Interband Transition Selection Rules

From Bloch's theorem, we can write the conduction and valence electron wave equations of the form:

$$|\psi\rangle = u(\bar{r})\frac{e^{i\bar{k}\cdot\bar{r}}}{\sqrt{V}}$$

where $\sqrt{V}$ is for normalization. For an electron in a bulk semiconductor, $u(\bar{r})$ is a quickly varying periodic function due to the underlying atomic lattice and $e^{i\bar{k}\cdot\bar{r}}$ represents the much more slowly varying envelope of the electron's wavefunction. For electrons in the valence & conduction band, we have:

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

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

Recall that the matrix element corresponding to the rate of transition from the conduction to valence band is given by:

$$\mathcal{H}'_{ba} = -\frac{eA_0}{2m_0}e^{i\bar{k}_{op}\cdot\bar{r}}\,\hat{e}\cdot\langle b|\bar{P}|a\rangle \qquad (\text{Note: In general } \bar{k}_{op}\cdot\bar{r}\sim 0)$$

We know that the outer product $\langle b|\cdots|a\rangle$ can be expressed as an integral over real space and that $\bar{P}$ is the quantum mechanical momentum operator $-i\hbar\bar{\nabla}$, thus:

$$\mathcal{H}'_{ba} = -\frac{eA_0}{2m_0}\hat{e}\cdot\int d\bar{r}\,e^{i\bar{k}_{op}\cdot\bar{r}}\,u_c^*(\bar{r})\frac{e^{-i\bar{k}_c\cdot\bar{r}}}{\sqrt{V}}\left\{-i\hbar\bar{\nabla}_r\,u_v(\bar{r})\frac{e^{i\bar{k}_v\cdot\bar{r}}}{\sqrt{V}}\right\}$$

$$= +\frac{i\hbar eA_0}{2m_0V}\hat{e}\cdot\int d\bar{r}\,u_c^*(\bar{r})e^{i(\bar{k}_{op}-\bar{k}_c)\cdot\bar{r}}\left\{e^{i\bar{k}_v\cdot\bar{r}}\bar{\nabla}_r u_v(\bar{r}) + u_v(\bar{r})\bar{\nabla}_r e^{i\bar{k}_v\cdot\bar{r}}\right\}$$

We have two terms that we can consider independently.

Consider the 2nd term:

$$2^{nd} \text{ term } \propto \hat{e} \cdot \int d\bar{r}\, u_c^*(\bar{r})\, u_v(\bar{r})\, e^{i(\bar{k}_{op}-\bar{k}_c)\cdot\bar{r}}\, \bar{\nabla}_r e^{i\bar{k}_v\cdot\bar{r}}$$

Next note that the complex exponentials (and their derivatives) vary slowly compared to $u_c(\bar{r})$ and $u_v(\bar{r})$. We can thus invoke the slowly varying envelope approximation which states:

$$\int d\bar{r}\, A(\bar{r}) B(\bar{r}) \approx \int d\bar{r}\, A(\bar{r}) \int d\bar{r}\, B(\bar{r})$$

given that $A(\bar{r})$ is a quickly varying function and $B(\bar{r})$ is comparatively slowly varying. It follos that

$$2^{nd} \text{ term } \sim \hat{e} \cdot \int_\Omega d\bar{r}\, u_c^*(\bar{r}) u_v(\bar{r}) \int_V d\bar{r}\, e^{i(\bar{k}_{op}-\bar{k}_c)\cdot\bar{r}}\, \bar{\nabla}_r e^{i\bar{k}_v\cdot\bar{r}}$$

It turns out that we require that $u_c(\bar{r})$ and $u_v(\bar{r})$ be orthogonal functions (WHY??) thus it follows that the 2^{nd} term is approximately zero since:

$$\int_\Omega d\bar{r}\, u_c^*(\bar{r}) u_v(\bar{r}) = \langle u_c | u_v \rangle = 0$$

