Física de Semiconductores

Lección 11

Electromagnetic radiation

- Radiation in Coulomb gauge

$$\boldsymbol{A} = \tfrac{1}{2}\boldsymbol{A}_0\left[e^{i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)} + e^{-i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)}\right]$$

- The fields are

$$\boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} = \frac{i\omega_{\boldsymbol{k}}}{2c}\boldsymbol{A}_0\left[e^{i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)} - e^{-i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)}\right]$$

$$\boldsymbol{B} = \nabla\times\boldsymbol{A} = i\frac{\boldsymbol{k}\times\boldsymbol{A}_0}{2}\left[e^{i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)} - e^{-i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)}\right]$$

- Poynting vector is

$$\boldsymbol{S} = \frac{c}{4\pi}\left(\boldsymbol{E}\times\boldsymbol{B}\right) = \frac{c}{4\pi}\frac{i\omega_{\boldsymbol{k}}}{2c}\frac{i}{2}\left(\boldsymbol{A}_0\times\boldsymbol{k}\times\boldsymbol{A}_0\right)\left[e^{2i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)} - e^{-2i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)} - 2\right]$$

$$= \frac{\omega_{\boldsymbol{k}}}{16\pi}\left(\boldsymbol{A}_0\times\boldsymbol{k}\times\boldsymbol{A}_0\right)\left[2 + e^{-2i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)} - e^{2i\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t\right)}\right]$$

Average power

- Time average of Poynting vector is

$$\boldsymbol{S}_{\mathrm{av}} = \frac{\omega}{8\pi}\left(\boldsymbol{A}_0 \times \boldsymbol{k} \times \boldsymbol{A}_0\right)$$

- Then energy density is

$$\frac{\left|\boldsymbol{S}_{\mathrm{av}}\right| n}{c} = \frac{n\omega_{\boldsymbol{k}} k A_0^2}{8\pi c} = \frac{n^2\omega_{\boldsymbol{k}}^2 A_0^2}{8\pi c^2} = \frac{\hbar\omega_{\boldsymbol{k}} n_\omega}{V}$$

- Therefore:

$$A_0^2 = \frac{8\pi c^2}{n^2\omega_{\boldsymbol{k}}^2}\frac{\hbar\omega_{\boldsymbol{q}} n_\omega}{V} = 4\left(\frac{4\pi c^2}{n^2 V}\right)\left(\frac{\hbar}{2\omega_{\boldsymbol{k}}}\right) n_\omega$$

Vector potential in second quantization

- The above is consistent with

$$\boldsymbol{A} = \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \sum_{\boldsymbol{k}\lambda} \left(\frac{\hbar}{2\omega_{\boldsymbol{k}}}\right)^{1/2} \mathbf{e}_{\boldsymbol{k}\lambda} \left[a_{\boldsymbol{k}\lambda} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + a_{\boldsymbol{k}\lambda}^{+} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\right]$$

- where λ indicates polarization.

Electron radiation interaction

- We saw in Lección 3:

$$H = \frac{1}{2m}\left[\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right]^2 - e\varphi\left(\boldsymbol{r}\right)$$

$$H = \frac{1}{2m}\left[p^2 + \frac{e}{c}\left(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p}\right) + \left(\frac{e}{c}\right)^2 A^2\right]$$

One photon term

$$H_{eR} = \frac{e}{2mc}\left(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p}\right)$$

- But

$$\left(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p}\right)\psi = \left(2\boldsymbol{A}\cdot\boldsymbol{p}\psi - i\hbar\psi\nabla\cdot\boldsymbol{A}\right)$$

- But in Coulomb gauge

$$\nabla\cdot\boldsymbol{A} = 0$$

- so

$$H_{eR} = \frac{e}{mc}\boldsymbol{A}\cdot\boldsymbol{p}$$

Second quantization form of H_{eR}

- The one-electron hamiltonian is then

$$H_{eR} = \frac{e}{mc}\boldsymbol{A}\cdot\boldsymbol{p} = \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2}\left(\frac{e}{mc}\right)\sum_{\boldsymbol{k}\lambda}\left(\frac{\hbar}{2\omega_{\boldsymbol{k}}}\right)^{1/2}\mathbf{e}_{\boldsymbol{k}\lambda}\cdot\boldsymbol{p}\left[a_{\boldsymbol{k}\lambda}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + a^{+}_{\boldsymbol{k}\lambda}e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\right]$$

- and therefore, the many electron electron radiation hamiltonian becomes (using κ for radiation wave vectors).

$$\hat{H}_{eR} = \sum_{n\boldsymbol{k},n'\boldsymbol{k}'}\left\langle n\boldsymbol{k}\middle| H_{eR}\middle| n'\boldsymbol{k}'\right\rangle c^{\dagger}_{n\boldsymbol{k}}c_{n'\boldsymbol{k}'}$$

$$= \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2}\left(\frac{e}{mc}\right)\sum_{n\boldsymbol{k},n'\boldsymbol{k}'}\left\langle n\boldsymbol{k}\middle|\sum_{\boldsymbol{\kappa}\lambda}\left(\frac{\hbar}{2\omega_{\boldsymbol{\kappa}}}\right)^{1/2}\left[a_{\boldsymbol{\kappa}\lambda}e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}} + a^{+}_{\boldsymbol{\kappa}\lambda}e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\right]\mathbf{e}_{\boldsymbol{\kappa}\lambda}\cdot\boldsymbol{p}\middle| n'\boldsymbol{k}'\right\rangle c^{\dagger}_{n\boldsymbol{k}}c_{n'\boldsymbol{k}'}$$

Momentum matrix element between Bloch functions (I)

- We want to explore the matrix element

$$\left\langle n\boldsymbol{k}\right|e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\boldsymbol{p}\left|n'\boldsymbol{k}'\right\rangle = \int d\boldsymbol{r}\,\psi^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\boldsymbol{p}\psi_{n'\boldsymbol{k}'}\left(\boldsymbol{r}\right) =$$

$$= \int d\boldsymbol{r}\,e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\boldsymbol{p}e^{i\boldsymbol{k}'\cdot\boldsymbol{r}}u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}\right)$$

$$= \int d\boldsymbol{r}\,e^{i\left(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{\kappa}\right)\cdot\boldsymbol{r}}u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)\boldsymbol{p}u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}\right) + \hbar\boldsymbol{k}'\int d\boldsymbol{r}\,e^{i\left(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{\kappa}\right)\cdot\boldsymbol{r}}u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}\right)u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}\right)$$

$$= \sum_{\boldsymbol{R}} e^{i\left(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{\kappa}\right)\cdot\boldsymbol{R}}\int_{\text{cell}} d\boldsymbol{r}\,e^{i\left(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{\kappa}\right)\cdot\boldsymbol{r}}u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}+\boldsymbol{R}\right)\boldsymbol{p}u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}+\boldsymbol{R}\right)$$

$$+\hbar\boldsymbol{k}'\sum_{\boldsymbol{R}} e^{i\left(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{\kappa}\right)\cdot\boldsymbol{R}}\int_{\text{cell}} d\boldsymbol{r}\,e^{i\left(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{\kappa}\right)\cdot\boldsymbol{r}}u^*_{n\boldsymbol{k}}\left(\boldsymbol{r}+\boldsymbol{R}\right)u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}+\boldsymbol{R}\right)$$

$$= N\delta_{\boldsymbol{k},\boldsymbol{k}'+\boldsymbol{\kappa}}\int_{\text{cell}} d\boldsymbol{r}\,u^*_{n\boldsymbol{k}'+\boldsymbol{\kappa}}\left(\boldsymbol{r}\right)\boldsymbol{p}u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}\right) + \hbar\boldsymbol{k}'N\delta_{\boldsymbol{k},\boldsymbol{k}'+\boldsymbol{\kappa}}\int_{\text{cell}} d\boldsymbol{r}\,u^*_{n\boldsymbol{k}'+\boldsymbol{\kappa}}\left(\boldsymbol{r}\right)u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}\right)$$

