5. Electron-Photon Interaction

5.1 Spontaneous + Stimulated (transition) emission rates for two discrete electronic states

5.2 Absorption + gain coefficients

5.3 The Einstein treatment of induced (stimulated) and spontaneous transitions

5.4 Absorption spectrum in direct semiconductors

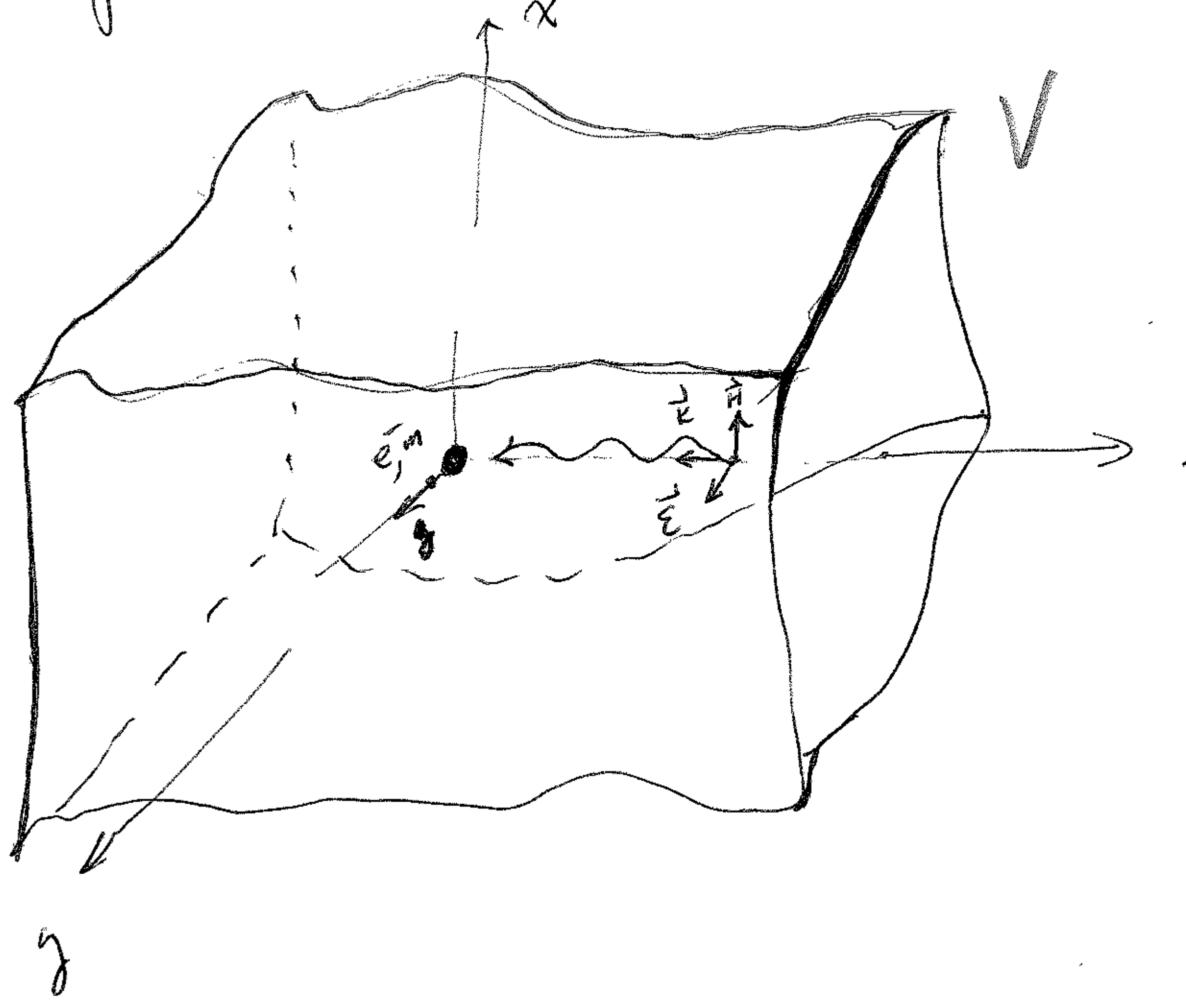
5.5 Spontaneous emission spectrum in direct semiconductors

