EE 232 Lightwave Devices
Lecture 9: Optical Matrix Element, k-Selection Rule, Quantum Well Gain / Absorption

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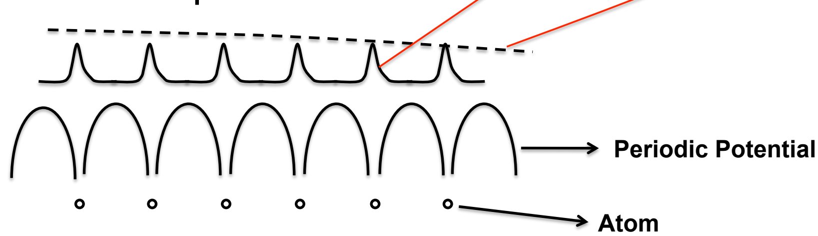
Bloch Function

- **Bloch function**
  - **Electron wavefunction in a periodic potential can be expressed as a product of a periodic function and a slowly varying plane wave envelop function**

$$|a\rangle = \psi_a(\vec{r}) = u_v(\vec{r})\frac{e^{i\vec{k}_v\cdot\vec{r}}}{\sqrt{V}}$$

$$|b\rangle = \psi_b(\vec{r}) = u_c(\vec{r})\frac{e^{i\vec{k}_c\cdot\vec{r}}}{\sqrt{V}}$$



Optical Matrix Element

$$H'_{ba} = \left\langle b \left| \left(-\frac{eA_0}{2m_0}\hat{e}\cdot\vec{P} \right) \right| a \right\rangle = -\frac{eA_0}{2m_0}\hat{e}\cdot\left\langle b \middle| \vec{P} \middle| a \right\rangle = -\frac{eA_0}{2m_0}\hat{e}\cdot\vec{P}_{ba}$$

Electron wavefunction can be expressed in Bloch functions:

$$\left|a\right\rangle = \psi_a(\vec{r}) = u_v(\vec{r})\frac{e^{i\vec{k}_v\cdot\vec{r}}}{\sqrt{V}}; \qquad \left|b\right\rangle = \psi_b(\vec{r}) = u_c(\vec{r})\frac{e^{i\vec{k}_c\cdot\vec{r}}}{\sqrt{V}}$$

$$H'_{ba} = -\frac{eA_0}{2m_0}\hat{e}\cdot\left\langle b \middle| \vec{P} \middle| a \right\rangle = -\frac{eA_0}{2m_0}\hat{e}\cdot\int u_c^*(\vec{r})e^{-i\vec{k}_v\cdot\vec{r}}e^{i\vec{k}_{op}\cdot\vec{r}}\left(-i\hbar\nabla\right)u_v(\vec{r})e^{i\vec{k}_v\cdot\vec{r}}\frac{d^3r}{V}$$

$$= -\frac{eA_0}{2m_0}\hat{e}\cdot\int u_c^*(\vec{r})e^{-i\vec{k}_c\cdot\vec{r}}e^{i\vec{k}_{op}\cdot\vec{r}}\left[\left(-i\hbar\nabla\right)u_v(\vec{r}) + (-i\hbar\vec{k}_v)u_v(\vec{r})\right]e^{i\vec{k}_v\cdot\vec{r}}\frac{d^3r}{V}$$

$$= -\frac{eA_0}{2m_0}\hat{e}\cdot\int u_c^*(\vec{r})\left(-i\hbar\nabla\right)u_v(\vec{r})\frac{d^3r}{\Omega}\int e^{-i\vec{k}_c\cdot\vec{r}}e^{i\vec{k}_{op}\cdot\vec{r}}e^{i\vec{k}_v\cdot\vec{r}}\frac{d^3r}{V}$$