Momentum matrix element between Bloch functions (II)

- We can neglect the second integral due to the orthogonality of different periodic parts, so

$$\left\langle n\boldsymbol{k}\middle| e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\boldsymbol{p}\middle| n'\boldsymbol{k}'\right\rangle = N\delta_{\boldsymbol{k},\boldsymbol{k}'+\boldsymbol{\kappa}}\int_{\text{cell}} d\boldsymbol{r}\, u^{*}_{n\boldsymbol{k}'+\boldsymbol{\kappa}}\left(\boldsymbol{r}\right)\boldsymbol{p}\, u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}\right)$$

$$= \delta_{\boldsymbol{k},\boldsymbol{k}'+\boldsymbol{\kappa}}\int_{\text{crystal}} d\boldsymbol{r}\, u^{*}_{n\boldsymbol{k}'+\boldsymbol{\kappa}}\left(\boldsymbol{r}\right)\boldsymbol{p}\, u_{n'\boldsymbol{k}'}\left(\boldsymbol{r}\right)$$

$$= \delta_{\boldsymbol{k},\boldsymbol{k}'+\boldsymbol{\kappa}}\boldsymbol{P}^{n,n'}_{\boldsymbol{k}'+\boldsymbol{\kappa},\boldsymbol{k}'}$$

Back to eR interaction (I)

- Inserting in e-R interaction

$$\hat{H}_{eR} = \hat{H}_{eR}^{+} + \hat{H}_{eR}^{-}$$

$$\hat{H}_{eR}^{-} =$$

$$= \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \left(\frac{e}{mc}\right) \sum_{n\boldsymbol{k},n'\boldsymbol{k}'} \sum_{\boldsymbol{\kappa}\lambda} \left(\frac{\hbar}{2\omega_{\boldsymbol{\kappa}}}\right)^{1/2} \delta_{\boldsymbol{k},\boldsymbol{k}'+\boldsymbol{\kappa}} a_{\boldsymbol{\kappa}\lambda} \mathbf{e}_{\boldsymbol{\kappa}\lambda} \cdot \boldsymbol{P}_{\boldsymbol{k}'+\boldsymbol{\kappa},\boldsymbol{k}'}^{n,n'} c_{n\boldsymbol{k}}^{\dagger} c_{n'\boldsymbol{k}'}$$

$$= \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \left(\frac{e}{mc}\right) \sum_{n,n'\boldsymbol{k}'} \sum_{\boldsymbol{\kappa}\lambda} \left(\frac{\hbar}{2\omega_{\boldsymbol{\kappa}}}\right)^{1/2} a_{\boldsymbol{\kappa}\lambda} \mathbf{e}_{\boldsymbol{\kappa}\lambda} \cdot \boldsymbol{P}_{\boldsymbol{k}'+\boldsymbol{\kappa},\boldsymbol{k}'}^{n,n'} c_{n\boldsymbol{k}'+\boldsymbol{\kappa}}^{\dagger} c_{n'\boldsymbol{k}'}$$

$$= \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \left(\frac{e}{mc}\right) \sum_{n\boldsymbol{k},n'} \sum_{\boldsymbol{\kappa}\lambda} \left(\frac{\hbar}{2\omega_{\boldsymbol{\kappa}}}\right)^{1/2} a_{\boldsymbol{\kappa}\lambda} \mathbf{e}_{\boldsymbol{\kappa}\lambda} \cdot \boldsymbol{P}_{\boldsymbol{k}+\boldsymbol{\kappa},\boldsymbol{k}}^{n',n} c_{n'\boldsymbol{k}+\boldsymbol{\kappa}}^{\dagger} c_{n\boldsymbol{k}}$$

Back to eR interaction (II)

$$\hat{H}^{+}_{eR} =$$

$$= \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \left(\frac{e}{mc}\right) \sum_{n\boldsymbol{k},n'\boldsymbol{k}'} \sum_{\boldsymbol{\kappa}\lambda} \left(\frac{\hbar}{2\omega_{\boldsymbol{\kappa}}}\right)^{1/2} \delta_{\boldsymbol{k},\boldsymbol{k}'-\boldsymbol{\kappa}} a^{+}_{\boldsymbol{\kappa}\lambda} \mathbf{e}_{\boldsymbol{\kappa}\lambda} \cdot \boldsymbol{P}^{n,n'}_{\boldsymbol{k}'+\boldsymbol{\kappa},\boldsymbol{k}'} c^{\dagger}_{n\boldsymbol{k}} c_{n'\boldsymbol{k}'}$$

$$= \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \left(\frac{e}{mc}\right) \sum_{n,n'\boldsymbol{k}'} \sum_{\boldsymbol{\kappa}\lambda} \left(\frac{\hbar}{2\omega_{\boldsymbol{\kappa}}}\right)^{1/2} a^{+}_{\boldsymbol{\kappa}\lambda} \mathbf{e}_{\boldsymbol{\kappa}\lambda} \cdot \boldsymbol{P}^{n,n'}_{\boldsymbol{k}'-\boldsymbol{\kappa},\boldsymbol{k}'} c^{\dagger}_{n\boldsymbol{k}'-\boldsymbol{\kappa}} c_{n'\boldsymbol{k}'}$$

$$= \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \left(\frac{e}{mc}\right) \sum_{n\boldsymbol{k},n'} \sum_{\boldsymbol{\kappa}\lambda} \left(\frac{\hbar}{2\omega_{\boldsymbol{\kappa}}}\right)^{1/2} a^{+}_{\boldsymbol{\kappa}\lambda} \mathbf{e}_{\boldsymbol{\kappa}\lambda} \cdot \boldsymbol{P}^{n',n}_{\boldsymbol{k}-\boldsymbol{\kappa},\boldsymbol{k}} c^{\dagger}_{n'\boldsymbol{k}-\boldsymbol{\kappa}} c_{n\boldsymbol{k}}$$

Direct transitions

- The photon wave vector is

$$\left|\boldsymbol{\kappa}\right| = \frac{2\pi}{\lambda} \simeq \frac{2\pi}{500\ \mathrm{nm}} \ll \left|\boldsymbol{k}\right|_{\max} \simeq \frac{2\pi}{0.5\ \mathrm{nm}}$$