5.6 example of H atom

5.1 Spontaneous & stimulated emission rates for two discrete electronic states

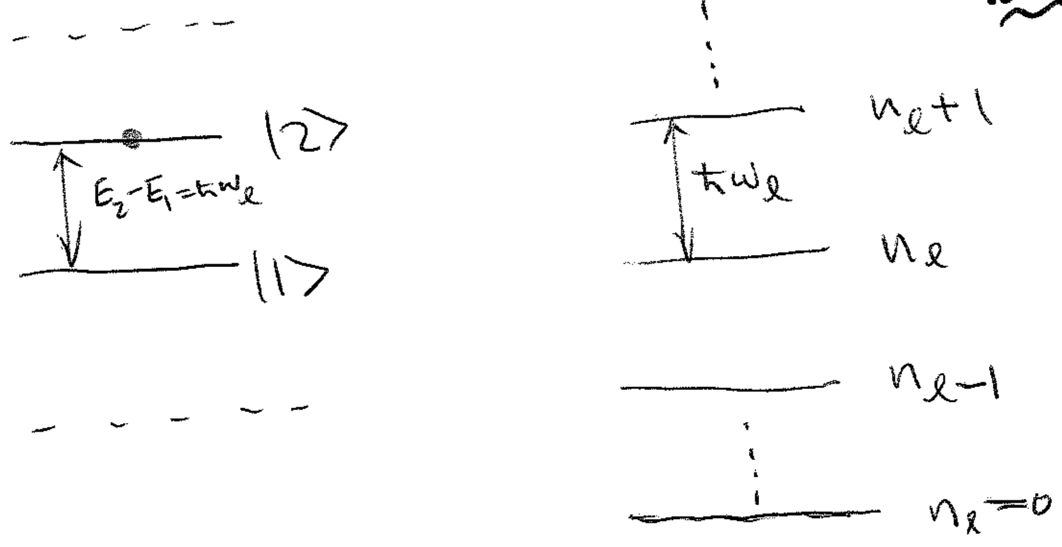
* system under consideration =
consists of ① one electromagnetic mode l with frequency ω_l and # of photons, n_l within the mode l inside a large optical enclosure with a volume V; ② an electron with two discrete energy states (E_1 & E_2) associated with an ion inside the optical enclosure.

* the physical layout of the system =



* The energy levels of the system =

(electron) (photons) (model) resonant



* Assuming electron is <u>in state $|2\rangle$</u>,

<u>what to find</u> = the optical transition probability per unit time (rate) for a transition from <u>state $|2\rangle$</u> <u>to state $|1\rangle$</u>, <u>induced by the interaction of the electromagnetic mode ℓ</u>. $\frac{|0\rangle}{|n_\ell\rangle}$

* <u>Method</u> (tool) = <u>quantum mechanics</u>

→ <u>time-dependent perturbation theory</u>

→ <u>Fermi-Golden's rule</u>

$$P_{21} = \frac{2\pi}{\hbar} \cdot \left| H'_{21} \right|^2 \cdot \underline{\delta(E_2 - E_1 \mp \hbar\omega_\ell)}$$

$$\left(\frac{1}{J \cdot S} \cdot J^2 \cdot J^{-1} \right) \rightarrow \frac{1}{S}$$

<u>with assumption of</u> $H_{int} = 2H' \sin(\omega_\ell t - \vec{k} \cdot \vec{r})$, $\vec{k} \cdot \vec{r} \approx 0$

$\vec{K}\cdot\vec{r} \simeq 0$ stands for the long-wavelength approximation, i.e. the electron wave function spread over a linear dimension that is much short than optical wave length. good for IR

* How to find H_{int}, interaction Hamiltonian ?

