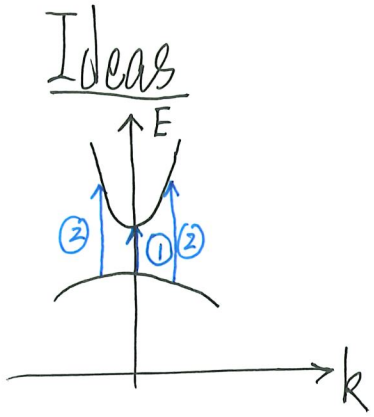
F. Interband Transitions

Ideas



① start to see absorption when $\hbar\omega \gtrsim E_g$

② for $\hbar\omega > E_g$, transitions from VB to CB can occur over pairs of states (joint density of states)

③ time-dependent perturbation theory (Fermi Golden rule)

④ Formal QM, light enters through vector potential $\vec{A}$

$$\hat{H}_0 = \frac{\vec{p}^2}{2m} + V(\vec{r})$$

↖ periodic (band problem)

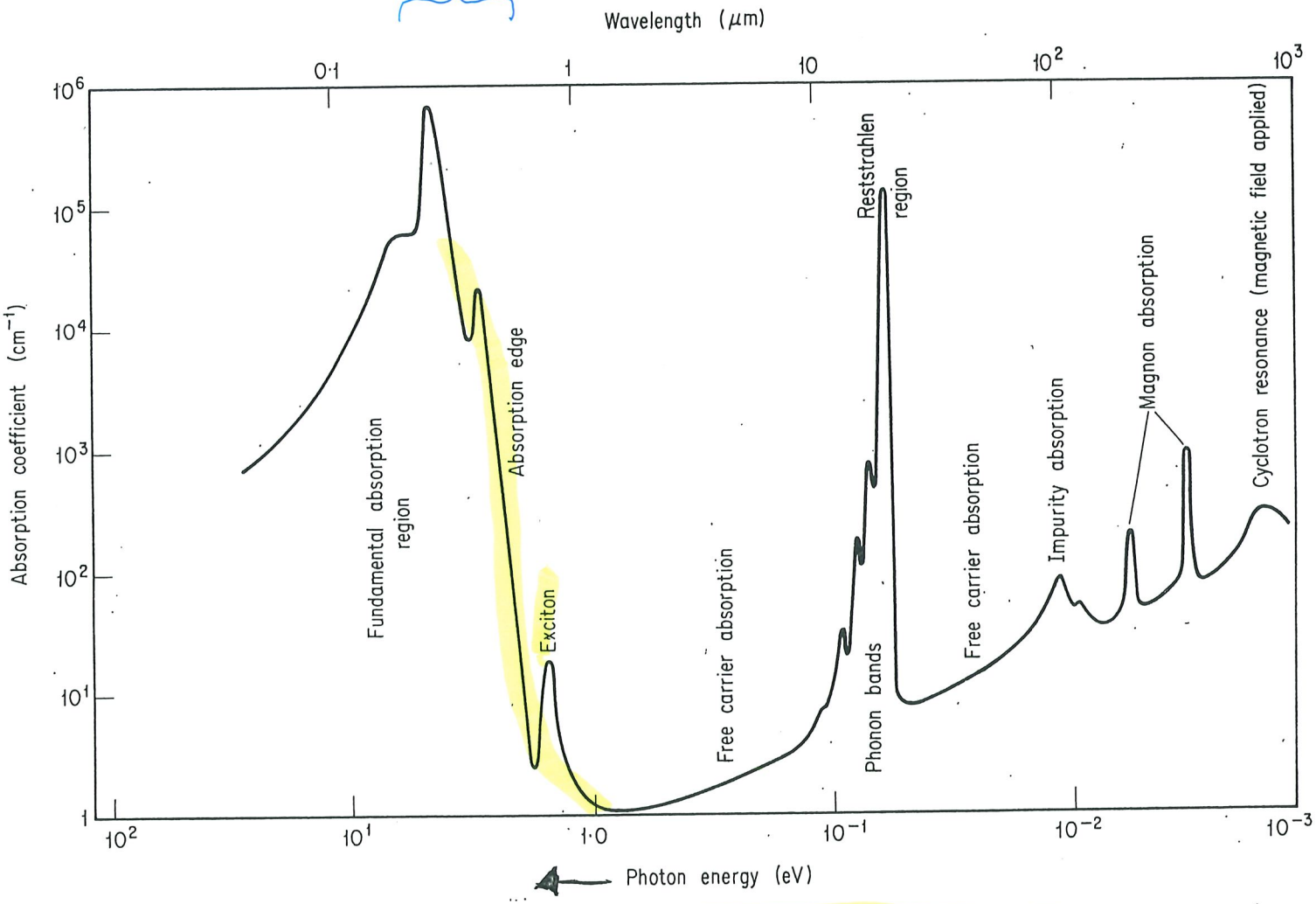
Recipe: $\vec{p} \to \vec{p} - q\vec{A}$ ← Vector potential in Hamiltonian

↖ carrier charge "-e" for electron

(using Coulomb gauge can avoid ϕ)

↗ scalar potential

Interband Transitions



Absorption spectrum of a hypothetical semiconductor

$$\hat{H} = \left[\frac{\vec{p}}{2m} + V(\vec{r})\right] + i\hbar\frac{q}{m}\vec{A}\cdot\vec{\nabla} = \hat{H}_0 - \frac{e}{m}i\hbar\vec{A}\cdot\vec{\nabla} = \hat{H}_0 + \frac{e}{m}\vec{A}\cdot\hat{\vec{p}} = \hat{H}_0 + \hat{H}' \quad (24)$$