- Therefore I can set it to zero without much error:

$$\hat{H}^{+}_{eR} = \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2}\left(\frac{e}{mc}\right)\sum_{n\boldsymbol{k},n'}\sum_{\lambda}\left(\frac{\hbar}{2\omega}\right)^{1/2} a^{+}_{\omega\lambda}\mathbf{e}_{\omega\lambda}\cdot\boldsymbol{P}^{n',n}_{\boldsymbol{k},\boldsymbol{k}}c^{\dagger}_{n'\boldsymbol{k}}c_{n\boldsymbol{k}}$$

$$\hat{H}^{-}_{eR} = \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2}\left(\frac{e}{mc}\right)\sum_{n\boldsymbol{k},n'}\sum_{\lambda}\left(\frac{\hbar}{2\omega}\right)^{1/2} a_{\omega\lambda}\mathbf{e}_{\omega\lambda}\cdot\boldsymbol{P}^{n',n}_{\boldsymbol{k},\boldsymbol{k}}c^{\dagger}_{n'\boldsymbol{k}}c_{n\boldsymbol{k}}$$

Valence and conduction bands

- We are interested in transitions from the filled valence band to the empty conduction band by absorption of one photon. It is convenient to name the operators in the valence band *v*⁺ and *v*, instead of *c*⁺ and *c*. We then use *c* instead of *n*' and *v* instead of *n*. Then the relevant operator is

$$\hat{H}_{eR}^{-} = \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \left(\frac{e}{mc}\right) \sum_{cv\boldsymbol{k}} \sum_{\lambda} \left(\frac{\hbar}{2\omega}\right)^{1/2} a_{\omega\lambda} \mathbf{e}_{\omega\lambda} \cdot \boldsymbol{P}_{\boldsymbol{k},\boldsymbol{k}}^{c,v} c_{\boldsymbol{k}}^{\dagger} v_{\boldsymbol{k}}$$

Polarized light

- Assume that the light is polarized in the *x*-direction. Then

$$\hat{H}_{eR}^{-} = \left(\frac{4\pi c^2}{Vn^2}\right)^{1/2} \left(\frac{\hbar}{2\omega}\right)^{1/2} \left(\frac{e}{mc}\right) \sum_{cv\boldsymbol{k}} a_{\omega} \left(P_{\boldsymbol{k},\boldsymbol{k}}^{c,v}\right)_x c_{\boldsymbol{k}}^{\dagger} v_{\boldsymbol{k}}$$

The ground-electronic state

- The electronic ground state at zero temperature is

$$\left|G\right\rangle = \left(\prod_{v,\boldsymbol{k}} v_{\boldsymbol{k}}^{\dagger}\right)\left|0\right\rangle$$

Fermi's golden rule (I)

- Transition rate is

$$R_{i\to f} = \frac{2\pi}{\hbar}\sum_f \left|H_{\text{int}}\right|^2 \delta\left(E_f - E_i\right)$$

- Where $H_{\text{int}} = H_{eR}^{-}$

$$\left|i\right\rangle = \left|G\right\rangle\left|1_\omega\right\rangle; \quad E_i = E_G + \hbar\omega$$

$$\left|f\right\rangle = c_{\boldsymbol{k}}^{\dagger} v_{\boldsymbol{k}}\left|G\right\rangle\left|0_\omega\right\rangle; \quad E_f = E_G + E_{c\boldsymbol{k}} - E_{v\boldsymbol{k}}$$

The matrix element

- One matrix element is

$$\left\langle f \middle| H_{eR}^{-} \middle| i \right\rangle =$$

$$= \left\langle 0_{\omega} \middle| \left\langle G \middle| v_{\boldsymbol{k}}^{\dagger} c_{\boldsymbol{k}} \left(\frac{4\pi c^2}{Vn^2} \right)^{1/2} \left(\frac{\hbar}{2\omega} \right)^{1/2} \left(\frac{e}{mc} \right) \sum_{c'v'\boldsymbol{k}'} a_{\omega} \left(P_{\boldsymbol{k}',\boldsymbol{k}'}^{c,v} \right)_x c_{\boldsymbol{k}'}'^{\dagger} v_{\boldsymbol{k}'}' \middle| G \right\rangle \middle| 1_{\omega} \right\rangle$$

$$= \left(\frac{4\pi c^2}{Vn^2} \right)^{1/2} \left(\frac{\hbar}{2\omega} \right)^{1/2} \left(\frac{e}{mc} \right) \left\langle 0_{\omega} \middle| \left\langle G \middle| v_{\boldsymbol{k}}^{\dagger} c_{\boldsymbol{k}} a_{\omega} \left(P_{\boldsymbol{k},\boldsymbol{k}}^{c,v} \right)_x c_{\boldsymbol{k}}^{\dagger} v_{\boldsymbol{k}} \middle| G \right\rangle \middle| 1_{\omega} \right\rangle$$

$$= \left(\frac{4\pi c^2}{Vn^2} \right)^{1/2} \left(\frac{\hbar}{2\omega} \right)^{1/2} \left(\frac{e}{mc} \right) \left\langle 0_{\omega} \middle| \left\langle G \middle| a_{\omega} \left(P_{\boldsymbol{k},\boldsymbol{k}}^{c,v} \right)_x c_{\boldsymbol{k}} c_{\boldsymbol{k}}^{\dagger} v_{\boldsymbol{k}}^{\dagger} v_{\boldsymbol{k}} \middle| G \right\rangle \middle| 1_{\omega} \right\rangle$$

$$= \left(\frac{4\pi c^2}{Vn^2} \right)^{1/2} \left(\frac{\hbar}{2\omega} \right)^{1/2} \left(\frac{e}{mc} \right) \left(P_{\boldsymbol{k},\boldsymbol{k}}^{c,v} \right)_x$$