Three format of the interaction Hamiltonian:

1. Vector potential (or momentum) format
2. Dipole format
3. creation & annihilation operator format

* Vector potential format:

The Schrödinger equation for a single electron bounded by an ion:

$$i\hbar \frac{\partial}{\partial t}\psi = \hat{H}_0 \psi \,, \quad \hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 - eV(\vec{r})$$

- question = how to modify the above Schrödinger equation in order to include a photon with wave vector $\vec{k}$ and energy $\hbar\omega_\ell$?

(answer, no derivation available, like Shrödinger equation itself, only by reasonable analysis)

rewrite the Schrödinger equation ?

$$i\hbar\frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 - eV\right)\psi$$

$$\rightarrow \left(i\hbar\frac{\partial}{\partial t} + eV\right)\psi = \frac{(-i\hbar\vec{\nabla})\cdot(-i\hbar\vec{\nabla})}{2m}\psi$$

$$-i\hbar\vec{\nabla} \equiv \vec{p}$$ (defined as momentum operator)

(from quantum field theory) $\underbrace{-i\hbar\vec{\nabla}}_{e^-} \Rightarrow \underbrace{-i\hbar\vec{\nabla} + e\vec{A}}_{e^- + \text{field}}$, (if E.M. field is present)

$$\Rightarrow \left(i\hbar\frac{\partial}{\partial t} + eV\right)\psi = \frac{(-i\hbar\vec{\nabla} + e\vec{A})\cdot(i\hbar\vec{\nabla} + e\vec{A})}{2m}\psi$$

- Work out the dot product =

$$\rightarrow \underbrace{i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 - eV\right)\psi}_{\text{without photon}} - \underline{\frac{ie\hbar}{m}\vec{A}\cdot\vec{\nabla}\psi}$$

$$+ \underline{\frac{e^2}{m}\vec{A}\cdot\vec{A}\psi}$$

$$\rightarrow i\hbar \frac{\partial}{\partial t}\psi = (H_0 + H_{int})\psi$$

$\frac{1}{2m}(e\vec{A})\cdot(e\vec{A})$

$$\rightarrow \underline{H_{int} \equiv -\frac{ie\hbar}{m}\vec{A}\cdot\vec{\nabla}} + \frac{e^2}{2m}\vec{A}\cdot\vec{A}$$

for weak field approx. the second term is often neglected. (for strong laser-situation, valid? 6/10/05)

$$\rightarrow H_{int} \equiv +\frac{1}{m}\left[(e\vec{A})\cdot(-i\hbar\vec{\nabla})\right]$$

He-photon

(photon momentum) (electron momentum)

[Sign indicates that energy is ~~lower~~ higher than the bare electron case]

- how to find $\vec{A}$?

assumption : $\vec{\mathcal{E}} = E_0 \vec{a_y} \cos(\omega t - \vec{k} \cdot \vec{r})$

We need to relate the ~~raw~~ magnitude of E_0 to energy flux of photon system

from EE331, the energy flux of electromagnetic wave is given by $S = |\langle \vec{\mathcal{E}} \times \vec{H} \rangle|$ averaged over one optical cycle

$$\rightarrow \quad S = \frac{1}{2} E_0^2 n \epsilon_0 c \qquad (\text{Watts}/m^2)$$

On the other hand, if we consider one photon in the system, then, the energy flux should be :

$$S(\text{one photon}) = \frac{\hbar\omega}{V} \cdot \frac{c}{n}$$

(energy density (ρ_E)) $\cdot$ (velocity)

$$\Rightarrow \frac{1}{2} E_0^2 n \epsilon_0 c = \frac{\hbar\omega}{V} \cdot \frac{c}{n}$$

$$\rightarrow \quad E_0 = \left(\frac{2\hbar\omega}{V n^2 \epsilon_0} \right)^{1/2}$$

