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

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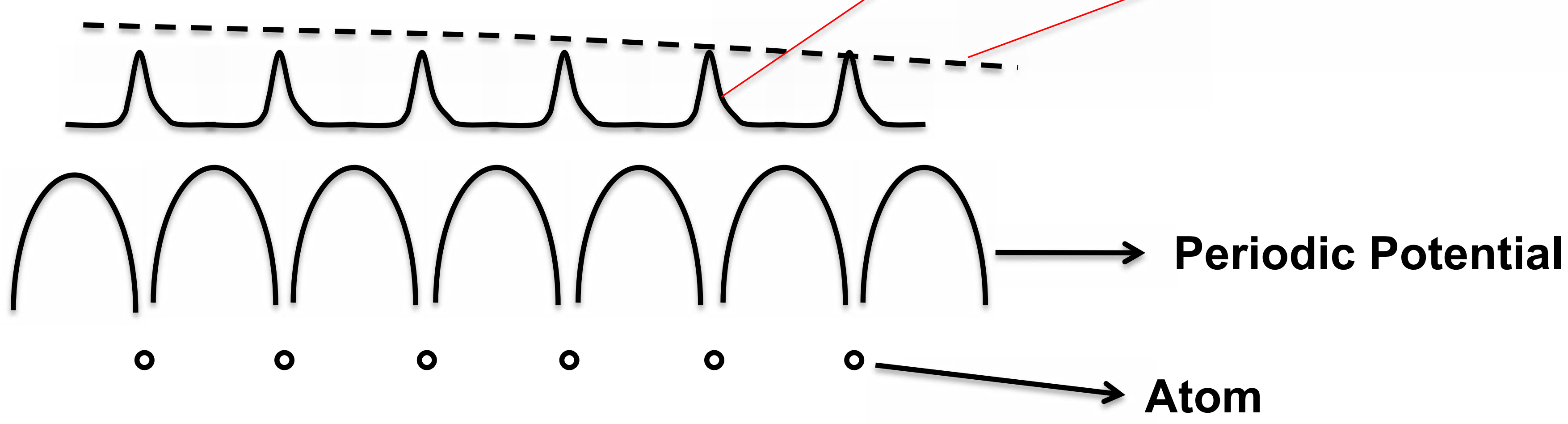
Bloch Function

- **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**

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

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



Optical Matrix Element

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

Electron wavefunction can be expressed in Bloch functions:

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

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

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

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

Slowly Varying Envelop Approx

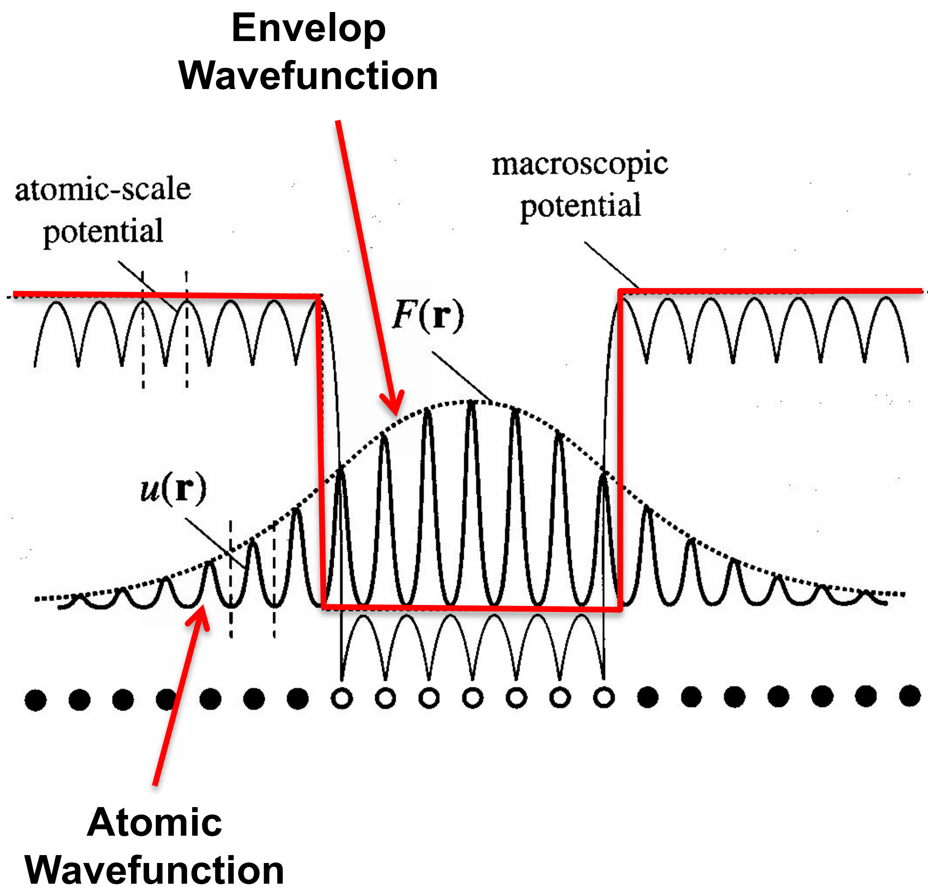
$$= -\frac{eA_0}{2m_0} \hat{e} \cdot \vec{p}_{cv} \cdot \delta_{\vec{k}_c, \vec{k}_{op} + \vec{k}_v}$$