"-e" is electron's charge

ignored A^2 term

EM field

momentum operator

gives a perturbation

For† $\vec{A}(\vec{r},t) = A_0(\omega)\,\hat{a}_0\, e^{i(\vec{q}\cdot\vec{r}-\omega t)} + c.c.$

polarization

real

amplitude

using $\vec{q}$ here to avoid "$\vec{k}$" as used for electrons in bands

complex conjugate

(i) Work out $\vec{\mathcal{E}}(\vec{r},t) = -\frac{\partial}{\partial t}\vec{A}(\vec{r},t)$ and $\vec{B}(\vec{r},t) = \vec{\nabla}\times\vec{A}(\vec{r},t)$

(ii) Find energy density $\langle u\rangle = \frac{1}{2}\varepsilon\varepsilon_0\mathcal{E}^2 + \frac{1}{2}\mu_0 H^2$ (with time average)

(iii) $|\text{Poynting vector}| = \frac{c}{n}\cdot\langle u\rangle$ ← incident energy per unit area per unit time

† The equations that follow may be off by some constants as it has been difficult to keep track of (i) SI units against gaussian units, and (ii) the $\vec{A}(\vec{r},t)$ here against $\vec{A}(\vec{r},t) = A_0(\omega)\,\hat{a}\cos(\vec{q}\cdot\vec{r}-\omega t)$.

Let $W(\omega)^{\dagger}$ = # photons absorbed per unit volume per unit time

(this is analogous to $W_{kk'}$ in transport theory, but off by "per unit volume")

$\therefore$ $\hbar\omega W(\omega)$ = energy absorbed per unit volume per unit time

α = Absorption coefficient $= \dfrac{\hbar\omega W(\omega)}{\frac{c}{n}\langle u(\omega)\rangle}$ (has $\frac{1}{\text{length}}$ unit, cm^{-1})

It turns out

$$\alpha(\omega) = \frac{2\pi}{\varepsilon_0 n c \omega A_0^2} W(\omega) \qquad (25)$$

[As $\hat{H}' = \frac{e}{m}\vec{A}\cdot\vec{p}$, $W \sim \frac{2\pi}{\hbar}|\langle f|\hat{H}'|i\rangle|^2 \delta(\text{energy criterion}) \sim A_0^2$
and the A_0 terms in α will cancel out, as expected]

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† $W(\omega)$ is to be dealt with by the Fermi Golden Rule (time-dependent perturbation theory)

From Eqs. (4) $\left(\alpha = \frac{2\omega}{c}K\right)$ and (5) $\left(\varepsilon_2 = 2nK\right)$,

$$\varepsilon_2(\omega) = 2nK = 2n \cdot \frac{c}{2\omega}\alpha = \frac{nc}{\omega}\cdot\alpha(\omega)$$

$$\Rightarrow \boxed{\varepsilon_2(\omega) = \frac{2\hbar}{\varepsilon_0 \omega^2 A_0^2} W(\omega)} \qquad (2b)$$

ε_2: imaginary part of (relative) dielectric constant

$W(\omega)$: related to a quantity (# photons absorbed per volume per unit time) that is handled by QM

Unit is OK!

$$\mathcal{E} \sim \frac{\partial \vec{A}}{\partial t} \Rightarrow \omega^2 A_0^2 \sim \mathcal{E}_0^2 \Rightarrow \varepsilon_0 \omega^2 A_0^2 \sim \text{energy density} \sim \frac{\text{energy}}{\text{Volume}}$$

$$\frac{\hbar}{\left(\frac{\text{energy}}{\text{Volume}}\right)} \cdot \frac{\#}{(\text{Volume}\cdot\text{time})} \sim \text{no units!}$$

Key Point: $\alpha(\omega)$ and $\varepsilon_2(\omega)$ are related to $W(\omega)$, which can be treated by QM.

From Eq. (24), $\hat{H}' = \frac{e}{m}\vec{A}\cdot\vec{p} = \frac{e\hbar A_0}{mi}\left[e^{i\vec{q}\cdot\vec{r}-i\omega t} + e^{-i\vec{q}\cdot\vec{r}+i\omega t}\right]\hat{a}_0\cdot\vec{\nabla}$ (27)

absorption (c.f. time dependent perturbation) — emission — operate on electron wavefunction

- From transition from one unperturbed state ψ_i to another state ψ_f

(we need to consider many possible initial states and final states, but that comes later)

Initial: $\psi_i(\vec{r})$ = a state in VB $= \langle\vec{r}|v\vec{k}\rangle = \psi_{v\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}u_{v\vec{k}}(\vec{r})$ (28a)

(v: VB; $\vec{k}\in 1^{st}$ B.Z.; $\frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}u_{v\vec{k}}(\vec{r})$: Bloch state)

evolves in time as $e^{-iE_v(\vec{k})t/\hbar}$

Final: $\psi_f(\vec{r})$ = a state in CB $= \langle\vec{r}|c\vec{k}'\rangle = \psi_{c\vec{k}'}(\vec{r}) = \frac{1}{\sqrt{V}}e^{i\vec{k}'\cdot\vec{r}}u_{c\vec{k}'}(\vec{r})$ (28b)

evolves in time as $e^{-iE_c(\vec{k}')t/\hbar}$

$$W_{fi} = \frac{2\pi}{\hbar} \left| \text{matrix element (spatial)} \right|^2 \delta(E_f - E_i - \hbar\omega) \qquad (29)$$