<u>Since</u> $\vec{\mathcal{E}} = -\frac{\partial \vec{A}}{\partial t}$ (EE331)

$$\vec{A} = -\int E_0 \vec{a_y} \cos(\omega t - \vec{K} \cdot \vec{r})\, dt$$

$$= -\underline{\vec{a_y}} \left(\frac{2\hbar}{V n^2 \epsilon_0 \omega} \right)^{1/2} \sin(\omega t - \vec{K} \cdot \vec{r})$$

$$\rightarrow H_{int} = -\frac{e}{m} \underline{\vec{A}} \cdot \underline{\vec{p}}$$

ē momentum

[m, should be free ē mass here, effective mass concept applies on when you deal with band. 1/9/98]

$$= \frac{e}{m} \left(\frac{2\hbar}{V n^2 \epsilon_0 \omega} \right)^{1/2} \underbrace{\sin(\omega t - \vec{K} \cdot \vec{r})}_{(\sim 0)} \underline{(\vec{a_y} \cdot \vec{p})}$$

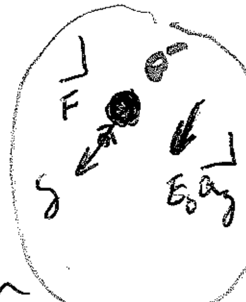
Compare to Fermi-Golden's rule

$$\boxed{P_{21} = \frac{e^2}{m^2} \cdot \frac{\pi}{V n^2 \epsilon_0 \omega} |M_{21}|^2 \delta(E_2 - E_1 + \hbar\omega_e)} \quad \boxed{1/5}$$

where $|M_{21}|^2 = |\langle 2 | \vec{a_y} \cdot \vec{p} | 1 \rangle|^2$

(momentum matrix) $\quad \vec{p} = \frac{\hbar}{i} \vec{\nabla} = \frac{\hbar}{i} \left(\frac{\partial}{\partial x} \vec{a_x} + \frac{\partial}{\partial y} \vec{a_y} + \frac{\partial}{\partial z} \vec{a_z} \right)$

* Dipole format



Since $\vec{E} = E_0 \vec{a_y} \cos(\omega t - \vec{k}\cdot\vec{r})$

the force ~~ex~~ excert'n on the electron can experience is =

$$\vec{F} = -e\vec{E}$$

the energy increase (or decrease) if electron moves ($\vec{r}$) against (or following) field is given by =

$$\left(\vec{r} = x\vec{a_x} + y\vec{a_y} + z\vec{a_z}\right)$$

$$\underline{H_{int}} \equiv +\vec{F}\cdot\vec{r}$$

$$= -eE_0\vec{a_y}\cos(\omega t - \vec{k}\cdot\vec{r})\cdot\vec{r}$$

$$= -\frac{eE_0 y}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)\cancel{\vec{a_y}\cdot\vec{r}}$$

• Use Fermi-Golden's rule again

$$\boxed{P_{21} = \frac{\pi e^2 E_0^2}{2\hbar}\,|y_{21}|^2\,\delta(E_2 - E_1 \mp \hbar\omega_e)} \quad \frac{1}{3}$$

$$|y_{21}|^2 \equiv |\langle 2|y|1\rangle|^2$$

In <u>Comparison</u> with <u>two format</u>

$$\rightarrow \quad |\gamma_{21}|^2 = \frac{|M_{21}|^2}{m^2 \omega_{21}} \quad , \quad (\omega_{21} = \omega_\ell)$$

or

$$\boxed{|M_{21}|^2 = |\gamma_{21}|^2 m^2 \omega_{21}^2}$$

✱ Creation & annihilation operator format ✱

In this format, electric field $\vec{E}$ (or $\vec{A}$) become operators itself, [ref. "An introduction to theory and application of quantum mechanics" A. Yariv, John Wiley 1988]

$$H_{int} = -e E_y(z,t) y$$

$$= -e i \sqrt{\frac{\hbar\omega}{V\epsilon_0}} \left(\hat{a}_\ell^* e^{-i\vec{k}\cdot\vec{r}} - \hat{a}_\ell e^{i\vec{k}\cdot\vec{r}} \right) y$$

