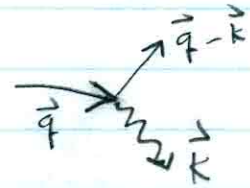
Lecture #20 Average electron phonon scattering time, electron - photon interactions

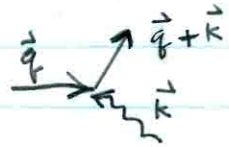
Average time for phonon emission or absorption by an electron with wavevector $\vec{q}$:
(Deformation potential)

$$\frac{1}{\tau_q} = \frac{2\pi}{\hbar} \left| \langle \Psi_f | \mathcal{H}_{e-ph} | \Psi_i \rangle \right|^2 \delta(E_f - E_i)$$

$$= \frac{2\pi}{\hbar} \sum_{\vec{k}} D^2 k^2 \frac{\hbar}{2\rho V \omega_k} \left| \langle N_k + 1 | a_k^+ c_{q-k}^+ c_q | N_k \rangle \right|^2 \delta\Big(\underbrace{(E_{q-k} + \hbar\nu k)}_{E_f} - \underbrace{E_q}_{E_i}\Big)$$



$$+ \frac{2\pi}{\hbar} \sum_{\vec{k}} D^2 k^2 \frac{\hbar}{2\rho V \underbrace{\omega_k}_{\nu k}} \left| \langle N_k - 1 | a_k c_{q+k}^+ c_q | N_k \rangle \right|^2 \delta\Big(\underbrace{E_{q+k}}_{E_f} - \underbrace{(E_q + \hbar\nu k)}_{E_i}\Big)$$



$$\frac{1}{\tau_q} = \frac{2\pi}{\hbar} D^2 \frac{\hbar}{2\rho V \nu} \int \frac{d^3k}{\underbrace{(2\pi)^3}_{V}} k \Big[N_q (1 - N_{q-k})(N_k + 1)\, \delta(E_{q-k} + \hbar\nu k - E_q)$$
$$+ N_q (1 - N_{q+k}) N_k \;\; \delta(E_{q+k} - E_q - \hbar\nu k) \Big]$$

Assume high temperatures: $N_q, N_{q-q} \ll 1$

Also assume: $\frac{\hbar^2 k^2}{2m} \gg \hbar\nu k$ (high electron energies)

$$E_{q\pm k} \mp \hbar\nu k - E_q = \frac{\hbar^2}{2m}(\vec{k} \pm \vec{q})^2 \mp \hbar\nu k - \frac{\hbar^2}{2m} q^2 \approx \pm \frac{\hbar^2}{m} k q \cos\theta + \frac{\hbar^2}{2m} k^2$$

$$\underbrace{\frac{1}{N_q}\frac{1}{\tau_q}}_{\text{Rate per electron}} = \frac{2\pi}{\hbar}\frac{D^2\hbar}{2\rho V v}\frac{V}{8\pi^3}\, 2\pi\int_{-1}^{1} d(\cos\theta)\int_0^\infty dk\, k^2\, k\,(1+2N_k)\,\delta\left(\frac{\hbar^2}{m}k^2 \pm \frac{\hbar^2}{m}kq\cos\theta\right)$$

$$= \frac{D^2}{4\pi\rho v}\int_0^\infty dk\, k^3\,(1+2N_k)\,\frac{1}{\frac{\hbar^2}{m}kq}\int_{-1}^{1} d(\cos\theta)\,\delta\left(\cos\theta \mp \frac{k}{2q}\right)$$

$$k \leq 2q$$

$$= \frac{D^2}{4\pi\rho v}\left(\frac{m}{\hbar^2 q}\right)\int_0^{2q} dk\, k^2\,(1+2N_k)$$

$$N_k = \frac{1}{e^{\frac{\hbar v k}{k_B T}}-1} \overset{\text{HIGH } T}{\approx} \frac{k_B T}{\hbar v k} \gg 1$$