Fermi Golden Rule

this is $\frac{1}{\text{time}}$

(not $\frac{1}{\text{Volume} \cdot \text{time}}$)

(the "Volume" is taken care of in working with DOS)

from absorption term, picks up

$$\int_0^t e^{+iE_f t'/\hbar} e^{-i\omega t'} e^{-iE_i t'/\hbar} dt'$$

selects $E_f = E_i + \hbar\omega$

when getting $a_f(t)$

prob. in state ψ_f after $\hat{H}'$ acting for time t

The matrix element in Eq. (29) is:

$$\langle \psi_f | \hat{H}' | \psi_i \rangle = \frac{e\hbar}{mi} A_0 \langle \psi_f | e^{i\vec{q}\cdot\vec{r}} \hat{a}_0 \cdot \vec{\nabla} | \psi_i \rangle$$

$$= \frac{e\hbar}{mi} A_0 \langle c\vec{k}' | e^{i\vec{q}\cdot\vec{r}} \hat{a}_0 \cdot \vec{\nabla} | v\vec{k} \rangle$$

$\hat{a}_0$: polarization of incident wave

$\vec{\nabla} \sim \left(\frac{\hbar}{i}\vec{\nabla}\right)$ ← momentum operator

$$\langle c\vec{k}' | \hat{H}' | v\vec{k} \rangle = -\frac{ie\hbar}{m}\frac{A_0}{V}\int u^*_{c\vec{k}'}(\vec{r})\, e^{-i\vec{k}'\cdot\vec{r}} \left[e^{i\vec{q}\cdot\vec{r}}\,\hat{a}_0\cdot\vec{\nabla}\right] e^{i\vec{k}\cdot\vec{r}}\, u_{v\vec{k}}(\vec{r})\, d^3r$$

gives 2 terms

$$= -\frac{ie\hbar}{m}\frac{A_0}{V}\int_{\text{all crystal } V} u^*_{c\vec{k}'}(\vec{r}) \left(\hat{a}_0\cdot\vec{\nabla}\, u_{v\vec{k}}(\vec{r}) + i\, u_{v\vec{k}}(\vec{r})\, \hat{a}_0\cdot\vec{k}\right) e^{i(\vec{k}+\vec{q}-\vec{k}')\cdot\vec{r}}\, d^3r \qquad (30)$$

- $u_{c\vec{k}'}(\vec{r})$, $u_{v\vec{k}}(\vec{r})$ are periodic functions (unit cell by unit cell)
- Each location $\vec{r}$ can be written as $\vec{r} = \vec{R}_n + \vec{r}'$
  - $\vec{r}$: some place
  - $\vec{R}_n$: which unit cell
  - $\vec{r}'$: relative to $\vec{R}_n$ ($\vec{r}'$ goes through only one unit cell)

Eq. (30): $\langle c\vec{k}' | \hat{H}' | v\vec{k} \rangle$

$$= \int_{\text{all crystal } V} (\cdots)\, d^3r \;\rightarrow\; \left(\int_{\text{one unit cell (Wigner-Seitz cell)}} \cdots\, d^3r'\right) \cdot \left(\sum_{\vec{R}_n} e^{i(\vec{k}+\vec{q}-\vec{k}')\cdot\vec{R}_n}\right) \qquad (31)$$

sum over all lattice vectors

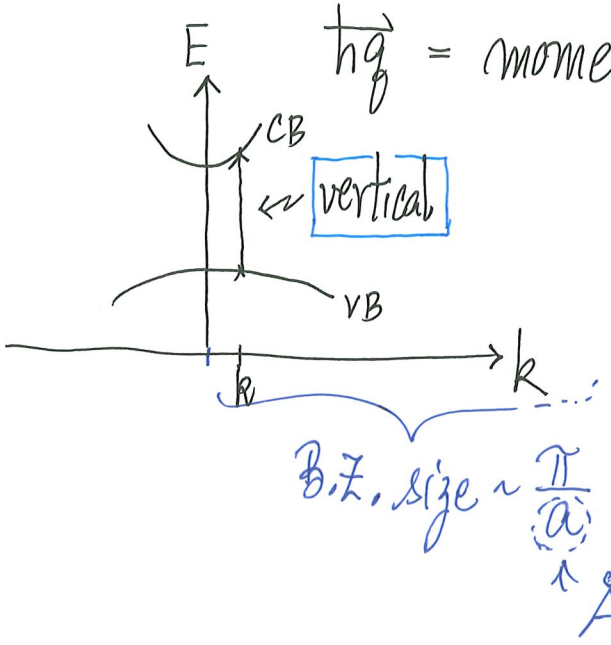
Recall: $e^{i\vec{G}\cdot\vec{R}} = 1$, $\sum_{\vec{R}_n} e^{i(\vec{k}+\vec{q}_f-\vec{k}')\cdot\vec{R}_n} \neq 0$ only when

$\vec{k} + \vec{q}_f - \vec{k}' = \vec{G}$ = some reciprocal lattice vector

Most relevant here is $\vec{G} = 0$, so

$$\boxed{\vec{k} + \vec{q}_f = \vec{k}'} \qquad (32)$$

condition for $|\langle f|\hat{H}'|i\rangle|^2 \neq 0$ (dominant term in (30)), "conservation of momentum"



