6.730 Physics for Solid State Applications

Lecture 31: Electron-photon Scattering

Outline

Electron-photon Matrix Element

- State-State Scattering Rate
- Scattering Time
- Absorption Coefficient
- Momentum Matrix Element
- Optical Gain

April 26, 2004

Scattering Rate Calculations

Overview

Step 1: Determine Scattering Potential

$$U_S(r,t) = U^a(r)e^{-i\omega t} + U^e(r)e^{+i\omega t}$$

Step 2: Calculate Matrix Elements

$$H^a_{k'k} = \int_V \psi_{nk'}(r)\ U^a_s(r)\ \psi_{nk}(r)\ d^3r$$

Step 3: Calculate State-State Transition Rates

$$S(k,k') = \frac{2\pi}{\hbar}\left[|H^a_{k'k}|^2\delta(E(k')-E(k)-\hbar\omega) + |H^e_{k'k}|^2\delta(E(k')-E(k)+\hbar\omega)\right]$$

Step 4: Calculate State Lifetime

$$\frac{1}{\tau(k)} = \sum_{k'} S(k,k')\left(1-f(k')\right)$$

Step 5: Calculate Ensemble Lifetime

$$<\tau>$$

Relating Forces to Potentials

For velocity independent potentials...

$$F_x = -\frac{\partial U_s}{\partial x}$$

For velocity *dependent* potentials...

$$F_x = -\frac{\partial U_s}{\partial x} + \frac{d}{dt}\left(\frac{\partial U_s}{\partial v_x}\right)$$

For electron-photon interactions...

$$\overline{F} = q(\overline{E} + \overline{v} \times \overline{B})$$

... there is an explicit velocity dependence in the force

Vector Potentials

Maxwell's Equations and Vector Potentials...

$$\overline{\nabla} \cdot \overline{B} = 0 \qquad \Rightarrow \overline{B} \equiv \overline{\nabla} \times \overline{A}$$

$$\overline{\nabla} \times \overline{E} = -\frac{\partial \overline{B}}{\partial t} = -\overline{\nabla} \times \frac{\partial \overline{A}}{\partial t} \qquad \Rightarrow \overline{E} = -\frac{\partial \overline{A}}{\partial t}$$

Lorentz Force and Vector Potentials...

$$\overline{F} = q(\overline{E} + \overline{v} \times \overline{B}) \qquad \Rightarrow q\left(-\frac{\partial A}{\partial t} + \overline{v} \times \overline{\nabla} \times \overline{A}\right)$$

Plane waves...

$$\overline{A}(r,t) = \frac{A_0}{2}\hat{\epsilon}\left(e^{i(\overline{\beta} \cdot \overline{r} - wt)} + c.c.\right)$$

Electron-Photon Scattering Potential

$$\overline{F} = q(\overline{E} + \overline{v}\times\mathrm{B}) \qquad \Rightarrow q\left(-\frac{\partial A}{\partial t} + \overline{v}\times\overline{\nabla}\times\mathrm{A}\right)$$

$$\left(\overline{v}\times\overline{\nabla}\times\overline{\mathrm{A}}\right)_x = \frac{\partial(\overline{v}\cdot\overline{A})}{\partial x} - \frac{dA_x}{dt} + \frac{\partial A_x}{\partial t} = \frac{\partial(\overline{v}\cdot\overline{A})}{\partial x} - \frac{d}{dt}\left(\frac{\partial(\overline{A}\cdot\overline{v})}{\partial v_x}\right) + \frac{\partial A_x}{\partial t}$$

$$\boxed{F_x = q\left(\frac{\partial(\overline{v}\cdot\overline{A})}{\partial x} - \frac{d}{dt}\left(\frac{\partial(\overline{A}\cdot\overline{v})}{\partial v_x}\right)\right)}$$

$$F_x = -\frac{\partial U_s}{\partial x} + \frac{d}{dt}\left(\frac{\partial U_s}{\partial v_x}\right) \Rightarrow \boxed{U_s(r,t) = -q\overline{A}(r,t)\cdot\overline{v} = -q\overline{A}(r,t)\cdot\frac{\overline{p}}{m_0}}$$