$$\frac{1}{N_q}\frac{1}{\tau_q} \approx \frac{D^2}{4\pi\rho v}\frac{m}{\hbar^2 q}\, 2\,\frac{k_B T}{\hbar v}\,\frac{(2q)^2}{2} = \frac{D^2 m k_B T}{\pi\rho v^2\hbar^3}\, q$$

$$\left\langle \frac{1}{N_q}\frac{1}{\tau_q}\right\rangle \approx \frac{D^2 m k_B T}{\pi\rho v^2\hbar^3}\underbrace{\langle q\rangle}_{\frac{\hbar^2\langle q^2\rangle}{2m}\approx\frac{3}{2}k_B T \;\Rightarrow\; \sqrt{\langle q^2\rangle}\approx\langle q\rangle\approx\sqrt{\frac{3mk_BT}{\hbar^2}}}$$

$$\left\langle \frac{1}{N_q}\frac{1}{\tau_q}\right\rangle \approx \frac{D^2}{\pi\rho v^2\hbar^3}\, m k_B T\,\frac{\sqrt{3}\sqrt{m}\sqrt{k_B T}}{\hbar} = \frac{\sqrt{3}\,D^2 m^{3/2}(k_B T)^{3/2}}{\pi\rho v^2\hbar^4}$$

$\Rightarrow$ Typical solid: $\rho \sim \frac{5g}{cm^3}$, $v \sim 5\times10^5\,\frac{cm}{s}$, $D \sim 1eV$, $m^* \sim m_e$, $T \approx 300K$:

$\Rightarrow \langle\tau\rangle \sim 10\,ps$ // Of course, this number varies depending on which e-ph interaction dominates.

↓ continued on Nov 26.

Electron-photon interactions

For EM waves in the coulomb gauge $\vec{\nabla}\cdot\vec{A}=0$ we have $\phi=0$ and $\vec{A}\neq 0$. This leads to the electron's Hamiltonian:

$$\mathcal{H} = \frac{1}{2m}\left(\vec{p}-q\vec{A}\right)^2 = \frac{p^2}{m} - \frac{q}{m}\underbrace{\left(\vec{A}\cdot\vec{p}+\vec{p}\cdot\vec{A}\right)}_{\substack{\nabla\cdot\vec{A}=0 \\ \Rightarrow \vec{p}\cdot\vec{A}=\vec{A}\cdot\vec{p}}} + \underbrace{\frac{1}{m}q^2A^2}_{\text{drop}}$$

$$\Rightarrow \mathcal{H}_{e\text{-photon}} = -\frac{q}{m}\vec{A}\cdot\vec{p}$$

Use

$$\vec{A}(\vec{r},t) = \sum_{\vec{k},\lambda}\hat{n}_{k,\lambda}\sqrt{\frac{\hbar}{2\varepsilon V\omega_k}}\left(\hat{a}_{k\lambda}e^{i(\vec{k}\cdot\vec{r}-\omega t)} + \hat{a}^{\dagger}_{k\lambda}e^{-i(\vec{k}\cdot\vec{r}-\omega t)}\right)$$

To describe interband transitions, use: (Set to 0 for simplicity)

$$\mathcal{H}^{m'm}_{e\text{-photon}} = \int d^3r\, \underbrace{\hat{\Psi}^{\dagger}_{m'}(\vec{r})}_{\sum_{k_2}\frac{e^{-i\vec{k}_2\cdot\vec{r}}}{\sqrt{V}}u^*_{m'k_2}(\vec{r})\hat{c}^{\dagger}_{m'k_2}}\,\mathcal{H}\,\underbrace{\hat{\Psi}_m(\vec{r})}_{\sum_{k_1}\frac{e^{+i\vec{k}_1\cdot\vec{r}}}{\sqrt{V}}u_{mk_1}(\vec{r})\hat{c}_{mk_1}}$$

$$= -\frac{e}{m}\sum_{k_1,k_2}\sum_{k,\lambda}\sqrt{\frac{\hbar}{2\varepsilon V\omega_k}}\left[a_{k\lambda}\hat{c}^{\dagger}_{m'k_2}\hat{c}_{mk_1}\left(\frac{1}{V}\int d^3r\, e^{i(k_1-k_2+k)\cdot\vec{r}}\, u^*_{m'k_2}(\vec{r})\left(\hat{n}_{k\lambda}\cdot\vec{p}\right)u_{mk_1}(\vec{r})\right)\right.$$