$\hbar\vec{q}_f$ = momentum of photon

$|\vec{q}_f|$ = wave vector of photon $\ll \frac{\pi}{a}$

$\Rightarrow |\vec{q}_f|$ is tiny comparing with B.Z. size

$\Rightarrow \boxed{\vec{k} \approx \vec{k}'}$ (33) Optical transitions are vertical transition (also Direct Transition)

initial (VB) — final (CB)

Let's say Condition (32) is satisfied, then $\sum_{\vec{R}_n} e^{i(\vec{k}+\vec{q}-\vec{k}')\cdot\vec{R}_n} = N = \#$ unit cells in crystal

Then Eq. (31) becomes

$$\langle c\vec{k}'|\hat{H}'|v\vec{k}\rangle = \frac{-ie\hbar}{m}\frac{A_0}{(V/N)}\int_{cell} u^*_{c\vec{k}+\vec{q}}\left[\hat{a}_0\cdot\vec{\nabla}u_{v\vec{k}}(\vec{r}) + i(\hat{a}_0\cdot\vec{k})u_{v\vec{k}}(\vec{r})\right] d^3r$$

term ① term ②

$\vec{k}' = \vec{k}+\vec{q}$ formally

(there is a factor $e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} = 1$ here)

$$= \frac{-ie\hbar}{m}\frac{A_0}{v_{cell}}\left[\int_{cell} u^*_{c\vec{k}}(\vec{r})\left[\hat{a}_0\cdot\vec{\nabla}u_{v\vec{k}}(\vec{r})\right]d^3r + \int_{cell} u^*_{c\vec{k}+\vec{q}}(\vec{r})\,(i\hat{a}_0\cdot\vec{k})\,u_{v\vec{k}}(\vec{r})\,d^3r\right] \quad (34)$$

used $\vec{k}'=\vec{k}$ here

term ①: if this term $\neq 0$ $\Rightarrow$ allowed transition (strong)

term ② (when term ① = 0, then look at this term) (weak)

$$\text{term}\,② \propto \int_{\text{cell}} u^*_{c\vec{k}+\vec{q}}(\vec{r})\, u_{v\vec{k}}(\vec{r})\, d^3r \approx \int_{\text{cell}} u^*_{c\vec{k}}(\vec{r})\, u_{v\vec{k}}(\vec{r})\, d^3r = 0$$

used $\vec{q} \approx 0$

Allowed transition: term ① $\neq 0$ [term ② negligible]

$$\langle c\vec{k}|\hat{H}'|v\vec{k}\rangle = \frac{eA_0}{m}\,\hat{a}_0 \cdot \underbrace{\frac{1}{U_{\text{cell}}}\int_{\text{cell}} u^*_{c\vec{k}}(\vec{r})\left(\frac{\hbar}{i}\vec{\nabla}\right) u_{v\vec{k}}(\vec{r})\, d^3r}$$

{retains term ①

Saw this before in $\vec{k}\cdot\vec{p}$ band theory†

$$= \frac{eA_0}{m}\,\hat{a}_0 \cdot \vec{P}_{cv} \qquad (35)$$

polarization

$\vec{P}_{cv}$ (momentum matrix element) $\neq 0$ [symmetry of $u_{c\vec{k}}$ and $u_{v\vec{k}}$]

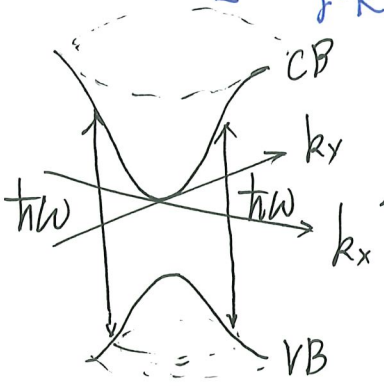
e.g. s-character and p-character

† Recall: $\frac{2|P_{cv}|^2}{m} \approx 20\ \text{eV}$ for wide range of materials (see Ch. VI)

From Eq. (29), $\mathcal{W}_{fi} = \frac{2\pi}{\hbar}\frac{e^2\hbar^2}{m^2}A_0^2\,|\hat{a}_0\cdot\vec{p}_{cv}|^2\,\delta(E_f - E_i - \hbar\omega)$

$\frac{1}{\text{time}} = \frac{2\pi e^2\hbar}{m^2}A_0^2\,|\hat{a}_0\cdot\vec{p}_{cv}|^2\,\delta(E_f - E_i - \hbar\omega)$ (36)

[$\mathcal{W}_{fi}$ ← from one state i to another state f]



← one value of ω ($\hbar\omega$) can lead to transitions from a group of states (in VB) to a group of states (in CB)

Key Point: leads to the idea of Joint Density of States

$\sum_{\substack{\text{states } i \text{ in VB and} \\ \text{states } f \text{ in CB}}} \delta(E_f - E_i - \hbar\omega)$ such that $E_f = E_i + \hbar\omega$

this is the Joint Density of States

$$W_{cv}(\omega) = \frac{1}{V}\frac{2\pi e^2\hbar}{m^2}A_0^2 \int \frac{V}{(2\pi)^3}\cdot 2\, d^3k \; |\hat{a}_0\cdot\vec{p}_{cv}|^2\,\delta(E_f - E_i - \hbar\omega)$$

(spin)

