Transition Rate for Direct Absorption

First calculate the "Density of Directly Associated States".
DDAS (E_{photon})

\[ E(k) = E_c + \frac{\hbar^2 k^2}{2m_e} \]

\[ E(k) = E_v + \frac{\hbar^2 k^2}{2m_v} \]

Step 1: How does the # of k-states increase with wave vector, \( k \)?

\[ \eta_{3d}(k) = \frac{k^3 L^3}{3\pi^2} \quad \Rightarrow \quad \frac{d\eta_{3d}}{dk} = \frac{k^2 L^3}{\pi^2} \]

Step 2: How does \( E_{photon} \) depend on \( k \)?

\[ E_{photon} = (E_c + \frac{\hbar^2 k^2}{2m_e}) - (E_v + \frac{\hbar^2 k^2}{2m_v}) \]

\[ = E_g + \frac{\hbar^2 k^2}{2} \left( \frac{1}{m_c} + \frac{1}{m_v} \right) = E_g + \frac{\hbar^2 k^2}{2 \mu} \]

\( \mu \) is the reduced mass.
Step 3  \[ \text{DDAS}(E_{ph}) = \frac{dn}{dk} / \frac{dE_{ph}}{dk} \]

\[ = \frac{k^2L^3}{\pi^2} \frac{\mu}{\hbar^2k} \]

\[ = \frac{L^3\mu}{\hbar^2\pi^2} \]

\[ = \frac{L^3\mu}{\hbar^2\pi} \sqrt{\frac{2\mu (E_{photon} - E_g)}{\hbar^2}} \]

Now need a

Quantitative relationship between \( \alpha \) & DDAS

Time-dependent perturbation theory is

summarized by Fermi's Golden Rule:

\[ W_{i-f} = \frac{2\pi}{\hbar^2} |\langle f | H' | i \rangle|^2 \text{DDAS}(E_{photon}) \]

transition rate between initial & final state that have \( E_f - E_i = E_{photon} \)

\( H' \) is perturbation Hamiltonian related to the photon's electric field.

\( \langle f | H' | i \rangle \) is called the "transition matrix element"
Conclusion \[ \alpha = (\text{constant})(E_{\text{photon}} - E_g)^{1/2} \]

Example: GaAs

\[ \alpha (\text{m}^{-1}) \]

\[ \begin{array}{c}
0 \\
2 \times 10^6 \\
\end{array} \]

\[ \begin{array}{c}
1.4 \text{eV} \\
2.4 \text{eV} \\
E_{\text{photon}} \\
E_g \\
\end{array} \]

Question: How thick should I make a GaAs solar cell?

Recall \[ I_o e^{-\alpha x} \]

I'd like 90% absorption \( \Rightarrow \alpha x \approx 2 \).

High absorption even when \( E_{\text{photon}} = 1.5 \text{eV} \)

where \( \alpha = 0.4 \times 10^6 \text{ m}^{-1} \)

Therefore, thickness > 5 \mu m.
COMMENTS ABOUT $\langle f | H' | i \rangle$, THE TRANSITION MATRIX ELEMENT

$$H' = V'(x) = eE_x x$$

Electric field of light polarized along the $x$-axis.

$$\langle f | H' | i \rangle = eE_x \int \phi_f^*(\vec{r}) x \phi_i(\vec{r}) \, d^3\vec{r}$$

consider an isolated hydrogen atom

Initial state $\rightarrow$ Final state

$1s \rightarrow 2p_x$ large transition matrix element

$1s \rightarrow 2s$ zero transition matrix element

The symmetry of the atomic orbitals determines allowed / forbidden transition, also called "selection rules"

For allowed transitions $\langle f | H' | i \rangle \sim eE_*(\text{size of atom})$

The energy change associated with moving an electron an atomic distance through an electric field $E$. 
The atomic selection rules say $\Delta l = 1$

\[ \text{i.e. } \begin{align*}
    s \rightarrow s & \times \\
    s \rightarrow p & \checkmark \\
    s \rightarrow d & \times
\end{align*} \]

These selection rules also apply to crystals that have 1 atom per primitive unit cell.

For diatomic molecules (and crystals that have 2 atoms per primitive unit cell) the selection rules are different.

For example

\[
|\phi_i\rangle = \frac{1}{\sqrt{2}} (|A\text{;}s\rangle + |B\text{;}s\rangle) \quad \text{"s-like" molecular orbital}
\]
\[
|\phi_f\rangle = \frac{1}{\sqrt{2}} (|A\text{;}2s\rangle - |B\text{;}2s\rangle) \quad \text{"s-like" molecular orbital}
\]

This transition is allowed because the symmetry of the wavefunction changed to ensure $\int \phi_i^*(r) \times \phi_f^*(r) d^3r \neq 0$
CALCULATING $\alpha$ USING WIEN 2K

Review electromagnetic wave theory inside materials

$$k_{\text{mat}}^{\text{photon}} = n k_{\text{vac}}^{\text{photon}}$$

The wave number of a photon changes when it goes from vacuum to inside material.

- $n$ is called refractive index.
- If the material absorbs light, then $n$ is a complex number, $\tilde{n}$.

Inside the material, the electric field of the electromagnetic wave is

$$\vec{E}(x) = \vec{E}_0 \exp \left( i \left( k_{\text{mat}}^{\text{photon}} x - wt \right) \right)$$

The imaginary component of $k_{\text{mat}}^{\text{photon}}$ causes the $E$-field to decay exponentially.

$$\alpha = 2 \text{Im}(\tilde{n}) k_{\text{vac}}^{\text{photon}}$$

factor 2 because $\text{Intensity}(\alpha) \propto |\vec{E}(x)|^2$
\[ \tilde{n}(\omega) = \sqrt{\frac{\tilde{\varepsilon}(\omega)}{\varepsilon_0}} \]

Wien 2k tells you the real & imaginary components of \( \tilde{\varepsilon} \).

In the limit of weak absorption \( (\alpha < k_{\text{photon}}) \)

\[ \alpha(\omega) \approx \frac{\text{Im } \varepsilon(\omega)}{\text{Re } \varepsilon(\omega)} \frac{\text{Re } k_{\text{photon}}(\omega)}{\text{Im } \varepsilon(\omega)} \]

Which means that people often say, in a loose sense,

\[ \alpha(\omega) \approx \text{Im } \varepsilon(\omega) \]

(See page 310, Jackson)