Electron-Photon Matrix Element

$$H_{kk'} = \int u^*_{c,k'}\mathrm{e}^{-i\overline{k'}\cdot\overline{r}}\left(\frac{-q\overline{A}(r,t)\cdot\overline{p}}{m_0}\right) u_{v,k}\,\mathrm{e}^{i\overline{k}\cdot\overline{r}}\,d^3\overline{r}$$

$$\overline{A}(r,t) = \frac{A_0}{2}\,\hat{\epsilon}\left(\mathrm{e}^{i(\overline{\beta}\cdot\overline{r}-wt)} + \mathrm{e}^{-i(\overline{\beta}\cdot\overline{r}-wt)}\right)$$

Photon Absorption Matrix Element...

$$H_{kk'} = \frac{-qA_0}{2m_0}\int u^*_{c,k'}(r)\mathrm{e}^{-i\overline{k'}\cdot\overline{r}}\mathrm{e}^{+i\overline{\beta}\cdot\overline{r}}(\hat{\epsilon}\cdot\overline{p})\;u_{v,k}(r)\mathrm{e}^{i\,\overline{k}\cdot\overline{r}}\;d^3\overline{r}$$

Electron-Photon Matrix Element

Photon Absorption Matrix Element...

$$H_{kk'} = \frac{-qA_0}{2m_0} \int u^*_{c,k'}(r) e^{-i\overline{k'}\cdot\overline{r}} e^{+i\overline{\beta}\cdot\overline{r}} (\hat{\epsilon}\cdot\overline{p})\ u_{v,k}(r) e^{i\,\overline{k}\cdot\overline{r}}\ d^3\overline{r}$$

$$= \frac{-qA_0}{2m_0} \int u^*_{c,k'}(r) e^{-i\,\overline{k}'\cdot\overline{r}} e^{+i\overline{\beta}\cdot\overline{r}} (-i\hbar\overline{\nabla})\ u_{v,k}(r) e^{i\,\overline{k}\cdot\overline{r}}\ d^3\overline{r}$$

(chain rule for derivative)

$$= \frac{-qA_0}{2m_0} \int [u^*_{c,k'}(r) e^{-i\overline{k}'\cdot\overline{r}} e^{i\overline{\beta}\cdot\overline{r}} e^{+ik\cdot\overline{r}} (-i\hbar\overline{\nabla})\, u_{v,k}(r)$$

$$+ u^*_{ck'}(r) e^{-i\,\overline{k}'\cdot\overline{r}} e^{i\overline{\beta}\cdot\overline{r}} (\hbar\overline{k})\, u_{vk}(r) e^{+i\overline{k}\cdot\overline{r}} d^3r]$$

Electron-Photon Matrix Element

Photon Absorption Matrix Element...

$$H_{kk'} = \frac{-qA_0}{2m_0} \int [u^*_{c,k'}(r) e^{-i\overline{k}'\cdot\overline{r}} e^{i\overline{\beta}\cdot\overline{r}} e^{+ik\cdot\overline{r}} (-i\hbar\overline{\nabla})\, u_{v,k}(r)$$

$$+ u^*_{ck'}(r) e^{-i\,\overline{k}'\cdot\overline{r}} e^{i\overline{\beta}\cdot\overline{r}} (\hbar\overline{k})\, u_{vk}(r) e^{+i\overline{k}\cdot\overline{r}} d^3r]$$

(separate slowly varying envelopes)

$$H_{kk'} = \frac{-qA_0}{2m_0} [\left(\sum_{R_m} e^{-i(k'-k-\beta)\cdot R_m}\right) \int u^*_{c,k'}(r)(-i\hbar\overline{\nabla})\, u_{v,k}(r) d^3r$$

$$+ \left(\sum_{R_m} e^{-i(k'-k-\beta)\cdot R_m}\right) \int u^*_{ck'}(r)(\hbar\overline{k})\, u_{vk}(r) d^3r]$$

$$\approx \frac{-qA_0\ \ < c|\hat{e}\cdot\overline{p}|v >}{2m_0} \delta_{k'=k+\beta} = \frac{-qA_0\ p_{cv}}{2m_0} \delta_{k'=k+\beta}$$