$$\left. + a^{\dagger}_{k\lambda}\hat{c}^{\dagger}_{m'k_2}\hat{c}_{mk_1}\left(\frac{1}{V}\int d^3r\, e^{i(k_1-k_2-k)\cdot\vec{r}}\, u^*_{m'k_2}(\vec{r})\left(\hat{n}_{k\lambda}\cdot\vec{p}\right)u_{mk_1}(\vec{r})\right)\right]$$

Again assume $k \ll (V_{cell})^{1/3}$ so that $u_{mk}(\vec{r}) \approx u_{m0}(\vec{r})$:

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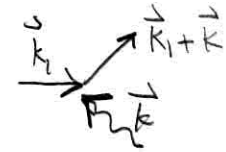
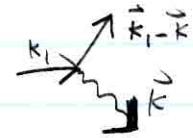


$$\mathcal{H}_{n'n} = -\frac{e}{m}\sum_{\vec{k}_1}\sum_{\vec{k},\lambda}\sqrt{\frac{\hbar}{2\varepsilon V\omega_k}}\left(\hat{\eta}_{k\lambda}\cdot\langle n'|\vec{p}|n\rangle\right)\left(\hat{a}_{k\lambda}\hat{c}^{\dagger}_{n'\vec{k}_1+\vec{k}}\,\hat{c}_{n\vec{k}_1} + a^{\dagger}_{k\lambda}\,\hat{c}^{\dagger}_{n'\vec{k}_1-\vec{k}}\,\hat{c}_{n\vec{k}_1}\right)$$



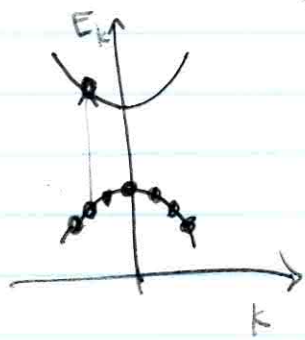
where $\boxed{\langle n'|\vec{p}|n\rangle = \frac{1}{V_{cell}}\int d^3r\, u^*_{n'0}(\vec{r})\left(\frac{i}{\hbar}\vec{\nabla}\right)u_{n0}(\vec{r})}$

$\hbar\omega \approx E_g$

$\hbar c k = E_g$

$k = \frac{E_g}{\hbar c} << k_c$

<u>Interband transitions in a semiconductor</u>



Absorption Rate for interband transitions per photon per valence electron:

$\sim \sum_k$ and divide by N_k

$$\frac{1}{\tau} = \frac{1}{N_k}\frac{2\pi}{\hbar}\sum_{\vec{k}_c}\frac{\hbar e^2}{2\varepsilon V\omega m^2}\left|\langle v|\vec{p}|\vec{c}\rangle\cdot\vec{\eta}\right|^2 N_k\, \underbrace{N_{\vec{k}_v}}_{=1}\,\underbrace{(1-N_{\vec{k}_c})}_{=1}\,\delta(E_{k_c}-E_{k_v}-\hbar\omega)$$

$\vec{k}_c$ conduction

and $\vec{k}_v + \vec{k} = \vec{k}_c$.

Use $E_{k_c} = E_{gap} + \frac{\hbar^2}{2m_c}k_c^2$, $E_{k_v} = -\frac{\hbar^2}{2m_h}k_h^2$

$$(E_{k_c}-E_{k_v}) = E_{gap} + \frac{\hbar^2}{2m_c}k_c^2 + \frac{\hbar^2}{2m_v}\underbrace{|\vec{k}_c-\vec{k}|^2}_{\approx k_c^2 + O(k_c k)}$$ tiny!