This leaves us w/ the first term only:

$$\mathcal{H}_{ba}' \simeq -\frac{eA_0}{2m_0} \hat{e} \cdot \int d\bar{r}\, u_c^*(\bar{r}) [-i\hbar \bar{\nabla}_r] u_v(\bar{r}) \frac{1}{V} e^{i(\bar{k}_{op}-\bar{k}_c+\bar{k}_v)\cdot\bar{r}}$$

Once again, we can separate the integral into a slowly varying integral & quickly varying integral:

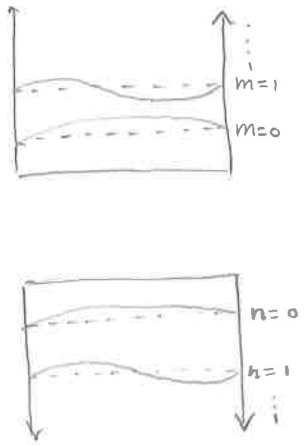
$$\mathcal{H}_{ba}' \simeq -\frac{eA_0}{2m_0} \hat{e} \cdot \int_\Omega d\bar{r}\, u_c^*(\bar{r}) [-i\hbar \bar{\nabla}] u_v(\bar{r}) \int_V d\bar{r} \frac{1}{V} e^{i(\bar{k}_{op}-\bar{k}_v+\bar{k}_c)\cdot\bar{r}}$$

$$\approx \boxed{-\frac{eA_0}{2m_0} \hat{e} \cdot \langle u_c | \bar{P} | u_v \rangle\, \delta(\bar{k}_{op} - \bar{k}_c + \bar{k}_v) \approx \mathcal{H}_{ba}'}$$

polarization information contained in here.

conservation of momentum

Transitions in 2D Quantum Wells :



For a 2D Quantum well, the wavefunction has a non-periodic Z-dependence:

$$|a\rangle = u_v(\bar{r}) \frac{e^{i\bar{k}_t \cdot \bar{r}}}{\sqrt{A}} \varphi_n(z)$$

$$|b\rangle = u_c(\bar{r}) \frac{e^{i\bar{k}_t \cdot \bar{r}}}{\sqrt{A}} \psi_m(z)$$

First we consider <u>interband transitions</u>:

$$\mathcal{H}'_{ba} = -\frac{eA_0}{2m_0} \hat{e} \cdot \int d\bar{r}\, e^{i\bar{k}_{op} \cdot \bar{r}} u_c^*(\bar{r}) e^{-i\bar{k}_{tc} \cdot \bar{r}} \psi_m^*(z) \left[-i\hbar \bar{\nabla}\right] u_v(\bar{r}) e^{i\bar{k}_{tv} \cdot \bar{r}} \varphi_n(z) \frac{1}{A}$$

As previously shown, the only non-zero term is:

$$\mathcal{H}'_{ba} = -\frac{eA_0}{2m_0} \hat{e} \cdot \int_\Omega d\bar{r}\, u_c^*(\bar{r}) [-i\hbar \bar{\nabla}] u_v(\bar{r}) \int_V d\bar{r}\, e^{i(\bar{k}_{op} - i\bar{k}_{tc} + i\bar{k}_{tv}) \cdot \bar{r}} \psi_m^*(z) \varphi_n(z) \frac{1}{A}$$

Let us make the approximation that $\bar{k}_{op} \cdot \bar{r} << \bar{k}_t \cdot \bar{r}$. This allows us to write:

$$\mathcal{H}'_{ba} = -\frac{1}{V}\frac{eA_0}{2m_0} \hat{e} \cdot \int_\Omega d\bar{r}\, u_c^*(\bar{r}) [-i\hbar \bar{\nabla}] u_v(\bar{r}) \iint_A dx\,dy \frac{e^{i(\bar{k}_{tv} - \bar{k}_{tc}) \cdot \bar{r}}}{\sqrt{A}} \int_L dz\, \psi_m^*(z) \varphi_n(z)$$

$$= \boxed{-\frac{eA_0}{2m_0} \hat{e} \cdot \bar{P}_{cv}\, \delta_{\bar{k}_{tc}, \bar{k}_{tv}}\, I_{mn} \simeq \mathcal{H}'_{ba}}$$

Where I_{mn} is the overlap integral of $\psi_m(z)$ & $\varphi_n(z)$. Notice that since $\psi_m(z)$ and $\varphi_n(z)$ are even for even m, n and odd for odd m, n, $I_{mn} \simeq 0$ when m and n have <u>different parity</u>.

