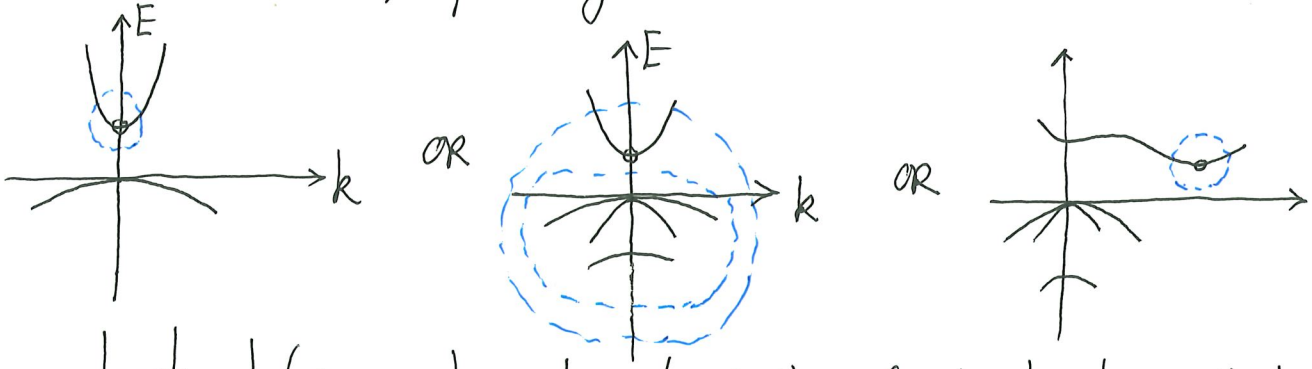
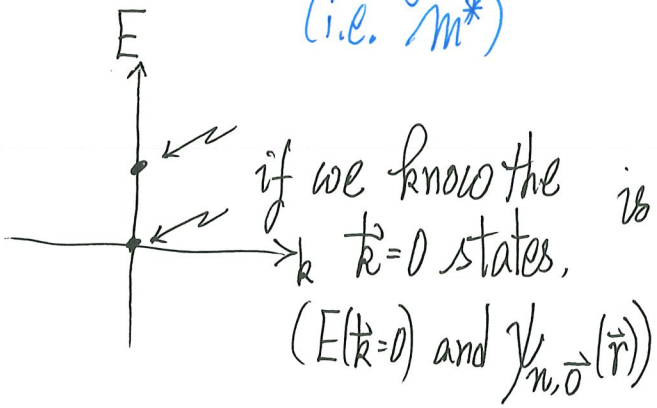
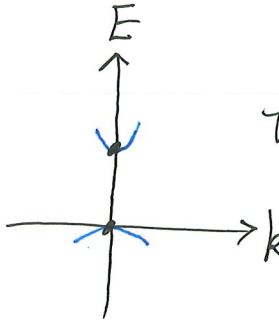
D. Simpler Ways to describe key part of semiconductor bands

Motivation:

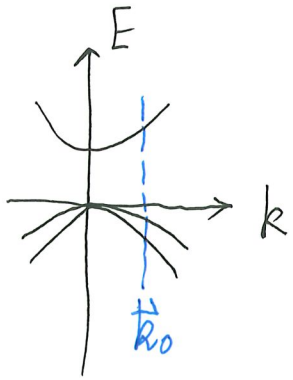


Q: Could we understand (more physical picture) the band structures that are most relevant?





band structure about $\vec{k}=0$?

More generally, 

if we know solution ($E_n(\vec{k}_0)$ and $u_{n\vec{k}_0}(\vec{r})$) at the point $\vec{k}_0$, is it possible to get something for $\vec{k} \approx \vec{k}_0$?

Preparation

The Periodic Part $u_{\vec{k}}(\vec{r})$ of Bloch Functions obeys the equation

$$\left[-\frac{\hbar^2}{2m}(\vec{\nabla}+i\vec{k})^2 + U(\vec{r})\right] u_{\vec{k}}(\vec{r}) = E(\vec{k})\, u_{\vec{k}}(\vec{r}) \qquad (37)$$

See p.Ⅳ-51

or equivalently $\left[\frac{1}{2m}(\hat{p}+\hbar\vec{k})^2 + U(\vec{r})\right] u_{\vec{k}}(\vec{r}) = E(\vec{k})\, u_{\vec{k}}(\vec{r})$

or equivalently and most explicitly,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) - i\frac{\hbar^2}{m}\vec{k}\cdot\vec{\nabla} + \frac{\hbar^2 k^2}{2m}\right] u_{\vec{k}}(\vec{r}) = E(\vec{k})\, u_{\vec{k}}(\vec{r}) \qquad (38)$$

with $U(\vec{r}+\vec{R}_n) = U(\vec{r})$ (8)

(a) Simplest Case [knowing $\vec{k}=0$ solutions, what about $\vec{k}\approx 0$?]