Slowly Varying Envelop Approx

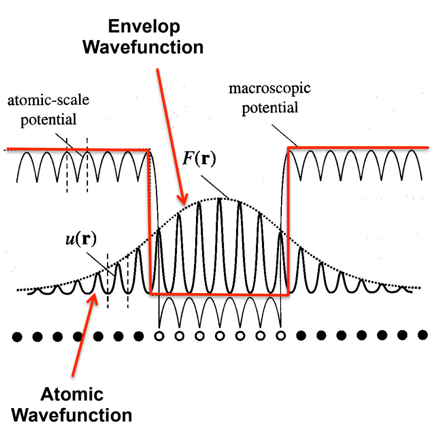
$$= -\frac{eA_0}{2m_0}\hat{e}\cdot\vec{p}_{cv}\cdot\delta_{\vec{k}_c,\vec{k}_{op}+\vec{k}_v}$$

k-Selection Rule

Matrix element of periodic function over unit cell

Optical Matrix Element for Quantum Wells

Quantum Well Wavefunction



$$\left|a\right\rangle = \psi_a(\vec{r}) = u_v(\vec{r})\frac{e^{i\vec{k}_t\cdot\vec{\rho}}}{\sqrt{A}}g_m(z)$$

$$\left|b\right\rangle = \psi_b(\vec{r}) = u_c(\vec{r})\frac{e^{i\vec{k}_{t'}\cdot\vec{\rho}}}{\sqrt{A}}\phi_n(z)$$

$$H'_{ba} = -\frac{eA_0}{2m_0}\hat{e}\cdot\left\langle b \middle| \vec{P} \middle| a \right\rangle$$

$$= -\frac{eA_0}{2m_0}\hat{e}\cdot\vec{p}_{cv}\cdot\delta_{\vec{k}_t,\vec{k}_{t'}}\cdot I_{hm}^{en}$$

Slowly Varying Envelop

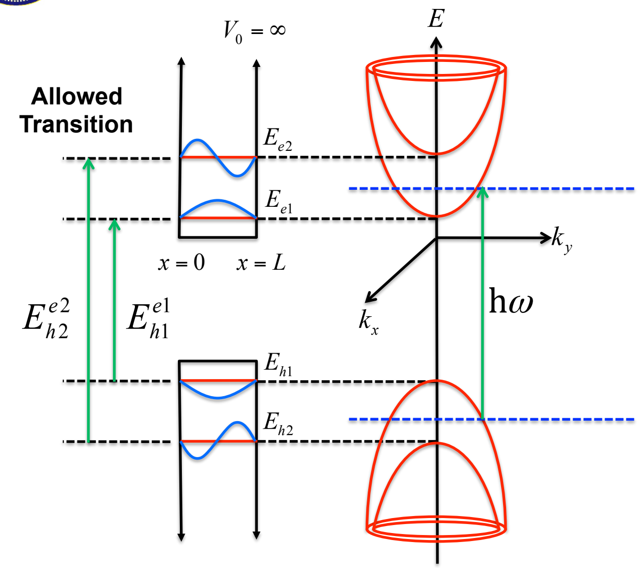
$$I_{hm}^{en} = \int_{-\infty}^{\infty}\phi_n^*(z)g_m(z)\,dz$$

Overlap integral of

QW envelop wavefunctions

$I_{hm}^{en} = \delta_{mn}$ for infinite potential well

Interband Transitions in Quantum Wells (1)



$E_{h1}^{e1} < \hbar\omega < E_{h2}^{e2}$

Only transition from m=1 hole subband to n=1 electron subband is allowed

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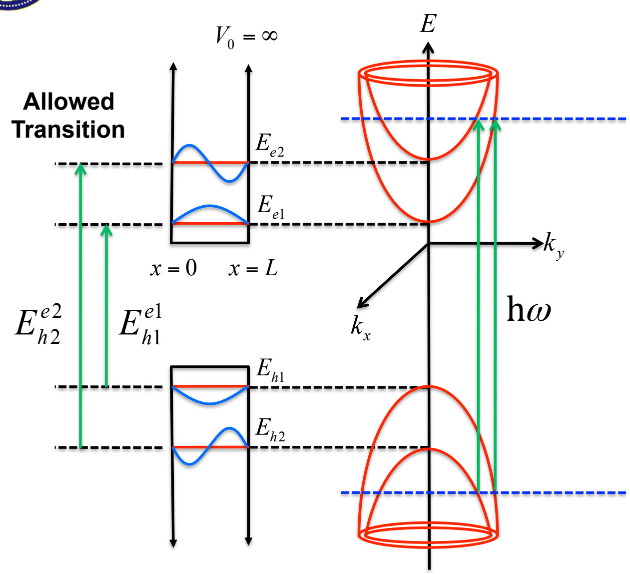
Interband Transitions in Quantum Wells (2)