$\frac{1}{V}$: per unit volume

$\frac{V}{(2\pi)^3}\cdot 2\, d^3k$: DOS in $\vec{k}$-space

$\left[\frac{1}{(\text{time})\cdot(\text{Volume})}\right]$: this is

goes into α and $\varepsilon_2(\omega)$

Putting this into Eq. (26) for $\varepsilon_2(\omega)$:

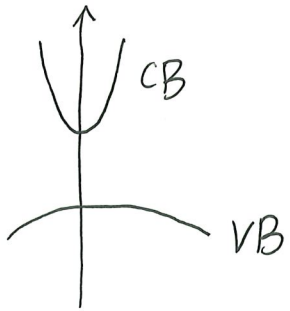
$$\varepsilon_2(\omega) = \frac{4\pi\hbar^2e^2}{\varepsilon_0 m^2\omega^2}\int \frac{1}{(2\pi)^3}\cdot 2\, d^3k \; |\hat{a}_0\cdot\vec{p}_{cv}|^2\,\delta(E_f - E_i - \hbar\omega) \qquad (37)$$

[meaning: go over 1st B.Z. to look for $(E_c(\vec{k}) - E_v(\vec{k}) = \hbar\omega)$ pairs of states]

$$= \frac{4\pi\hbar^2e^2}{\varepsilon_0 m^2\omega^2}\; |\hat{a}_0\cdot\vec{p}_{cv}|^2 \cdot g_{cv}(\hbar\omega) \qquad (38)$$

$g_{cv}(\hbar\omega)$: Joint DOS per unit volume of CB and VB

E.g.: Parabolic CB and VB



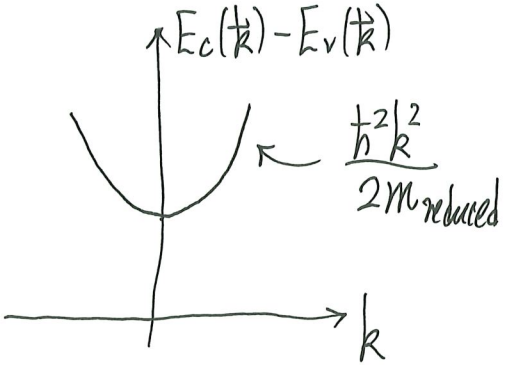
$$E_c(\hbar k) = E_g + \frac{\hbar^2 k^2}{2m_e}$$

$$E_v(\hbar k) = -\frac{\hbar^2 k^2}{2m_h}$$

↖ effective mass

↖ effective mass

Consider $E_c(\hbar k) - E_v(\hbar k) = E_g + \frac{1}{2}\underbrace{\left(\frac{1}{m_e} + \frac{1}{m_h}\right)}_{\frac{1}{m_{reduced}}} \hbar^2 k^2 = E_g + \frac{\hbar^2 k^2}{2m_{reduced}}$



We want to know the DOS per unit volume
for $(E_c(\hbar k) - E_v(\hbar k) = \hbar\omega)$
two photon can lead to transitions

The answer is:

$$g_{cv}(\hbar\omega) = \frac{1}{2\pi^2}\left(\frac{2m_{reduced}}{\hbar^2}\right)^{3/2}\sqrt{\hbar\omega - E_g} \sim \sqrt{\hbar\omega - E_g} \quad (39)$$

↙ this is DOS per volume

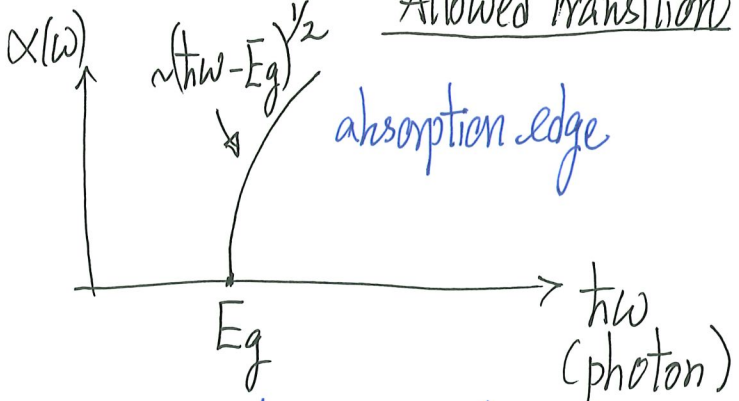
(for $\hbar\omega \geq E_g$)

Eqs. (38) and (39) give allowed interband transition contribution to $\varepsilon_2(\omega)$

Recall: $$\alpha(\omega) = \frac{\omega}{c}\frac{1}{n}\varepsilon_2(\omega) = \frac{4\pi\hbar^2 e^2}{\varepsilon_0 m^2 c\, n\, \omega}\,|\hat{a}_0\cdot\vec{p}_{cv}|^2\cdot\left[\frac{1}{2\pi^2}\left(\frac{2m_{red}}{\hbar^2}\right)^{3/2}\sqrt{\hbar\omega - E_g}\right]$$