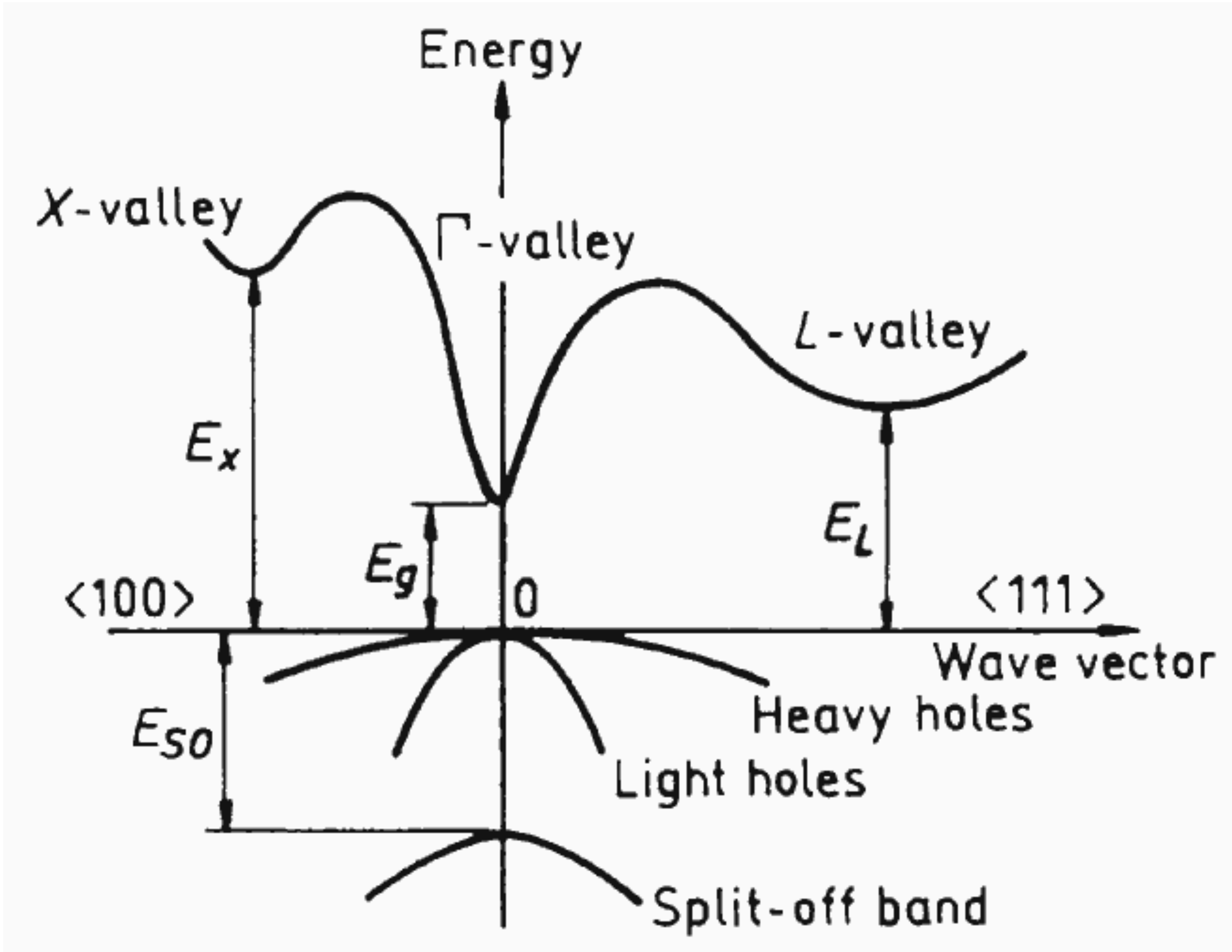
Transition rate

- Therefore, the transition rate is

$$R = \frac{2\pi}{\hbar}\left(\frac{4\pi c^2}{Vn^2}\right)\left(\frac{\hbar}{2\omega}\right)\left(\frac{e}{mc}\right)^2 \sum_{cv\boldsymbol{k}} \left| \left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}}\right)_x \right|^2 \delta\left(E_{c\boldsymbol{k}} - E_{v\boldsymbol{k}} - \hbar\omega\right)$$

- We would like to obtain an analytical expression. Therefore, we need further simplification.

Near band gap band structure



States involved

- The states involved

$$c : \left| S, \pm \tfrac{1}{2} \right\rangle$$

$$hh : \left| \tfrac{3}{2}, \pm \tfrac{3}{2} \right\rangle$$

$$lh : \left| \tfrac{3}{2}, \pm \tfrac{1}{2} \right\rangle$$

$$so : \left| \tfrac{1}{2}, \pm \tfrac{1}{2} \right\rangle$$

Transition rate

$$R = \frac{2\pi}{\hbar}\left(\frac{4\pi c^2}{Vn^2}\right)\left(\frac{\hbar}{2\omega}\right)\left(\frac{e}{mc}\right)^2 \times$$

$$\left(\sum_{c,hh,\boldsymbol{k}}\left|\left(P^{c,hh}_{\boldsymbol{k},\boldsymbol{k}}\right)_x\right|^2 \delta\left(E_{c\boldsymbol{k}} - E_{hh\boldsymbol{k}} - \hbar\omega\right)\right.$$

$$+\sum_{c,lh,\boldsymbol{k}}\left|\left(P^{c,lh}_{\boldsymbol{k},\boldsymbol{k}}\right)_x\right|^2 \delta\left(E_{c\boldsymbol{k}} - E_{lh\boldsymbol{k}} - \hbar\omega\right)$$

$$\left.+\sum_{c,so,\boldsymbol{k}}\left|\left(P^{c,so}_{\boldsymbol{k},\boldsymbol{k}}\right)_x\right|^2 \delta\left(E_{c\boldsymbol{k}} - E_{so\boldsymbol{k}} - \hbar\omega\right)\right)$$

p-matrix element $\left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}}\right)_x$

- We want to take the matrix element of *p* out of the summation, so we mayassume

$$\left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}}\right)_x \simeq \lim_{|\boldsymbol{k}|\to 0}\left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}}\right)_x$$

- This means that we can write the matrix element in terms of the k.p matrix elements for ***k=0***

k.p hamiltonian

	$\lvert S_a \uparrow\rangle$	$\lvert \frac{3}{2},-\frac{3}{2}\rangle_b$	$\lvert \frac{3}{2},\frac{1}{2}\rangle_b$	$\lvert \frac{1}{2},\frac{1}{2}\rangle_b$	$\lvert S_a \downarrow\rangle$	$\lvert \frac{3}{2},\frac{3}{2}\rangle_b$	$\lvert \frac{3}{2},-\frac{1}{2}\rangle_b$	$\lvert \frac{1}{2},-\frac{1}{2}\rangle_b$
$\lvert S_a \uparrow\rangle$	E_0	0	$\frac{i\hbar Pk_z}{m}\sqrt{\frac{2}{3}}$	$\frac{i\hbar Pk_z}{m}\frac{1}{\sqrt{3}}$	0	0	0	0
$\lvert \frac{3}{2},-\frac{3}{2}\rangle_b$	0	0	0	0	0	0	0	0
$\lvert \frac{3}{2},\frac{1}{2}\rangle_b$	$-\frac{i\hbar Pk_z}{m}\sqrt{\frac{2}{3}}$	0	0	0	0	0	0	0
$\lvert \frac{1}{2},\frac{1}{2}\rangle_b$	$\frac{i\hbar Pk_z}{m}\frac{1}{\sqrt{3}}$	0	0	$-\Delta_0$	0	0	0	0
$\lvert S_a \downarrow\rangle$	0	0	0	0	E_0	0	$\frac{i\hbar Pk_z}{m}\sqrt{\frac{2}{3}}$	$\frac{i\hbar Pk_z}{m}\frac{1}{\sqrt{3}}$
$\lvert \frac{3}{2},\frac{3}{2}\rangle_b$	0	0	0	0	0	0	0	0
$\lvert \frac{3}{2},-\frac{1}{2}\rangle_b$	0	0	0	0	$-\frac{i\hbar Pk_z}{m}\sqrt{\frac{2}{3}}$	0	0	0
$\lvert \frac{1}{2},-\frac{1}{2}\rangle_b$	0	0	0	0	$-\frac{i\hbar Pk_z}{m}\frac{1}{\sqrt{3}}$	0	0	$-\Delta_0$

Recipe for states near k =0 (I)

- First choose the z-axis in the direction of ***k*.**
- Then heavy hole bands are (approx) given by the states

$$\left|\tfrac{3}{2},\tfrac{3}{2}\right\rangle_b = \frac{1}{\sqrt{2}}X_b\uparrow + \frac{i}{\sqrt{2}}Y_b\uparrow; \quad \left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle_b = \frac{1}{\sqrt{2}}X_b\downarrow - \frac{i}{\sqrt{2}}Y_b\downarrow$$