$\hbar\omega > E_{h2}^{e2}$

$$\begin{cases} m=1 \rightarrow n=1 \\ m=2 \rightarrow n=2 \end{cases}$$

Since the density of states for each subband is the same, the maximum optical gain is twice of that of a single-band transition

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Optical Gain for Interband Transition in Quantum Wells

$$\boxed{g(\hbar\omega) = C_0 \left|\hat{e}\cdot\vec{P}_{cv}\right|^2 \rho_r^{2d}(\hbar\omega) f_g(\hbar\omega)}$$

$$\rho_r^{2d}(E) = \frac{m_r^*}{\pi\hbar^2 L_z}\sum_{n=1}^{\infty} H(E - E_{hn}^{en})$$

$$f_g(\hbar\omega) = f_C\left(E_{en} + \left(\hbar\omega - E_{hn}^{en}\right)\frac{m_r^*}{m_e^*}\right) - f_V\left(-E_{hm} - \left(\hbar\omega - E_{hn}^{en}\right)\frac{m_r^*}{m_h^*}\right)$$

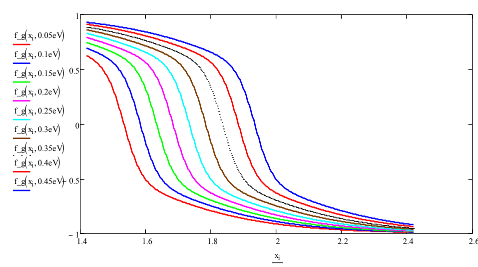
For more general case:

$$\Rightarrow g(\hbar\omega) = C_0 \left|\hat{e}\cdot\vec{P}_{cv}\right|^2 \sum_{m,n}\left|I_{hm}^{en}\right|^2 \rho_r^{2d} H(\hbar\omega - E_{hm}^{en}) f_g(\hbar\omega)$$

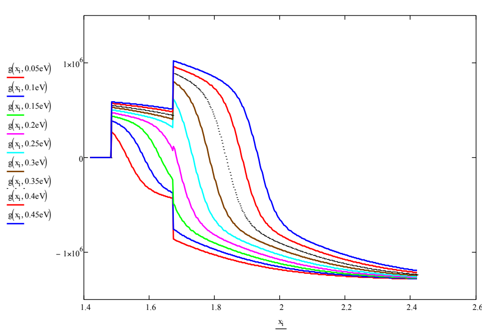
$$\rho_r^{2d} = \frac{m_r^*}{\pi\hbar^2 L_z}$$

Quantum Well Gain

Fermi Inversion Factor



Gain



Solving Quasi-Fermi Level in Quantum Well

Electron concentration:

$$N = \int dE \rho_e^{2d}(E) f_C^n(E)$$

$$\rho_e^{2d}(E) = \frac{m_e^*}{\pi\hbar^2 L_z} \sum_{n=1}^{\infty} H(E - E_{en})$$

$$f_C^n(E) = \frac{1}{1 + e^{\frac{E_{en}+E_t-F_C}{k_B T}}}$$

Use $\int \frac{dx}{1+e^x} = -\ln(1+e^{-x})$

$$N = \sum_n \frac{m_e^* k_B T}{\pi\hbar^2 L_z} \ln\left(1 + e^{\frac{F_C - E_{en}}{k_B T}}\right)$$

For large quasi-Fermi Energy:

$F_C \gg E_{en}$

$$\ln\left(1 + e^{\frac{F_C - E_{en}}{k_B T}}\right) \approx \frac{F_C - E_{en}}{k_B T}$$

$$N = \sum_n \frac{m_e^*}{\pi\hbar^2 L_z}\left(F_C - E_{en}\right)$$

For small quasi-Fermi Energy:

$F_C \ll E_{en}$

$$\ln(1 + e^{\frac{F_C - E_{en}}{k_B T}}) \approx e^{\frac{F_C - E_{en}}{k_B T}} = e^{-\frac{E_{en} - F_C}{k_B T}}$$

$$\boxed{N = \frac{m_e^* k_B T}{\pi\hbar^2 L_z} e^{-\frac{E_{e1} - F_C}{k_B T}} = N_C e^{-\frac{E_{e1} - F_C}{k_B T}}}$$