$\hat{a}_\ell^*$, & $\hat{a}_\ell$ are the creation and <u>annihilation</u> operators, respectively.

they follow (rules) :

$$\langle n_\ell + 1 | a_\ell^+ | n_\ell \rangle = \sqrt{n_\ell + 1}$$

$$\langle n_\ell + 1 | a_\ell | n_\ell \rangle = 0$$

Using Fermi-Golden's rule:

$$\boxed{P_{21} = \frac{\pi e^2 \omega_l}{V \epsilon_0} \left| b_{21} \right|^2 (n_l + 1)\, \delta(E_2 - E_1 - \hbar\omega_l)}$$

$$\equiv P_{21}^{spont} + P_{21}^{ind} = \underline{P_{21}^{spont}(1 + n_l)}$$

$$P_{21}^{spont} = \frac{\pi e^2 \omega_l}{V \epsilon_0} \left| b_{21} \right|^2 \delta(E_2 - E_1 - \hbar\omega_l)$$

$$P_{21}^{ind} = \frac{\pi e^2 \omega_l}{V \epsilon_0} \left| b_{21} \right|^2 \cdot n_l \cdot \delta(E_2 - E_1 - \hbar\omega_l)$$

easily, $\boxed{P_{21}^{ind} = P_{21}^{spont} \cdot n_l}$

* Note: all three format are consistent! provide no half photon concept, ?

[One photon minimum eventhough $n_l = 0$]

* Question = If more than one mode l exist in the optical enclosure, what is the total optical transition probability per unit time? P.60

** also, radiation energy density $\rho(\nu) = \frac{8\pi n^3 \nu^2}{c^3} \cdot h\nu \cdot \frac{1}{e^{h\nu/kT}-1}$ (J/m^3)

Since # of modes of E.M. field per unit frequency is given by =

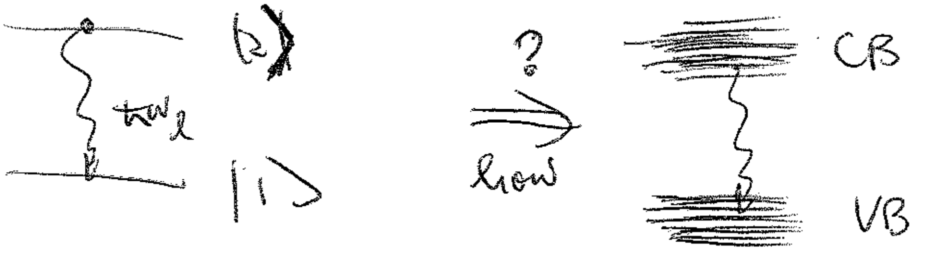
$$\boxed{\rho(\nu) = \frac{8\pi n^3 V}{c^3}\nu^2}$$ * ** (see previous notes on photon)

* to be not confused with the total # of modes between ν_0 to ν = $N_\nu = \frac{8\pi n^3 V}{3c^3}\nu^3$ (with usual assumption)

$$\rightarrow W_{21}^{spont} = \int_0^\infty P_{21}^{spont}(\omega)\,\rho(\nu)\,d\nu$$

$$\boxed{W_{21}^{spont} = \frac{4\pi e^2 n E_{21}}{m^2 \epsilon_0 c^3 \hbar^2}\left|M_{21}\right|^2} \quad (1/s)$$

(#6) find out the value of $|M_{21}|^2$



(H)

$3p \to 1S$: Oscillator Strength (~~Is this right?~~)