$$\approx E_{gap} + \frac{\hbar^2}{2}\underbrace{\left(\frac{1}{m_c}+\frac{1}{m_v}\right)}_{\frac{1}{m_R}}k_c^2$$

k_c^2 → exciton momentum $= \vec{k}_v + \vec{k}$

$\frac{1}{m_R}$ → exciton reduced mass

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \int \frac{d^3k}{\frac{(2\pi)^3}{V}} \frac{\hbar e^2}{2\varepsilon V \omega m^2} \left|\langle v|\vec{p}|c\rangle \cdot \vec{n}\right|^2 \delta\left(\hbar\omega - \left(E_{gap} + \frac{\hbar^2}{m_r} k^2\right)\right)$$

$$\delta(f(k)) = \frac{\delta(k-k_0)}{|f'(k_0)|} \quad \text{where } f(k_0)=0$$

$$= \frac{2\pi}{\hbar} \frac{\hbar e^2}{2\varepsilon V \omega m^2} \left|\langle v|\vec{p}|c\rangle \cdot \vec{n}\right|^2 \frac{V}{(2\pi)^3} \int_0^\infty 4\pi k^2 dk \, \frac{\delta\left(k - \sqrt{\frac{2m_r}{\hbar^2}(\hbar\omega - E_{gap})}\right)}{\frac{\hbar^2}{m_r} k}$$

$$= \frac{2\pi}{\hbar} \frac{\hbar e^2}{2\varepsilon V \omega m^2} \left|\langle v|\vec{p}|c\rangle \cdot \vec{n}\right|^2 \underbrace{\left(\frac{V}{(2\pi)^3} \frac{m_r}{\hbar^2} 4\pi \sqrt{\frac{2m_r}{\hbar^2}(\hbar\omega - E_{gap})}\right)}_{D_{EXCITON}(\hbar\omega - E_{gap})}$$

$$\boxed{\frac{1}{\tau_{interband}} = \sqrt{(\hbar\omega - E_{gap})} \, \frac{e^2 m_r^{3/2}}{\pi \hbar^2 \varepsilon m^2} \frac{\left|\langle v|\vec{p}|c\rangle \cdot \hat{n}\right|^2}{\hbar\omega}}$$

//

Valid for $\hbar\omega \gg E_{gap}$, otherwise formation of excitons bound state need to be considered.

<u>Alternative form of e-photon interaction:</u>

From the $\vec{A}\cdot\vec{p}$ coupling we got:

$$H_{m'm} = -\frac{e}{m} \sum_{\vec{k}_1} \sum_{\vec{k},\lambda} \sqrt{\frac{\hbar}{2\varepsilon V \omega_{k\lambda}}} \left(\hat{n}_{\vec{k}\lambda} \cdot \langle m'|\vec{p}|m\rangle\right) \Big[\hat{a}_{k\lambda} c^{\dagger}_{m'\vec{k}_1+\vec{k}} \hat{c}_{m\vec{k}_1} e^{-i\omega t}$$

$$+ \hat{a}^{\dagger}_{k\lambda} c^{\dagger}_{m'\vec{k}_1-\vec{k}} \hat{c}_{m\vec{k}_1} e^{i\omega t} \Big]$$

Before, we had $t=0$ here

Plug $\vec{p} = m\frac{\partial \vec{x}}{\partial t} = \mp m i \omega \vec{x}$:

$$H_{n'n} = ie \sum_{\vec{k}_1} \sum_{\vec{k}\lambda} \sqrt{\frac{\hbar\omega_{k\lambda}}{2\varepsilon V}} \left(\hat{n}_{\vec{k}\lambda} \cdot \langle n'|\vec{x}|n\rangle\right)\left[\hat{a}_{k\lambda}\hat{c}^{+}_{n'k_1+k}\hat{c}_{nk_1}e^{-i\omega t} - \hat{a}^{+}_{k\lambda}\hat{c}^{+}_{n'k_1-k}\hat{c}_{nk_1}e^{i\omega t}\right]$$

"Electric dipole", equivalent to $\vec{A}\cdot\vec{p}$ interaction.

Formally, one may derive this from multipole expansion instead of $\vec{A}\cdot\vec{p}$.