k-Selection Rule

Matrix element of periodic function over unit cell

Optical Matrix Element for Quantum Wells

Quantum Well Wavefunction



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

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

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

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

Slowly Varying Envelop

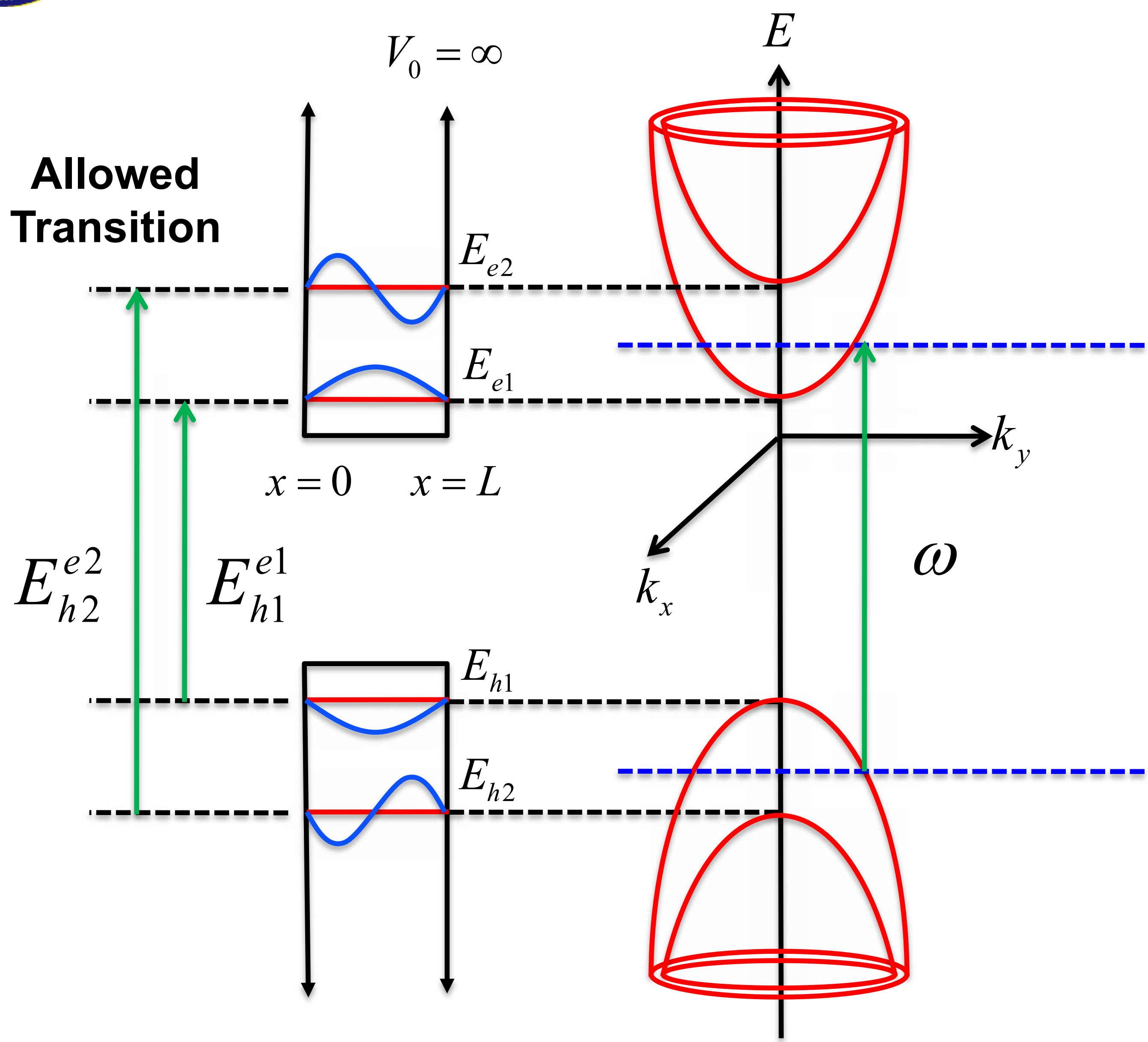
$$I_{hm}^{en} = \int_{-\infty}^{\infty} \phi_n^*(z) g_m(z)\, dz$$