$\cdot\ \frac{2|\vec{p}_{cv}|^2}{m}$ almost the same for many semiconductors

$g_{cv}(\hbar\omega) \sim \sqrt{\hbar\omega - E_g}$



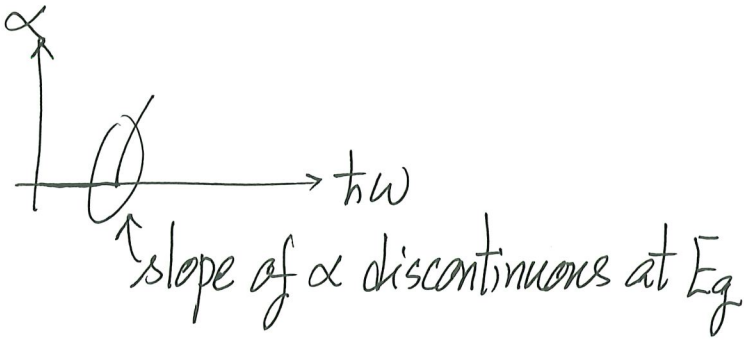
provides a way to determine E_g experimentally

$$\varepsilon_2(\omega) \propto \frac{1}{(\hbar\omega)^2}|\vec{p}_{cv}|^2\cdot(\hbar\omega - E_g)^{1/2} \quad \text{for allowed transitions} \qquad (40)$$

$\varepsilon_2(\omega)$ and $\alpha(\omega)$ reflect $|\vec{p}_{cv}|^2$ and $g_{cv}(\hbar\omega)$ [joint DOS]

Features in DOS: "Critical Points"

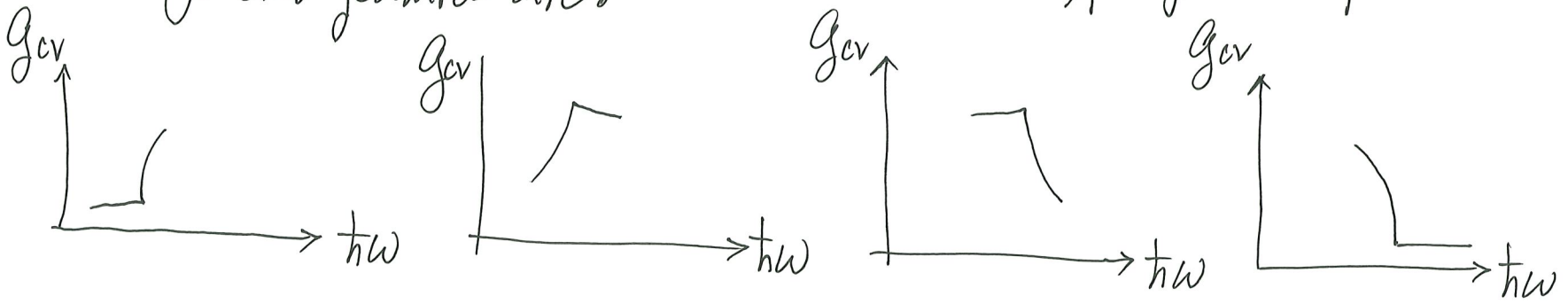
- If $\vec{\nabla}_{\vec{k}} E_c(\vec{k}) = 0$ AND $\vec{\nabla}_{\vec{k}} E_v(\vec{k}) = 0$, then



- If $\vec{\nabla}_{\vec{k}} E_c(\vec{k}) \neq 0$, $\vec{\nabla}_{\vec{k}} E_v(\vec{k}) = 0$,
  but $\vec{\nabla}_{\vec{k}} \underbrace{(E_c(\vec{k}) - E_v(\vec{k}))}_{\text{CB and VB are parallel in some range of } \vec{k}} = 0$ (≈ 0), Joint DOS is big.

General features are:

4 types of critical points in DOS



"Forbidden" Transition

Back to Eq.(34), term① = 0 ⇒ forbidden transition (due to symmetry of u_{ck} and u_{vk})

Then consider term②,

$$\langle ck'|\hat{H}'|vk\rangle = -\frac{ieh}{m}\frac{A_0}{v_{cell}}\int_{cell} u^*_{c\,k+q}(\vec{r})\,u_{vk}(\vec{r})\,d^3r\,(i\hat{a}_0\cdot\vec{k})$$

($\vec{q}$ kept; $\vec{k}$ [note "$\vec{k}$"])

$\therefore$ small $\equiv M_{cv}^{forbidden}$

$$\therefore W(\omega) \propto |M_{cv}^{forbidden}|^2 k^2 g_{cv}(\hbar\omega)$$

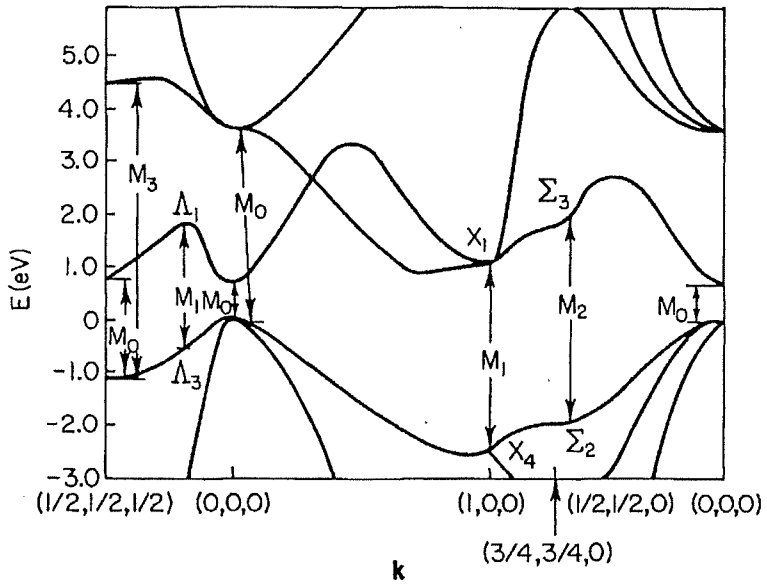
$$\propto |M_{cv}^{forbidden}|^2 \cdot (\hbar\omega - E_g)\,(\hbar\omega - E_g)^{1/2}$$

$$\therefore \propto \sim (\hbar\omega - E_g)^{3/2} \quad \text{forbidden transition}$$