Electron-Photon Scattering Rate

$$H_{kk'} = \frac{-qA_0\, p_{cv}}{2m_0}\, \delta_{k'=k+\beta}$$

$$S(K,K') = \frac{2\pi}{\hbar}\, |H_{kk'}|^2\, \delta\left(E_c(k') - E_v(k) - \hbar\omega_\beta\right)$$

$$= \frac{2\pi}{\hbar}\, \frac{q^2 A_0^2\, |p_{cv}|^2}{4m_0^2}\, \delta_{k'=k+\beta}\, \delta\left(E_c(k') - E_v(k) - \hbar\omega_\beta\right)$$

Momentum Conservation

$$\overline{k}' = \overline{k} + \overline{\beta}$$

Let E ~ $k_B T$ and for room temperature this is 1/40 eV

$$k \approx \frac{\sqrt{2m^* E}}{\hbar} = \frac{\sqrt{2 \cdot (0.067)(9\text{x}10^{-31})(26\text{x}10^{-3})(1.6\text{x}10^{-19})}}{(10^{-34} J \cdot s)} \approx 2.2\text{x}10^{8}\ \text{m}^{-1}$$

$$\beta = \frac{\hbar\omega_\beta}{\frac{c}{n}\hbar} = \frac{(1eV)(1.6x10^{-19})}{\frac{(3x10^8)}{3}(10^{-34})} = 10^7\ m^{-1}\ so\ \beta \ll k$$

Electron momentum is relatively unchanged... $k' \approx k$

Momentum and Energy Conservation

$$E_c + \frac{\hbar^2 k'^2}{2m_c^*} = E_v - \frac{\hbar^2 k^2}{2m_v^*} + \hbar\omega_\beta$$

$$k' \approx k$$

Combining the conditions for energy and momentum conservation...

$$E_c(k') - E_v(k) - \hbar\omega_\beta = E_c - E_v - \hbar\omega_\beta + \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_c^*} + \frac{1}{m_v^*}\right)$$

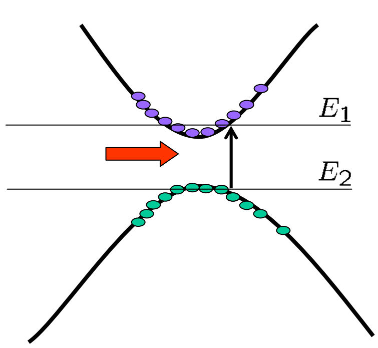
$$= E_g - \hbar\omega_\beta + \frac{\hbar^2 k^2}{2m_r}$$

m_r is called the reduced mass

Momentum and Energy Conservation

$$k' \approx k$$

$$E_c + \frac{\hbar^2 k'^2}{2m_c^*} = E_v - \frac{\hbar^2 k^2}{2m_v^*} + \hbar\omega_\beta$$

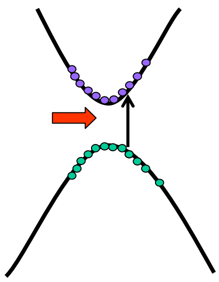


$$E_1 = \frac{\hbar^2 k^2}{2m_c^*} = \frac{\hbar\omega - E_g}{1 + m_c^*/m_v^*}$$

$$E_2 = \frac{\hbar^2 k^2}{2m_v^*} = \frac{\hbar\omega - E_g}{1 + m_v^*/m_c^*}$$

Electron-Photon Scattering Time

$$\frac{1}{\tau(k)} = \sum_{k'} S(k,k')$$



$$\frac{1}{\tau(k)} = \sum_{k'} \frac{2\pi\, q^2 A_0^2 |p_{cv}|^2}{\hbar\, m_0^2 4} \delta_{k'=k}\, \delta\left(E_c(k') - E_v(k) - \hbar\omega_\beta\right)$$

$$= \frac{2\pi\, q^2 A_0^2 |p_{cv}|^2}{\hbar\, m_0^2 4}\ \delta\left(E_g - \hbar\omega_\beta + \frac{\hbar^2 k^2}{2m_r}\right)$$

Photons only interact with a small set of k states...