Overlap integral of

QW envelop wavefunctions

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

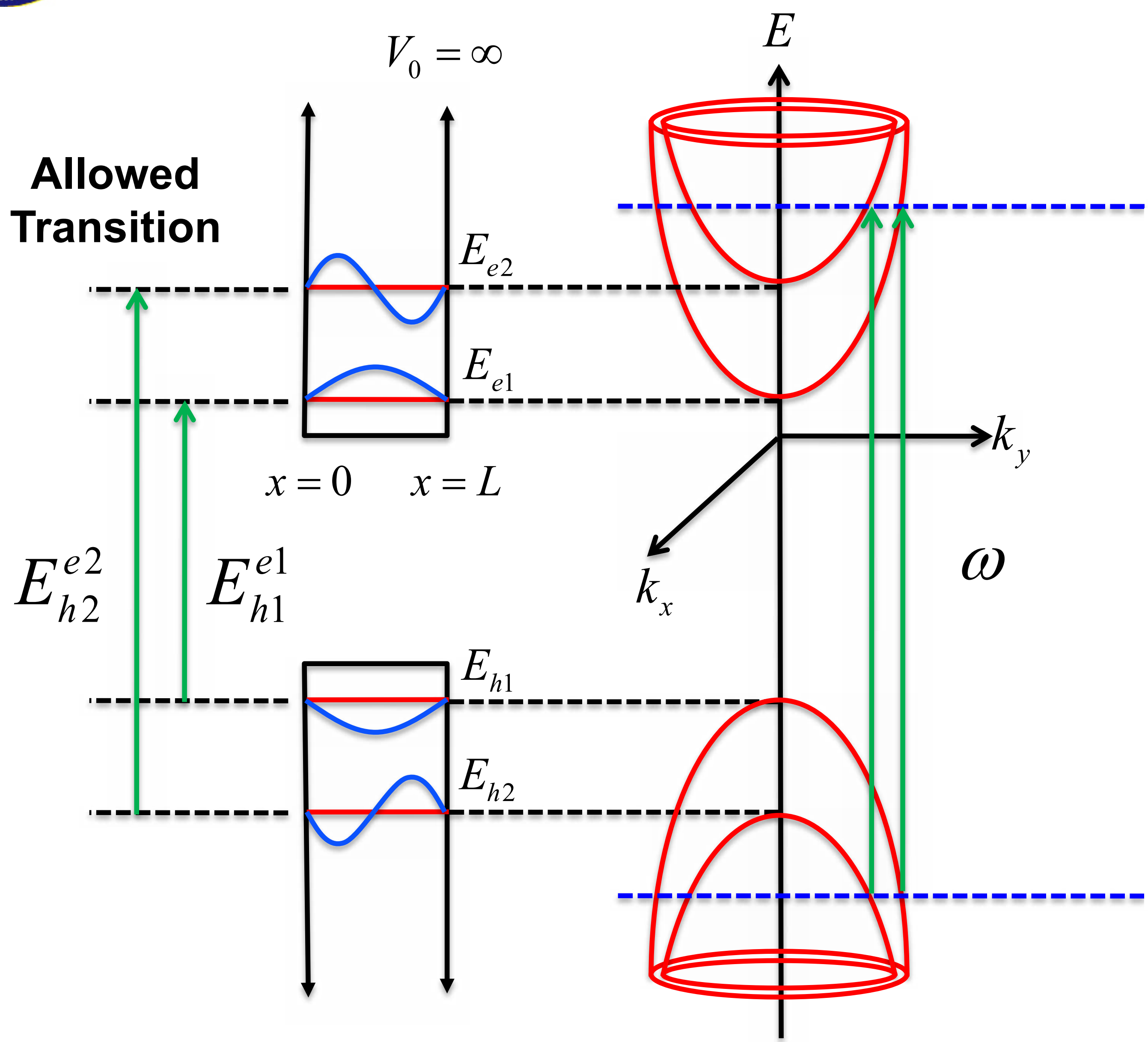
Interband Transitions in Quantum Wells (1)