- The light hole band is

$$\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle_b = \frac{1}{\sqrt{6}}X_b\uparrow - \frac{i}{\sqrt{6}}Y_b\uparrow + \sqrt{\frac{2}{3}}Z_b\downarrow; \quad \left|\tfrac{3}{2},\tfrac{1}{2}\right\rangle_b = \frac{1}{\sqrt{6}}X_b\downarrow + \frac{i}{\sqrt{6}}Y_b\downarrow + \sqrt{\frac{2}{3}}Z_b\uparrow$$

- The split-off band is

$$\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_b = -\frac{1}{\sqrt{3}}X_b\uparrow + \frac{i}{\sqrt{3}}Y_b\uparrow + \frac{1}{\sqrt{3}}Z_b\downarrow; \quad \left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle_b = -\frac{1}{\sqrt{3}}X_b\downarrow - \frac{i}{\sqrt{3}}Y_b\downarrow + \frac{1}{\sqrt{3}}Z_b\uparrow$$

Problem with matrix elements

- We would like to use

$$\left\langle S_a \middle| p_x \middle| X_b \right\rangle = \left\langle S_a \middle| p_y \middle| Y_b \right\rangle = \left\langle S_a \middle| p_z \middle| Z_b \right\rangle = iP$$

- But we need

$$\left(P_{\boldsymbol{k},\boldsymbol{k}}^{c,v} \right)_x \simeq \lim_{\left|\boldsymbol{k}\right| \to 0} \left(P_{\boldsymbol{k},\boldsymbol{k}}^{c,v} \right)_x$$

- The heavy and light-hole states are described with *x,y,z* chosen with *z* along ***k***, making an angle with the *x* direction of the cubic crystal.
- The solution is to rotate the basis and then average the angles. Cumbersome.

A clever solution (only for cubic materials)

- Because the material is cubic

$$\sum_{\boldsymbol{k}} \left| \left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}} \right)_x \right|^2 = \sum_{\boldsymbol{k}} \left| \left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}} \right)_y \right|^2 = \sum_{\boldsymbol{k}} \left| \left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}} \right)_z \right|^2$$

- and

$$\sum_{\boldsymbol{k}} \left(\left| \left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}} \right)_x \right|^2 + \left| \left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}} \right)_y \right|^2 + \left| \left(P^{c,v}_{\boldsymbol{k},\boldsymbol{k}} \right)_z \right|^2 \right)$$

- must be independent of the choice of axis orientation.
- Therefore, I can calculate the matrix element in the basis that diagonalizes the k.p interaction.

The matrix element of P

- It can be shown that

$$\left|\left\langle S\uparrow\middle|p_x^2\middle|J,J_z\right\rangle\right|^2+\left|\left\langle S\uparrow\middle|p_y^2\middle|J,J_z\right\rangle\right|^2+\left|\left\langle S\uparrow\middle|p_z^2\middle|J,J_z\right\rangle\right|^2$$
$$+\left|\left\langle S\uparrow\middle|p_x^2\middle|J,-J_z\right\rangle\right|^2+\left|\left\langle S\uparrow\middle|p_y^2\middle|J,-J_z\right\rangle\right|^2+\left|\left\langle S\uparrow\middle|p_z^2\middle|J,-J_z\right\rangle\right|^2=P^2$$

$$\left|\left\langle S\downarrow\middle|p_x^2\middle|J,J_z\right\rangle\right|^2+\left|\left\langle S\downarrow\middle|p_y^2\middle|J,J_z\right\rangle\right|^2+\left|\left\langle S\downarrow\middle|p_z^2\middle|J,J_z\right\rangle\right|^2$$
$$+\left|\left\langle S\downarrow\middle|p_x^2\middle|J,-J_z\right\rangle\right|^2+\left|\left\langle S\downarrow\middle|p_y^2\middle|J,-J_z\right\rangle\right|^2+\left|\left\langle S\downarrow\middle|p_z^2\middle|J,-J_z\right\rangle\right|^2=P^2$$

Final form

- Therefore

$$\sum_{c,v=hh} \lim_{|\boldsymbol{k}|\to 0} \left(P^{c,hh}_{\boldsymbol{k},\boldsymbol{k}}\right)_x = \frac{1}{3}\left(P^2 + P^2\right) = \frac{2}{3}P^2$$

$$\sum_{c,v=lh} \lim_{|\boldsymbol{k}|\to 0} \left(P^{c,lh}_{\boldsymbol{k},\boldsymbol{k}}\right)_x = \frac{1}{3}\left(P^2 + P^2\right) = \frac{2}{3}P^2$$

$$\sum_{c,v=so} \lim_{|\boldsymbol{k}|\to 0} \left(P^{c,lh}_{\boldsymbol{k},\boldsymbol{k}}\right)_x = \frac{1}{3}\left(P^2 + P^2\right) = \frac{2}{3}P^2$$

Transition rate (I)

- Therefore

$$R = \frac{2\pi}{\hbar}\left(\frac{4\pi c^2}{Vn^2}\right)\left(\frac{\hbar}{2\omega}\right)\left(\frac{e}{mc}\right)^2\left(\frac{2P^2}{3}\right)\times$$

$$\left(\sum_{\boldsymbol{k}}\delta\left(E_{c\boldsymbol{k}} - E_{hh\boldsymbol{k}} - \hbar\omega\right)\right.$$

$$+\sum_{\boldsymbol{k}}\delta\left(E_{c\boldsymbol{k}} - E_{lh\boldsymbol{k}} - \hbar\omega\right)$$

$$\left.+\sum_{\boldsymbol{k}}\delta\left(E_{c\boldsymbol{k}} - E_{so\boldsymbol{k}} - \hbar\omega\right)\right)$$

Transition rate (II)

- Converting into an integral

$$R=\left(\frac{V}{8\pi^3}\right)\frac{2\pi}{\hbar}\left(\frac{4\pi c^2}{Vn^2}\right)\left(\frac{\hbar}{2\omega}\right)\left(\frac{e}{mc}\right)^2\left(\frac{2P^2}{3}\right)\times$$

$$\left(\int d\boldsymbol{k}\,\delta\left(E_{c\boldsymbol{k}}-E_{hh\boldsymbol{k}}-\hbar\omega\right)\right.$$

$$+\int d\boldsymbol{k}\,\delta\left(E_{c\boldsymbol{k}}-E_{lh\boldsymbol{k}}-\hbar\omega\right)$$

$$\left.+\int d\boldsymbol{k}\,\delta\left(E_{c\boldsymbol{k}}-E_{so\boldsymbol{k}}-\hbar\omega\right)\right)$$

Transition rate (III)