Electron-Photon Scattering Time

$$\frac{1}{\tau_{total}} = \sum_k \frac{1}{\tau(k)} = \sum_k \frac{2\pi\, q^2 A_0^2 |p_{cv}|^2}{\hbar\, m_0^2 4}\, \delta\left(E_g - \hbar\omega_\beta + \frac{\hbar^2 k^2}{2m_r}\right)$$

$$= \frac{V}{8\pi^3} \int \left(\frac{2\pi\, q^2 A_0^2 |p_{cv}|^2}{\hbar\, m_0^2 4}\right) \delta\left(E_g - \hbar\omega_\beta + \frac{\hbar^2 k^2}{2m_r}\right) d^3\overline{k}$$

$$= V \left(\frac{2\pi\, q^2 A_0^2 |p_{cv}|^2}{\hbar\, m_0^2 4}\right) \rho_r(\hbar\omega - E_g)$$

Note: the reduced density of states differs from our ususal density of states by a factor of 2 since the electron doesn't scatter into both spin states necessarily

Absorption Coefficient

$$\alpha(\omega) = \frac{\text{\# of photons absorbed per unit time per unit volume}}{\text{\# of photons incident per unit time per unit area}}$$

$$= \frac{\frac{1}{\tau_{total}} \cdot \frac{1}{V}}{S/\hbar\omega} \qquad \text{cm}^{-1}$$

Where the intensity is the magnitude of the Poynting vector...

$$S = |E\text{x}\text{H}| \qquad \frac{\text{W}}{\text{cm}^2}$$

Light Intensity and Vector Potential

$$\alpha(\omega) = \frac{\frac{1}{\tau_{total}} \cdot \frac{1}{V}}{S/\hbar\omega}$$

$$S = |E\text{x}\text{H}| = \left| -\frac{\partial \text{A}}{\partial \text{t}} \text{x} \frac{1}{\mu_0} (\nabla \text{x} \text{A}) \right|$$

$$\overline{A}(r,t) = \frac{A_0}{2} \hat{\epsilon} \left(\text{e}^{i(\overline{\beta} \cdot \overline{r} - wt)} + c.c. \right)$$

$$S = |E\text{x}\text{H}| = \frac{\omega_\beta \beta}{2\mu_0} \text{A}_0^2$$

$$\omega_\beta = \frac{c}{n}\beta \Rightarrow \beta = \frac{n}{c}\omega_\beta$$

$$S = \frac{n\omega^2}{2c\mu_0} A_o^2$$

Absorption Coefficient

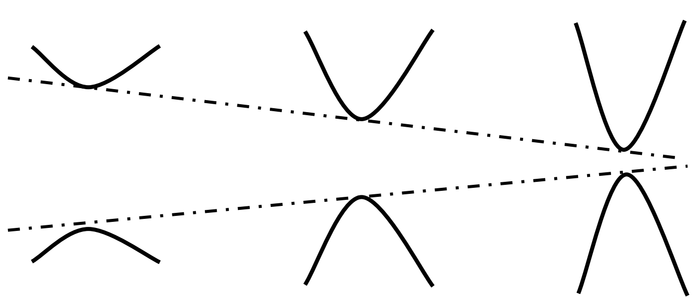
$$\frac{1}{\tau_{total}} = V\left(\frac{2\pi\, q^2 A_0^2 |p_{cv}|^2}{\hbar\, m_0^2 4}\right) \rho_r(\hbar\omega - E_g) \qquad S = \frac{n\omega^2}{2c\mu_0} A_o^2$$

$$\alpha(\omega) = \frac{\frac{1}{\tau_{total}}\frac{1}{V}}{S/\hbar\omega} = \frac{\pi\, q^2 A_0^2 |p_{cv}|^2}{2\hbar\, m_0^2} \frac{2c\mu_0 \hbar\omega}{n\omega^2 A_0^2} \rho_r(\hbar\omega - E_g)$$

$$= \frac{\pi\, q^2 c\mu_0}{m_0^2 \omega\, n} |p_{cv}|^2 \rho_r(\hbar\omega - E_g)$$

Independent of light intensity...think of it as a property of the solid.