P. 60a

and example

$$\langle r|1s\rangle = \frac{2}{a^{3/2}} e^{-r/a}$$

$$\langle r|3p\rangle = \frac{4\sqrt{2}}{9(3a)^{3/2}} \frac{r}{a}\left(1-\frac{r}{6a}\right)e^{-r/3a}$$

$$\langle 3p|r|1s\rangle = \left\langle \frac{4\sqrt{2}}{9(3a)^{3/2}} \frac{r}{a}\left(1-\frac{r}{6a}\right)e^{-r/3a} \middle| r \middle| \frac{2}{a^{3/2}} e^{-r/a} \right\rangle$$

$$= \frac{8\sqrt{2}}{9(3)^{3/2} a^3 a} \left\langle \frac{r}{1}\left(1-\frac{r}{6a}\right)e^{-r/3a} \middle| r \middle| e^{-r/a}\right\rangle$$

$$= \frac{.241925}{a^4} \left\langle r\left(1-\frac{r}{6a}\right)e^{-r/3a} \middle| r \middle| e^{-r/a}\right\rangle$$

$$= \frac{.241925}{a^4}\int_0^\infty r\left(1-\frac{r}{6a}\right)e^{-r/3a} \cdot r \cdot e^{-r/a} \; r^2\, dr$$

$$= \frac{.241925}{a^4}\int_0^\infty \left(r - \frac{r^2}{6a}\right) r^3 e^{-4r/3a}\, dr$$

$$= \frac{.241925}{a^4}\int_0^\infty \left(r^4 - \frac{r^5}{6a}\right) e^{-4r/3a}\, dr$$

$$= \frac{.241925}{a^4}\int_0^\infty r^4 e^{-4r/3a}\, dr - \frac{.241925}{6a^5}\int_0^\infty r^5 e^{-4r/3a}\, dr$$

$$u = 4r/3a, \quad du = \frac{4}{3a}\, dr$$

$$r = \left(\frac{3a}{4}\right) u, \quad dr = \left(\frac{3a}{4}\right) du$$

$$= \frac{.241925}{a^4}\int_0^\infty \left(\frac{3a}{4}\right)^4 u^4 e^{-u}\left(\frac{3a}{4}\right) du - \frac{.241925}{6a^5}\int_0^\infty \left(\frac{3a}{4}\right)^5 u^5 e^{-u}\left(\frac{3a}{4}\right) du$$

$$= \frac{.241925}{a^4}\left(\frac{3a}{4}\right)^5 \underbrace{\int_0^\infty u^4 e^{-u}\, du}_{4! = 24} - \frac{.241925}{6a^5}\left(\frac{3a}{4}\right)^6 \underbrace{\int_0^\infty u^5 e^{-u}\, du}_{5! = 120}$$

$$= \frac{.241925}{a^4} \cdot \frac{243a^5}{1024} \cdot 24 - \frac{.241925}{6a^5} \cdot \frac{729a^6}{4096} \cdot 120$$

$$= 1.377838\, a - .861149\, a = .516689\, a$$

$$f_{3p\to 1s} = \frac{2m\omega_{31}}{3\hbar}\langle 3p|r|1s\rangle^2$$

$$= \frac{2m\hbar\omega_{31}}{3\hbar^2}(.516\,689a)^2$$

$$= \frac{2(.2669675)}{3}\frac{E_{31}a^2 m}{\hbar^2}$$

$$= .1779783\,\frac{ma^2E_{31}}{\hbar^2}$$

$m = 9.1094\times10^{-31}$ kg

$a = .52918\times10^{-10}$ m

$\hbar = 1.0546\times10^{-34}$ J s

$E_1 = -13.6\,\text{eV}$

$E_3 = \frac{-13.6}{9} = -1.51\,\text{eV}$

$E_{31} = 12.09\,\text{eV} = 1.93706\times10^{-18}$ J

$f_{3p\to 1s} = .1779783\,(.44428)$

$= .07907$

$2p \to 1s$ Oscillator strength (~~Is this right?~~)

