = 4ab$$

$$\frac{1}{\tau(k)} = \frac{m^* D_0^2}{8\pi\hbar^2\rho\omega_0 k}\left[N_0 \cdot 4\sqrt{1+\frac{\hbar\omega_0}{E_K}} + (N_0+1)\,4\sqrt{1-\frac{\hbar\omega_0}{E_K}}\,\right]k^2$$

$$= \frac{m^* D_0^2}{2\pi\hbar^2\rho\omega_0}\,k\left[N_0\sqrt{1+\frac{\hbar\omega_0}{E_K}} + (N_0+1)\sqrt{1-\frac{\hbar\omega_0}{E_K}}\,\right]$$

We can reorganize slightly this final expression by multiplying and dividing by $\sqrt{E_K}$, to get for the constant upfront:

$$\frac{m^* D_0^2}{2\pi\hbar^2\rho\omega_0}\sqrt{\frac{2mE_K}{\hbar^2}}\,\frac{1}{\sqrt{E_K}} = \frac{m^{*\,3/2} D_0^2}{\sqrt{2}\,\pi\hbar^3\rho\,\omega_0}$$

This gives us the following result for the total scattering rate out of state $\vec{k}$:

$$\frac{1}{\tau(\vec{k})} = \frac{m^{*\,3/2} D_0^2}{\sqrt{2}\,\pi\hbar^3\rho\omega_0}\left[N_0\sqrt{E_K+\hbar\omega_0} + (N_0+1)\sqrt{E_K-\hbar\omega_0}\,\right]$$

- Important comments:

(a) The matrix element $|M(k,q)|^2$ is independent of q which means that optical phonon scattering (non-polar) is <u>ISOTROPIC</u> SCATTERING PROCESS $\Rightarrow \tau_m(k) = \tau(k)$

(b) The phonon energies involved in the scattering process are in the range between 20 to 60 meV, which means that nonpolar OP scattering is <u>inelastic</u> scattering process. Only for very energetic electrons it can be considered to be elastic process.

absorption process *emission process*

(c) In contrast to the simple change in volume of the unit cell produced by acoustic phonons (longitudinal), optical phonon scattering is sensitive to the symmetry of the crystal. Selection rules forbid optical phonon scattering of electrons at $\vec{p}=(0,0,0)$ and along <100> direction (which includes electrons in the conduction band of GaAs and Si). Optical phonon scattering does occur for holes and for conduction band electrons in Ge.

(d) Only those carriers that have energy $E_k > \hbar\omega_0$ can emit optical phonons.

(e) For the momentum relaxation time, we have the same expression as the one for $\tau(\vec{k})$ since the scattering process is <u>ISOTROPIC</u>.

(f) The energy relaxation time that is calculated as:

$$\frac{1}{\tau_E(k)} = \sum_{k'} S(\vec{k},\vec{k}')\left[1-\frac{E(k')}{E(k)}\right]$$

For very high energy carriers, for which emission dominates the absorption we have:

$$\frac{1}{\tau_E(k)} \cong \sum_{k'} S_{em}(\vec{k},\vec{k}')\left[1-\frac{E(k)-\hbar\omega_0}{E(k)}\right] = \frac{\hbar\omega_0}{E(k)}\sum_{k'} S_{em}(\vec{k},\vec{k}')$$

$$\frac{1}{\tau_E(k)} \simeq \frac{\hbar\omega_0}{E(k)}\frac{1}{\tau(k)} \Rightarrow \tau_E(\vec{k}) \approx \frac{E(\vec{k})}{\hbar\omega_0}\tau(\vec{k})$$

This last expression suggests that, because $E(k) \gg \hbar\omega_0$, the energy relaxation time might greatly exceed the momentum relaxation time since very many phonons are needed to remove carrier's kinetic energy.