Momentum Matrix Elements and k.p Effective Mass



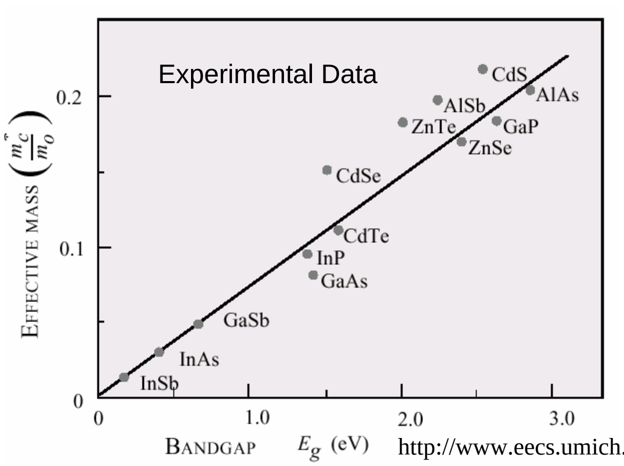
$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2}\frac{|p_{cv}|^2}{E_g}$$

$$E_n^{(2)} \approx E_n^0 + V_{nn} + \sum_{p \neq n} \frac{|V_{np}|^2}{E_n^0 - E_p^0}$$

Level repulsion causes bands to curve as bandgap is reduceed...

Momentum Matrix Elements and k.p Effective Mass

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2}\frac{|p_{cv}|^2}{E_g}$$



http://www.eecs.umich.edu/~singh/bk7ch03.pdf

$$\frac{2|p_{cv}|^2}{m_0} \approx 20eV$$

The momentum matrix is nearly constant for a wide range of materials..

Absorption Coefficient

$\underline{GaAs}$	$\underline{InP}$
$m_c^* = 0.067$	$m_c^* = 0.077$
$m_{v,HH}^* = 0.5$	$m_{v,HH}^* = 0.6$
$m_r^* = 0.059$	$m_r^* = 0.068$
$E_g = 1.424$	$E_g = 1.344$
$n_r = 3.606$	$n_r = 3.456$

$$\frac{\alpha_{GaAs}(1.5eV)}{\alpha_{InP}(1.5eV)} \approx \frac{n_{InP}}{n_{GaAs}} \frac{m_{r,GaAs}^{*3/2}(1.5eV - E_{g,GaAs})^{1/2}}{m_{r,InP}^{*3/2}(1.5eV - E_{g,InP})^{1/2}}$$

$= 0.51$ theory

$= 0.4$ Experiment (errors due to light-holes and p_{cv})

Optical Properties at High Carrier Concentrations

At high density, have to check to see if state at *k'* is empty....

$$\frac{1}{\tau(k)} = \sum_{k'} S(k,k') \Rightarrow \frac{1}{\tau(k)} = \sum_{k'} S(k,k')\,(1-f(k'))$$

...and also if there is a carrier at state *k*....

$$\frac{1}{\tau_{total}} = \sum_{k} \frac{1}{\tau(k)} = \sum_{k}\sum_{k'} S(k,k')\;(1-f(k'))f(k)$$

In general, we should redo the integrals account for Fermi functions...
...all the delta functions make this easy to do...

Gain Coefficient

Since $f(k) = f(k')$ under illumination, we can substitute $f(k) \to f(E)$

At high density, the absorption coefficient is...

$$\alpha(\omega) = \frac{\pi\, q^2 c\mu_0}{m_0^2 \omega\, n} |p_{cv}|^2\, \rho_r(\hbar\omega - E_g)\, f_v(E_2)\,(1-f_c(E_1))$$

At high density, the emission coefficient (stimulated emission) is...