p. 60C

$$\langle r | 1s \rangle = \frac{2}{a^{3/2}} e^{-r/a}$$

$$\langle r | 2p \rangle = \frac{1}{2\sqrt{6}\, a^{3/2}} \frac{r}{a} e^{-r/2a}$$

$$\langle 2p | r | 1s \rangle = \left\langle \frac{1}{2\sqrt{6}\, a^{3/2}} \frac{r}{a} e^{-r/2a} \middle| r \middle| \frac{2}{a^{3/2}} e^{-r/a} \right\rangle$$

$$= \frac{1}{\sqrt{6}\, a^4} \left\langle r e^{-r/2a} \middle| r \middle| e^{-r/a} \right\rangle$$

$$= \frac{1}{\sqrt{6}\, a^4} \int_0^\infty r e^{-r/2a}\, r\, e^{-r/a}\, r^2\, dr$$

$$= \frac{1}{\sqrt{6}\, a^4} \int_0^\infty r^4 e^{-3r/2a}\, dr$$

$$u = \frac{3r}{2a} \qquad du = \frac{3}{2a} dr$$

$$= \frac{1}{\sqrt{6}\, a^4} \int_0^\infty \left(\frac{2a}{3}\right)^4 u^4 e^{-u} \left(\frac{2a}{3}\right) du$$

$$= \frac{1}{\sqrt{6}\, a^4} \left(\frac{2a}{3}\right)^5 \underbrace{\int_0^\infty u^4 e^{-u}\, du}_{4! = 24}$$

$$= \frac{24}{\sqrt{6}\, a^4} \left(\frac{2a}{3}\right)^5 = \frac{768\, a^5}{\sqrt{6}\, a^4\, 243} = 1.29a$$

P. 60d

$$f_{2p\to 1s} = \frac{2m\omega_{21}}{3\hbar}\langle 2p|r|1s\rangle^2$$

$$= \frac{2m\hbar\omega_{21}}{3\hbar^2}(1.29a)^2$$

$\hbar\omega_{21} = E_{21} = 13.6 - \frac{13.6}{4} = 10.2\,eV = 1.632\times10^{-18}$

$1.29a = 68.26422\times10^{-12}$ where $a = .52918\times10^{-8}$

$f_{2p\to 1s} = .415269$

not invoke the **k**-selection rule for transitions involving band-tail states and, at the same time, should extrapolate to that obeying the **k**-selection rule for above-band-edge transitions involving parabolic band states. The model for such a matrix element has been considered by Stern.[14-16] Before discussing his model in the next section, we consider the simpler case where the **k**-selection rule holds and obtain the absorption coefficient and the spontaneous emission rate.

The k-Selection Rule When the **k**-selection rule is obeyed, $|M_{\mathrm{if}}|^2 = 0$ unless $\mathbf{k}_c = \mathbf{k}_v$. If we consider a volume V of the semiconductor, the matrix element $|M_{\mathrm{if}}|^2$ is given by

$$|M_{\mathrm{if}}|^2 = |M_b|^2 \frac{(2\pi)^3}{V}\, \delta(\mathbf{k}_c - \mathbf{k}_v). \tag{3.2.32}$$

The δ function accounts for the momentum conservation between the conduction-band and valence-band states. The quantity $|M_b|$ is an average matrix element for the Bloch states. Using the Kane model,[7] $|M_b|^2$ in bulk semiconductors is given by [7,17]

over energy

$$|M_b|^2 = \frac{m_0^2 E_g (E_g + \Delta)}{12 m_c (E_g + 2\Delta/3)} = \xi m_0 E_g \tag{3.2.33}$$

where m_0 is the free-electron mass, E_g is the band gap, and Δ is the spin-orbit splitting. For GaAs, using $E_g = 1.424$ eV, $\Delta = 0.33$ eV, $m_c = 0.067$ m₀, we get $\xi = 1.3$.