- Converting into an integral

$$R = \left(\frac{V}{8\pi^3}\right)\frac{2\pi}{\hbar}\left(\frac{4\pi c^2}{Vn^2}\right)\left(\frac{\hbar}{2\omega}\right)\left(\frac{e}{mc}\right)^2\left(\frac{2P^2}{3}\right)\times$$

$$\left(\int d\boldsymbol{k}\,\delta\left(E_0 + \frac{\hbar^2 k^2}{2m_e} - \left(0 - \frac{\hbar^2 k^2}{2m_{hh}}\right) - \hbar\omega\right)\right.$$

$$+\int d\boldsymbol{k}\,\delta\left(E_0 + \frac{\hbar^2 k^2}{2m_e} - \left(0 - \frac{\hbar^2 k^2}{2m_{lh}}\right) - \hbar\omega\right)$$

$$\left.+\int d\boldsymbol{k}\,\delta\left(E_0 + \frac{\hbar^2 k^2}{2m_e} - \left(-\Delta_0 - \frac{\hbar^2 k^2}{2m_{so}}\right) - \hbar\omega\right)\right)$$

Reduced mass

- We define the reduced masses

$$\frac{1}{\mu_{hh}} = \frac{1}{m_e} + \frac{1}{m_{hh}}$$

$$\frac{1}{\mu_{lh}} = \frac{1}{m_e} + \frac{1}{m_{lh}}$$

$$\frac{1}{\mu_{so}} = \frac{1}{m_e} + \frac{1}{m_{so}}$$

Transition rate (IV)

- Converting into an integral

$$R = \left(\frac{V}{8\pi^3}\right)\frac{2\pi}{\hbar}\left(\frac{4\pi c^2}{Vn^2}\right)\left(\frac{\hbar}{2\omega}\right)\left(\frac{e}{mc}\right)^2\left(\frac{2P^2}{3}\right)\times$$

$$\left(\int d\boldsymbol{k}\,\delta\left(E_0 + \frac{\hbar^2k^2}{2\mu_{hh}} - \hbar\omega\right)\right.$$

$$+\int d\boldsymbol{k}\,\delta\left(E_0 + \frac{\hbar^2k^2}{2\mu_{lh}} - \hbar\omega\right)$$

$$\left.+\int d\boldsymbol{k}\,\delta\left(E_0 + \Delta_0 + \frac{\hbar^2k^2}{2\mu_{so}} - \hbar\omega\right)\right)$$

Doing the integrals

$$\int d\boldsymbol{k}\,\delta\left(E_0 + \frac{\hbar^2 k^2}{2\mu_{hh}} - \hbar\omega\right) = 4\pi \int dk\, k^2 \delta\left(E_0 + \frac{\hbar^2 k^2}{2\mu_{hh}} - \hbar\omega\right)$$

Let $u = \dfrac{\hbar^2 k^2}{2\mu_{hh}} \Rightarrow du = \dfrac{\hbar^2 k}{\mu_{hh}} dk$

$$\Rightarrow k^2 dk = \left(\frac{2\mu_{hh} u}{\hbar^2}\right)^{1/2} \frac{\mu_{hh}}{\hbar^2} du = \frac{1}{2}\left(\frac{2\mu_{hh}}{\hbar^2}\right)^{3/2} u^{1/2} du$$

$$4\pi \int dk\, k^2 \delta\left(E_0 + \frac{\hbar^2 k^2}{2\mu_{hh}} - \hbar\omega\right) = \frac{4\pi}{2}\left(\frac{2\mu_{hh}}{\hbar^2}\right)^{3/2} \int du\, u^{1/2} \delta\left(E_0 + u - \hbar\omega\right)$$

$$= 2\pi \left(\frac{2\mu_{hh}}{\hbar^2}\right)^{3/2} \left(\hbar\omega - E_0\right)^{1/2}$$

Final expression for R (I)

$$R = \left(\frac{V}{8\pi^3}\right)\frac{2\pi}{\hbar}\left(\frac{4\pi c^2}{Vn^2}\right)\left(\frac{\hbar}{2\omega}\right)\left(\frac{e}{mc}\right)^2\left(\frac{2P^2}{3}\right)\times 2\pi\left(\frac{2\mu_{hh}}{\hbar^2}\right)^{3/2}$$

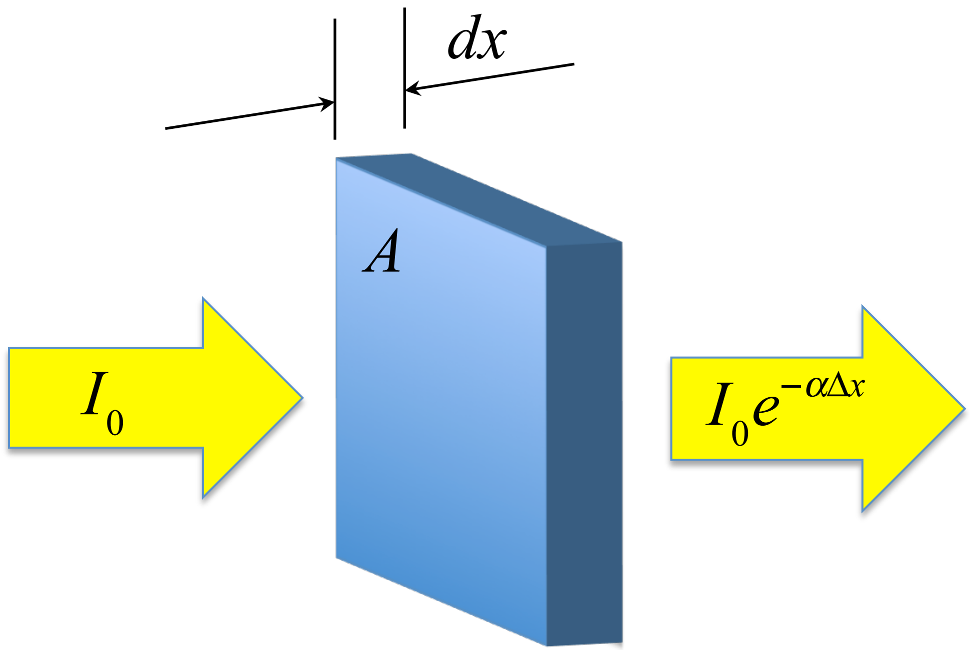
$$\left[\left(\mu_{hh}\right)^{3/2}\left(\hbar\omega - E_0\right)^{1/2} + \left(\mu_{lh}\right)^{3/2}\left(\hbar\omega - E_0\right)^{1/2} + \left(\mu_{so}\right)^{3/2}\left(\hbar\omega - E_0 - \Delta_0\right)^{1/2}\right]$$

$$= \left(\frac{4\sqrt{2}}{3}\right)\left(\frac{e^2P^2}{m^2n^2\hbar^3\omega}\right)\times$$

$$\left[\left(\mu_{hh}\right)^{3/2}\left(\hbar\omega - E_0\right)^{1/2} + \left(\mu_{lh}\right)^{3/2}\left(\hbar\omega - E_0\right)^{1/2} + \left(\mu_{so}\right)^{3/2}\left(\hbar\omega - E_0 - \Delta_0\right)^{1/2}\right]$$