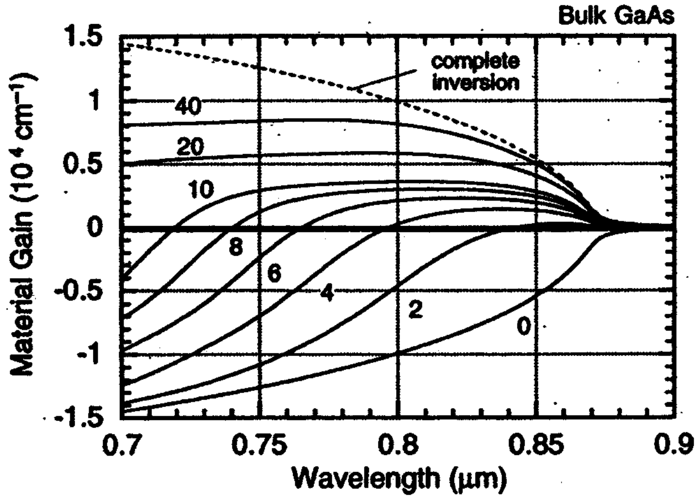
$$s(\omega) = \frac{\pi\, q^2 c\mu_0}{m_0^2 \omega\, n} |p_{cv}|^2\, \rho_r(\hbar\omega - E_g)\, f_c(E_1)\,(1-f_v(E_2))$$

...the net gain is...

$$g(\omega) = s(\omega) - \alpha(\omega)$$

$$g(\omega) = \frac{\pi\, q^2 c\mu_0}{m_0^2 \omega\, n} |p_{cv}|^2\, \rho_r(\hbar\omega - E_g)\,(f_c(E_1) - f_v(E_2))$$

Gain/Absorption Curves for Bulk GaAs



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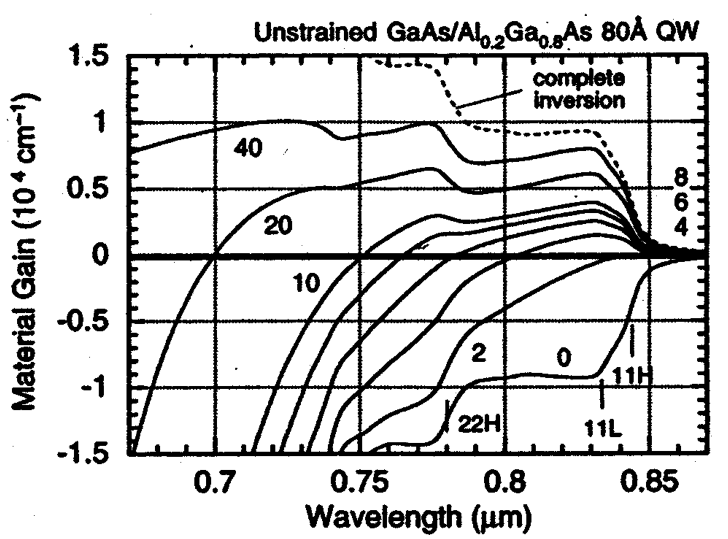
Gain/Absorption Curves for Quantum Wells



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Population Inversion in Solids

$$g(\omega) = \frac{\pi\, q^2 c \mu_0}{m_0^2 \omega\, n} |p_{cv}|^2 \rho_r(\hbar\omega - E_g)\,(f_c(E_1) - f_v(E_2))$$

$$g(\omega) > 0 \Rightarrow f_c(E_1) > f_v(E_2)$$

$$\frac{1}{e^{(E_1 - E_{fc})/kt} + 1} > \frac{1}{e^{(E_2 - E_{fv})/kt} + 1}$$

$$e^{(E_2 - E_{fv})/kt} + 1 > e^{(E_1 - E_{fc})/kt} + 1$$

$$E_2 - E_{fv} > E_1 - E_{fc}$$

$$E_{fc} - E_{fv} > E_1 - E_2 = \hbar\omega$$

Population inversion: $E_{fc} - E_{fv} > \hbar\omega$