↳ $I_{mn} \rightarrow \delta_{mn}$ in infinite square well approx

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Next, we consider intersubband transitions: Let us consider the matrix element for a transition between subbands of the conduction band. The relevant wavefunctions are:

$$|a\rangle = u_c(\bar{r}) \frac{e^{i\bar{k}_{tc}\cdot\bar{r}}}{\sqrt{A}} \psi_m(z)$$

$$|b\rangle = u_c(\bar{r}) \frac{e^{i\bar{k}_{tc}\cdot\bar{r}}}{\sqrt{A}} \psi_n(z)$$

The matrix element is thus (assuming $\bar{k}_{op}\cdot\bar{r} \simeq 0$)

$$H'_{ba} \simeq -\frac{eA_0}{2m_0}\hat{e}\cdot\int_V d^3\bar{r}\, u_c^*(\bar{r}) e^{-i\bar{k}_t\cdot\bar{r}} \psi_n^*(z) \left[-i\hbar\bar{\nabla}_r\right] u_c(\bar{r}) e^{i\bar{k}_t\cdot\bar{r}} \psi_m(z) \frac{1}{A}$$

Applying chain rule and our integral approximation we are left w/ two terms:

$$H'_{ba} \simeq -\frac{eA_0}{2m_0}\hat{e}\cdot\int_V d^3\bar{r}\, u_c^*(\bar{r}) u_c(\bar{r}) \psi_n^*(z) e^{-i\bar{k}_t\cdot\bar{r}} (-i\hbar) \left\{ \psi_m(z) \bar{\nabla}_t e^{i\bar{k}_t\cdot\bar{r}} + e^{i\bar{k}_t\cdot\bar{r}} \hat{z} \frac{\partial}{\partial z}\psi_m(z) \right\} \frac{1}{A}$$

Let's analyze the two terms separately. Consider the 1st term:

$$1^{st}\text{ term} \propto \hat{e}\cdot\int_V d^3\bar{r}\, u_c^*(\bar{r}) u_c(\bar{r}) \psi_n^*(z) \psi_m(z) e^{-i\bar{k}_t\cdot\bar{r}} \left[-i\hbar\bar{\nabla}\right] e^{i\bar{k}_t\cdot\bar{r}}$$

$$\sim \hat{e}\cdot\int_V d^3\bar{r}\, u_c^*(\bar{r}) u_c(\bar{r}) \int_A d^2\bar{r}\, e^{-i\bar{k}_t\cdot\bar{r}} \left[-i\hbar\bar{\nabla}\right] e^{i\bar{k}_t\cdot\bar{r}} \underbrace{\int_L dz\, \psi_n^*(z)\psi_m(z)}_{0}$$

$$= 0 \text{ for } m \neq n$$

Thus the 1st term is zero. Next consider the 2nd term:

$$H'_{ba} \simeq -\frac{eA_0}{2m_0}\hat{e}\cdot\int_V d^3\bar{r}\, u_c^*(\bar{r}) u_c(\bar{r}) (-i\hbar) \psi_n^*(z) \frac{\partial}{\partial z}\psi_m(z)\, \hat{z}$$

$$\approx -\frac{eA_0}{2m_0}\hat{e}\cdot\hat{z} \int d^3\bar{r}\, u_c^*(\bar{r}) u_c(\bar{r}) \int dz\, (-i\hbar) \psi_n^*(z) \frac{\partial}{\partial z}\psi_m(z)$$

$$\neq 0$$

$\Rightarrow$ TE Mode allowed for n, m w/ different parity