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

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

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

Optical Gain for Interband Transition in Quantum Wells

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

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

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

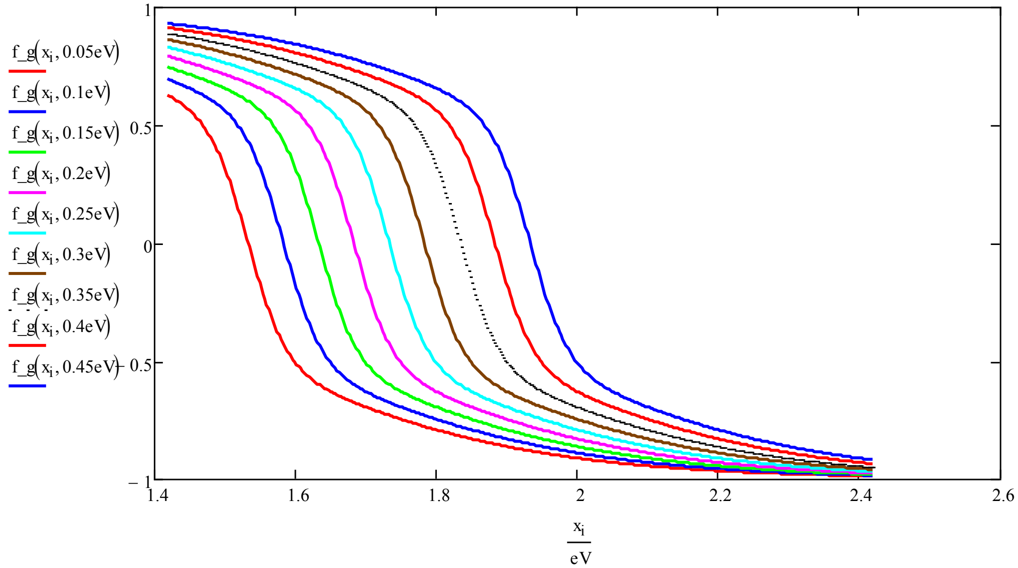
For more general case:

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

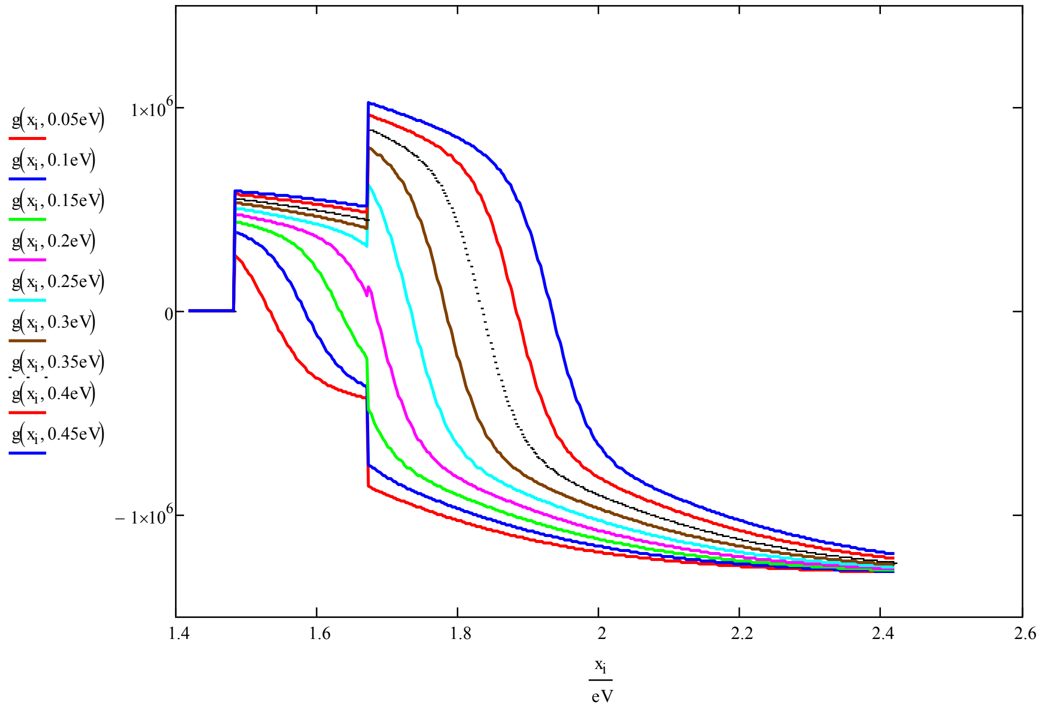
$$\rho_r^{2d} = \frac{m_r^*}{\pi\hbar^2 L_z}$$

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:

$$F_C \ll E_{en}$$

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

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