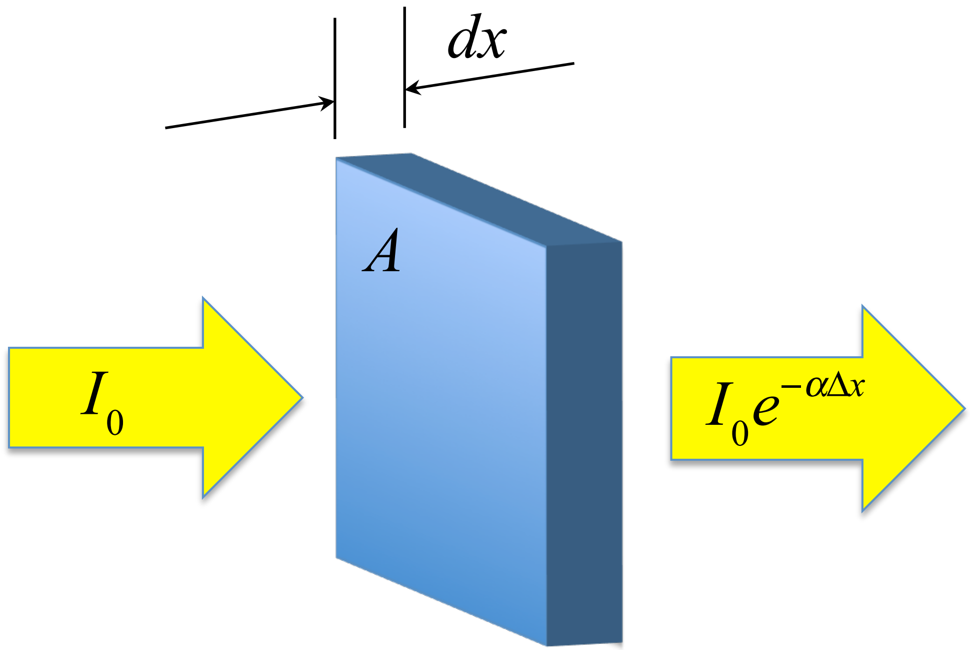
Absorption coefficient I

- The absorption coefficient is defined as



$$\alpha = \frac{\text{Number of photons absorbed per unit volume per second}}{\text{Number of photons incident per unit area per second}}$$

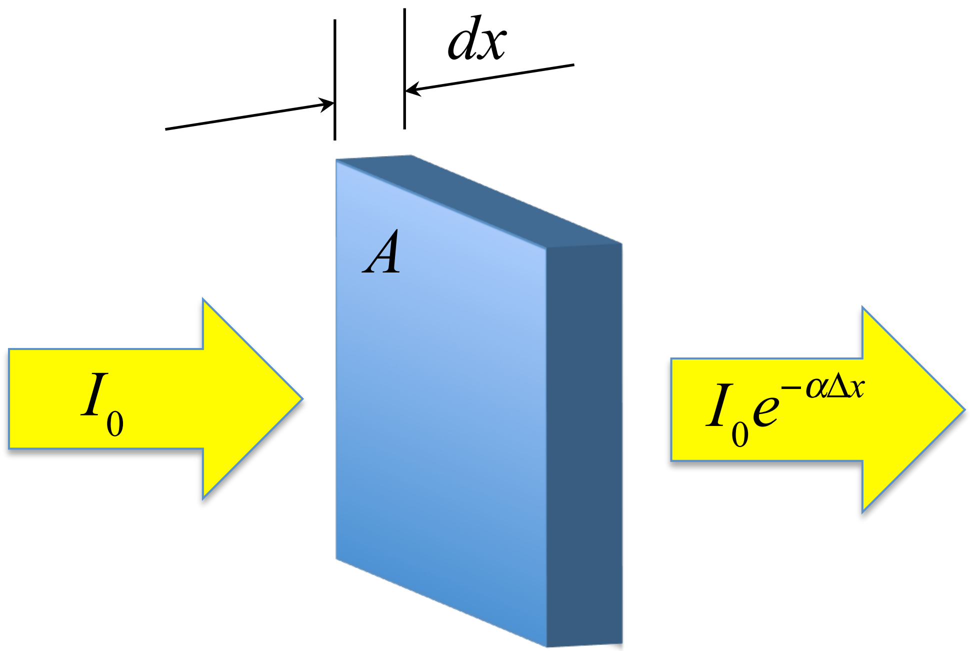
Absorption coefficient II



$$\alpha = \frac{\text{Number of photons absorbed per unit volume per second}}{\text{Number of photons incident per unit area per second}}$$

$$\alpha = \frac{\frac{(-dI)A}{\hbar\omega}\frac{1}{A\,dx}}{\frac{I}{\hbar\omega}} = -\frac{dI}{I\,dx} \Rightarrow I = I_0 \exp(-\alpha x)$$

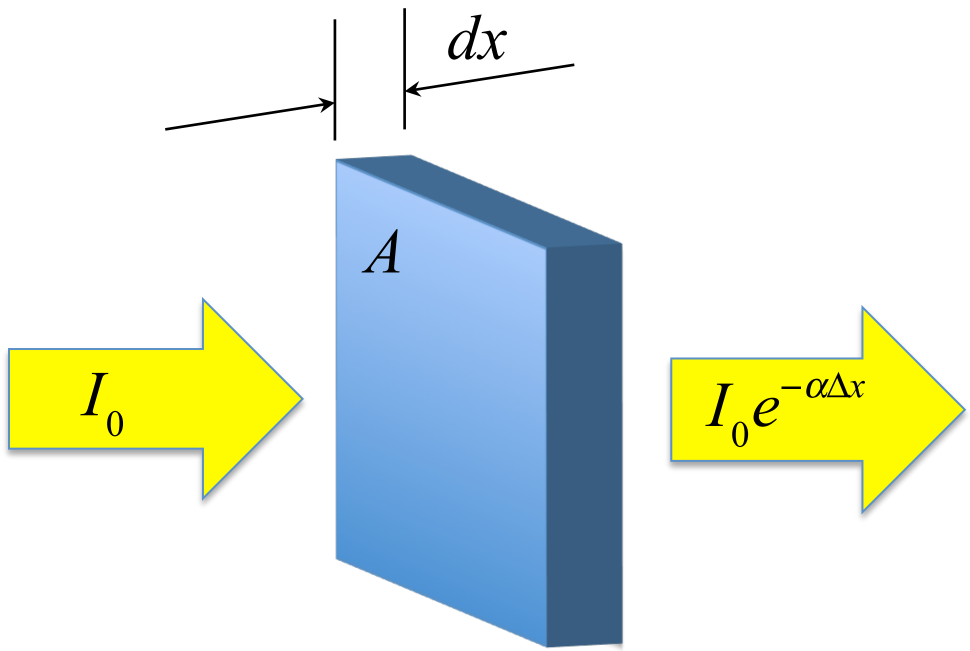
Absorption coefficient II



$$\alpha = \frac{\text{Number of photons absorbed per unit volume per second}}{\text{Number of photons incident per unit area per second}}$$

$$= \frac{\dfrac{P_{loss}}{\hbar\omega}\dfrac{1}{Adx}}{\dfrac{I_0}{\hbar\omega}} = \frac{P_{loss}}{I_0}\frac{1}{Adx}$$

Absorption coefficient III



If only one photon is incident

$$\alpha = \frac{P_{loss}}{I_0}\frac{1}{Adx} = \frac{P_{loss}}{\frac{\hbar\omega}{Adt}}\frac{1}{Adx} = \frac{P_{loss}}{\hbar\omega v} = \frac{P_{loss}n}{\hbar\omega c} = \frac{R\hbar\omega n}{\hbar\omega c} = \frac{Rn}{c}$$