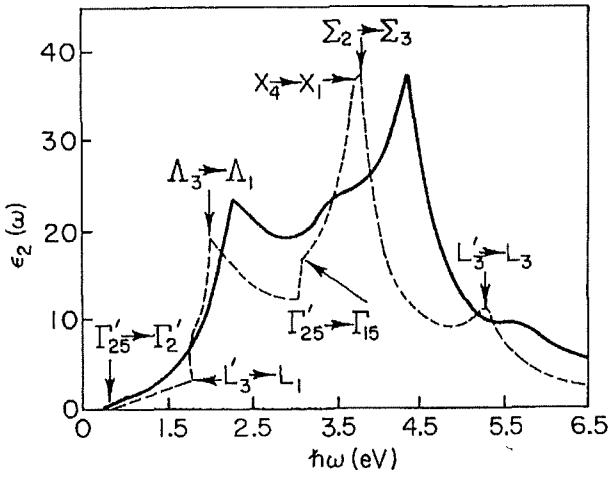
$$\varepsilon_2 \sim |M_{cv}^{forbidden}|^2 (\hbar\omega - E_g)^{3/2} \quad \text{forbidden transition} \qquad (41)$$

different power than allowed transition

One can relate band structure to $\varepsilon_2(\omega)$ through DOS and momentum matrix elements



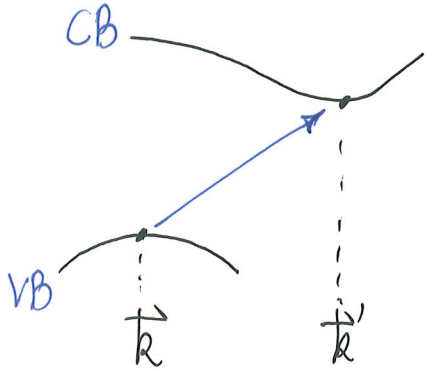
The band structure of Ge. [From J. C. Phillips, D. Brust, and G. F. Bassani, *Proc. Int. Conf. Phys. Semicond. Exeter London* p. 564 (1962).]



Imaginary part of the dielectric constant $\varepsilon_2(\omega)$ for Ge. (——) Experiment; (— — —) theory. [From D. Brust, J. C. Phillips, and G. F. Bassani, *Phys. Rev. Lett.* **9**, 94 (1962).]

Indirect Transitions

- Harder to analyze/understand (second order time-dependent perturbation)



Need some other elementary excitations (phonons) to help out

photon: $\vec{q}$, $\hbar\omega(\vec{q})$

phonon: $\vec{p}$, $\hbar\omega(\vec{p})$

Energy and momentum conservation:

$$E(\vec{k}') = E(\vec{k}) + \underbrace{\hbar\omega(\vec{q})}_{\text{photon}} \pm \underbrace{\hbar\omega(\vec{p})}_{\text{phonon}} \quad (42a)$$

(+ absorbs a phonon, − emits a phonon)

$$\vec{k}' = \vec{k} + \vec{q} \pm \vec{p} \quad (42b)$$

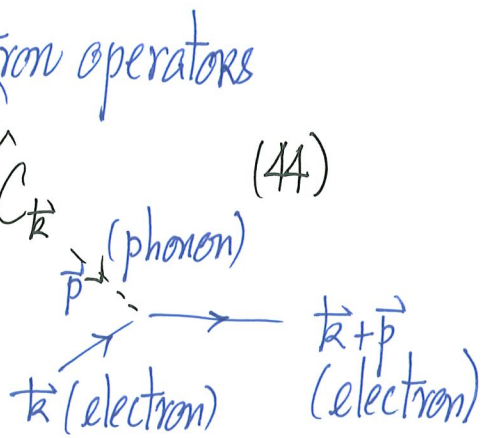
As one more entity is involved, probability is much smaller than direct transitions

$$\hat{H}' = \hat{H}'_{photon} + \hat{H}'_{phonon} \qquad (43)$$

$\hat{H}'_{photon}$: $\frac{e\hbar}{mi} A_0 e^{i\vec{q}\cdot\vec{r}} (\hat{a}_0 \cdot \vec{\nabla}) e^{-i\omega t}$ (see Eq. (27))

$$\hat{H}'_{phonon} \sim M_{\vec{k}\vec{p}} \left(\hat{a}^{+}_{-\vec{p}} e^{i\omega(\vec{p})t} + \hat{a}_{\vec{p}} e^{-i\omega(\vec{p})t} \right) \hat{C}^{+}_{\vec{k}+\vec{p}} \hat{C}_{\vec{k}} \qquad (44)$$

- $M_{\vec{k}\vec{p}}$: some electron-phonon matrix element
- $\hat{a}^{+}_{-\vec{p}}$, $\hat{a}_{\vec{p}}$: phonon operators
- $\hat{C}^{+}_{\vec{k}+\vec{p}}$, $\hat{C}_{\vec{k}}$: electron operators



$$\hat{H} = \hat{H}_0 + \hat{H}' \leftarrow \text{time-dependent}$$

$$\Psi(\vec{r},t) = \sum_{n,\vec{k}} a_n(\vec{k},t)\, e^{-iE_n(\vec{k})t/\hbar}\, \psi_{n\vec{k}}(\vec{r})$$