We are now in a position to calculate the spontaneous-emission rate and the absorption coefficient for a bulk semiconductor. Equations (3.2.22) and (3.2.32) can be used to obtain the total spontaneous-emission rate per unit volume. Summing over all states in the band, we obtain

$$r_{\mathrm{sp}}(E) = \frac{4\pi\bar{\mu} q^2 E}{m_0^2 \epsilon_0 h^2 c^3} |M_b|^2 \frac{(2\pi)^3}{V} (2) \left(\frac{V}{(2\pi)^3}\right)^2 \frac{1}{V} \times \Sigma \int\cdots\int f_c(E_c) f_v(E_v)\, d^3\mathbf{k}_c\, d^3\mathbf{k}_v\, \delta(\mathbf{k}_c - \mathbf{k}_v)\delta(E_i - E_f - E) \tag{3.2.34}$$

where f_c and f_v are the Fermi factors for electrons and holes. The factor 2 arises from the two spin states. In Eq. (3.2.34), Σ stands for the sum over the three valence bands (see Fig. 3.1). For definiteness, we first consider transitions involving electrons and heavy holes. The integrals in Eq. (3.2.34) can be evaluated with the following result:

$\bar{\mu}$ ← energy dependent ?

$$r_{\mathrm{sp}}(E) = \frac{2\bar{\mu} q^2 E |M_b|^2}{\pi m_0^2 \epsilon_0 h^2 c^3} \left(\frac{2m_r}{\hbar^2}\right)^{3/2} (E - E_g)^{1/2} f_c(E_c) f_v(E_v) \tag{3.2.35}$$

where

$$E_c = \frac{m_r}{m_c}(E - E_g)$$

$$E_v = \frac{m_r}{m_{hh}}(E - E_g)$$

$$m_r = \frac{m_c m_{hh}}{m_c + m_{hh}}$$

and m_{hh} is the effective mass of the heavy hole. Equations (3.2.35) give the spontaneous-emission rate at the photon energy E. To obtain the tota spontaneous-emission rate, a final integration should be carried out over al possible energies. Thus the total spontaneous-emission rate per unit volum due to electron-heavy-hole transitions is given by

$$R = \int_{E_g}^{\infty} r_{\mathrm{sp}}(E)\, dE = A|M_b|^2 I \qquad (3.2.36$$

where

$$I = \int_{E_g}^{\infty} (E - E_g)^{1/2} f_c(E_c) f_v(E_v)\, dE$$

and A represents the remaining constants in Eq. (3.2.35). A similar equatio holds for the electron–light-hole transitions if we replace m_{hh} by the effecti light-hole mass m_{lh}.

The absorption coefficient $\alpha(E)$ can be obtained in a similar way usin Eq. (3.2.19) and (3.2.32) and integrating over the available states in the co duction and valence bands. The resulting expression is

$$\alpha(E) = \frac{q^2 h}{2\epsilon_0 m_0^2 c\, \bar{\mu} E} |M_b|^2 \frac{(2\pi)^3}{V} (2) \left(\frac{V}{(2\pi)^3}\right)^2 \left(\frac{1}{V}\right) \times \int\cdots\int (1 - f_c - f_v)\, d^3\mathbf{k}_c d^3\mathbf{k}_v\, \delta(\mathbf{k}_c - \mathbf{k}_v)\, \delta(E_i - E_f - E) \qquad (3.2.3$$

$$= \frac{q^2 h |M_b|^2}{4\pi^2 \epsilon_0 m_0^2 c\, \bar{\mu} E} \left(\frac{2m_r}{\hbar^2}\right)^{3/2} (E - E_g)^{1/2} [1 - f_c(E_c) - f_v(E_v)] \qquad (3.2.3$$