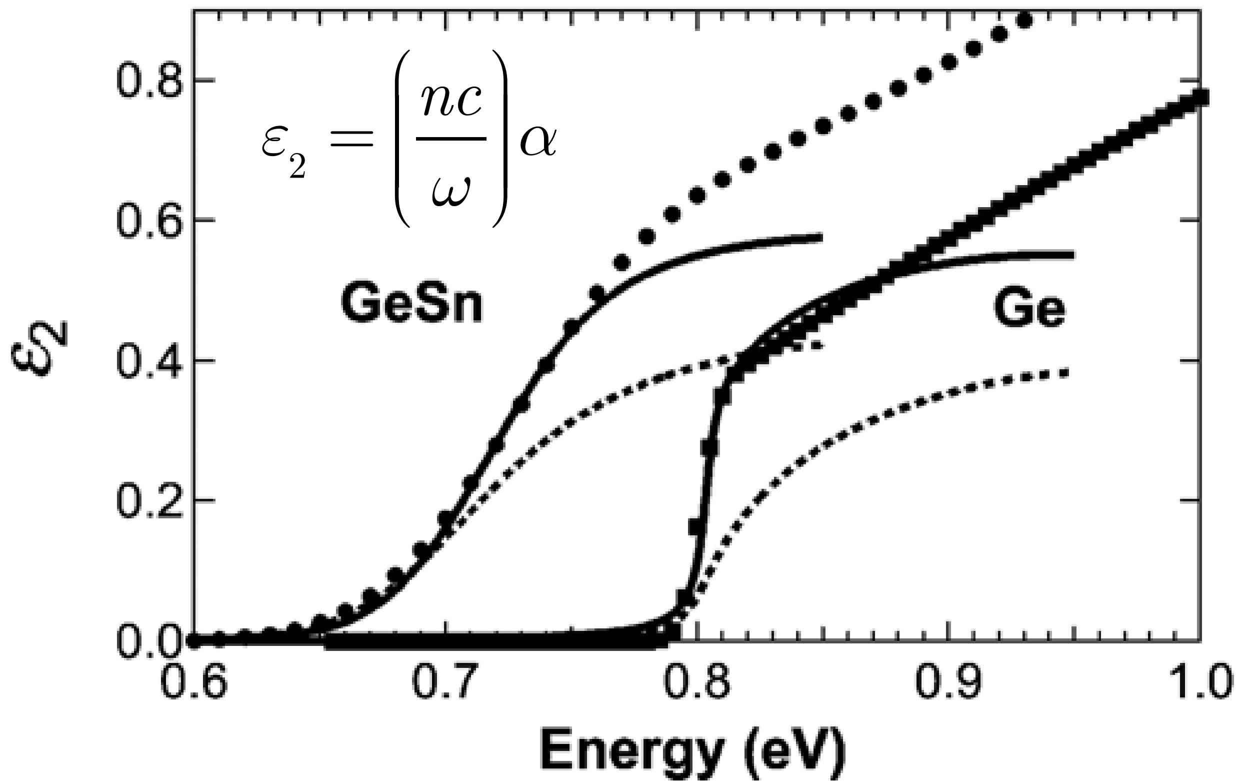
Theoretical absorption coefficient

$$\alpha = \left(\frac{4\sqrt{2}}{3}\right)\left(\frac{e^2P^2}{m^2nc\hbar^3\omega}\right)\times$$

$$\left\{\left[\left(\mu_{hh}\right)^{3/2} + \left(\mu_{lh}\right)^{3/2}\right]\left(\hbar\omega - E_0\right)^{1/2} + \left(\mu_{so}\right)^{3/2}\left(\hbar\omega - E_0 - \Delta_0\right)^{1/2}\right\}$$

Notice that α^2 is approximately linear in frequency.

Comparison with experiment



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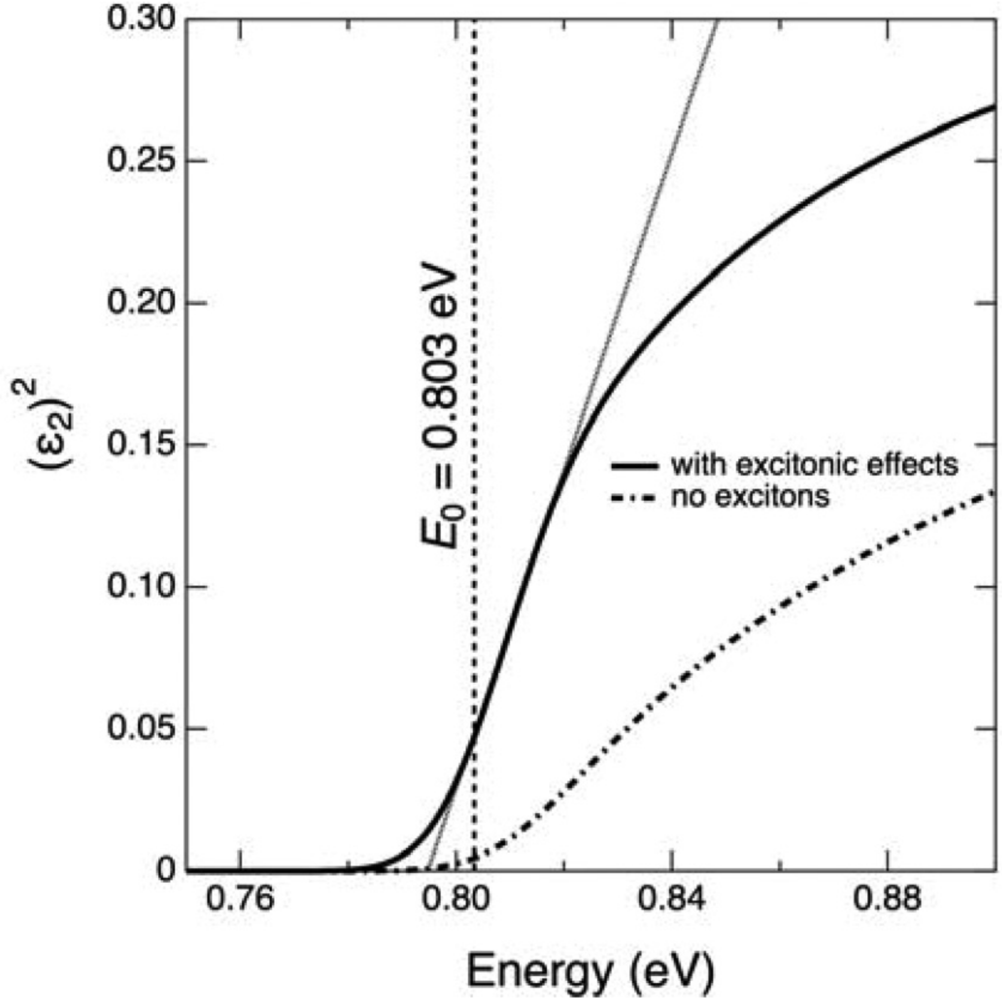
The linear plot



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