- n: bands
- $\vec{k} \in 1^{st}$ B.Z
- bands, $\vec{k} \in 1^{st}$ B.Z: as basis
- $a_n(\vec{k},t)$: time-dependence due to $\hat{H}'(t) = \hat{H}'_{photon}(t) + \hat{H}'_{phonon}(t)$
- $\psi_{n\vec{k}}(\vec{r})$: Bloch states

$\hat{H}\Psi = i\hbar\frac{\partial}{\partial t}\Psi \Rightarrow$ set of equations for $a_n(\vec{k},t)$

$$\frac{da_m(\vec{k}',t)}{dt} = \frac{1}{i\hbar}\sum_n a_n(\vec{k},t)\, e^{\frac{i}{\hbar}(E_m(\vec{k}')-E_n(\vec{k}))t} \langle m\vec{k}'|\hat{H}'|n\vec{k}\rangle \quad (45)$$ (exact)

- perturbation idea ← 0th order [initial conditions] ← 1st order
  - $a_n^{(0)}(\vec{k},t)$ into RHS, then $a_m^{(1)}(\vec{k}',t)$ come out in LHS
  - $a_n^{(1)}(\vec{k},t)$ into RHS, then $a_m^{(2)}(\vec{k}',t)$ come out in LHS, and so on

Think! $\hat{H}' = \hat{H}'_{photon} + \hat{H}'_{phonon}$

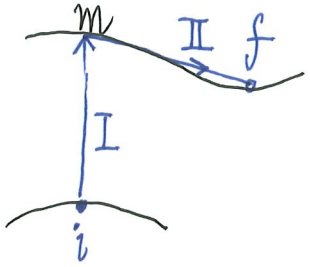
1st order: Can (only) pick up $\hat{H}'_{photon}$ (or $\hat{H}'_{phonon}$, but not both)

To pick up effects of $\hat{H}'_{photon}$ AND $\hat{H}'_{phonon}$ in a process, need 2nd order term!

For 2nd order processes, they can go through many intermediate states

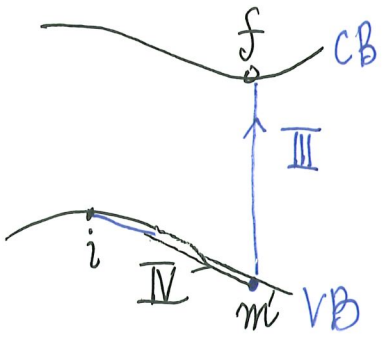
$$\sum_{\text{intermediate}} \langle \text{final} | \hat{H}'_{\text{photon}} | \text{intermediate} \rangle \langle \text{intermediate} | \hat{H}'_{\text{phonon}} | \text{initial} \rangle$$

Two intermediate states are of importance



I: Absorbs a photon to go to CB vertically to m

II: Electron makes a transition within CB to final state with absorption or emission of a phonon



III: Electron at m' absorbs a photon to go to final state

IV: Electron from i absorbs/emits a phonon to go to m'

equivalent description

III: Hole transition from CB (f state) to VB (m' state) by absorption of a photon

IV: Hole transition from m' to state i with absorption or emission of a phonon

Expected to have temperature dependence due to phonons

Prob. of phonon absorption $\propto N_{phonon} \sim \frac{1}{e^{\frac{\hbar\omega(\vec{p})}{kT}} - 1}$

Other topic: Two-photon processes

With enough background understanding...

how to turn Si into better optical material?

- quantum confinement? "squeeze CB minimum at $\vec{k} \neq 0$ higher"?
- Si/Ge superlattice? "Band folding: fold CB minimum to $\vec{k}=0$ by imposing a new period?"
- Making Si into direct bandgap (2020 "breakthrough")
  - Grow hexagonal Si or SiGe alloys

    band theory gives a direct gap

    (but hard to prepare samples)

Chosen a breakthrough by Institute of Physics UK in 2020

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Article

Direct-bandgap emission from hexagonal Ge and SiGe alloys

https://doi.org/10.1038/s41586-020-2150-y

Received: 25 October 2019

Accepted: 11 February 2020

Published online: 8 April 2020

Check for updates

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Silicon crystallized in the usual cubic (diamond) lattice structure has dominated the electronics industry for more than half a century. However, cubic silicon (Si), germanium (Ge) and SiGe alloys are all indirect-bandgap semiconductors that cannot emit light efficiently. The goal[1] of achieving efficient light emission from group-IV materials in silicon technology has been elusive for decades[2–6]. Here we demonstrate efficient light emission from direct-bandgap hexagonal Ge and SiGe alloys. We measure a sub-nanosecond, temperature-insensitive radiative recombination lifetime and observe an emission yield similar to that of direct-bandgap group-III–V semiconductors. Moreover, we demonstrate that, by controlling the composition of the hexagonal SiGe alloy, the emission wavelength can be continuously tuned over a broad range, while preserving the direct bandgap. Our experimental findings are in excellent quantitative agreement with ab initio theory. Hexagonal SiGe embodies an ideal material system in which to combine electronic and optoelectronic functionalities on a single chip, opening the way towards integrated device concepts and information-processing technologies.

Nature 580, 205 (2020)

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Growth of hexagonal Ge and SiGe alloys: GaAs nanowire → coat Ge on wire (forming a hexagonal substrate) → coat SiGe (hexagonal alloys)