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{r}) \qquad \text{[general, } V(\vec{r}) = V(\vec{r}+\vec{R}) \text{ periodic]} \qquad (4)$$

$$\hat{H}\psi_{n\vec{k}}(\vec{r}) = E_n(\vec{k})\,\psi_{n\vec{k}}(\vec{r}) \qquad \text{[this is the problem to solve]} \qquad (5)$$

$$\psi_{n\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}}\underbrace{e^{i\vec{k}\cdot\vec{r}}}_{\text{already know this plane wave form}}\underbrace{u_{n\vec{k}}(\vec{r})}_{\text{the hard part [Plane wave expansion, TBM, DFT, ...]}} \qquad \text{[Bloch's theorem]} \qquad (6)$$

Generally, $u_{n\vec{k}}(\vec{r})$ satisfies:

$$\left[\frac{1}{2m}(\hat{p}+\hbar\vec{k})^2 + V(\vec{r})\right]u_{n\vec{k}}(\vec{r}) = E_n(\vec{k})\,u_{n\vec{k}}(\vec{r}) \qquad (7a)\ \text{(exact)}$$

OR

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r}) - \frac{i\hbar^2}{m}\vec{k}\cdot\vec{\nabla} + \frac{\hbar^2k^2}{2m}\right]u_{n\vec{k}}(\vec{r}) = E_n(\vec{k})\,u_{n\vec{k}}(\vec{r}) \qquad (7b)$$

OR

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r}) + \frac{\hbar}{m}\vec{k}\cdot\hat{p} + \frac{\hbar^2k^2}{2m}\right]u_{n\vec{k}}(\vec{r}) = E_n(\vec{k})\,u_{n\vec{k}}(\vec{r}) \qquad (7c)$$

- The $\vec{k}=0$ (known (assumed)) problem:

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right] u_{n0}(\vec{r}) = E_n(\vec{0})\, u_{n0}(\vec{r}) \qquad (8)$$

($\vec{k}=0$)

  - all $E_n(\vec{0}) = E_n(0)$, and $u_{n0}(\vec{r})$ are assumed known

(For those who like to think in terms of perturbation, this is the unperturbated problem or $\hat{H}_0$ problem)

- The $\vec{k}\neq 0$ problem:

$$\left(\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right] + \underbrace{\left(\frac{\hbar}{m}\vec{k}\cdot\hat{p} + \frac{\hbar^2k^2}{2m}\right)}_{\text{extra term}}\right) \underbrace{u_{n\vec{k}}(\vec{r})}_{\text{unknowns}} = \underbrace{E_n(\vec{k})}_{\text{unknowns}}\, \underbrace{u_{n\vec{k}}(\vec{r})}_{\text{unknowns}} \qquad (7c)$$

(i) Short Cut: Perturbation Theory

Want the correction due to $\left(\hat{H}' = \frac{\hbar}{m}\vec{k}\cdot\hat{p} + \frac{\hbar^2k^2}{2m}\right)$ for the n^{th} band $E_n(\vec{k}\neq 0)$ to second order in k (because $\hat{H}'$ has $\frac{\hbar^2k^2}{2m}$ which is 2nd order)? (Meaning $\vec{k}\approx 0$)

$$E_n(\vec{k}) \cong E_n(0) + \frac{\hbar}{m}\vec{k}\cdot\langle u_{no}|\hat{\vec{p}}|u_{no}\rangle + \frac{\hbar^2|k|^2}{2m} + \frac{\hbar^2}{m^2}\sum_{n'(\neq n)}\frac{|\vec{k}\cdot\vec{p}_{nn'}|^2}{E_n(0)-E_{n'}(0)} \qquad (8)$$

this is 2nd order (non-degenerate) perturbation theory

1st order ($\sim k$)

$\because \langle u_{no}|u_{no}\rangle = 1$

$$\frac{1}{V}\int u_{no}^*(\vec{r})\left(\frac{\hbar}{i}\vec{\nabla}\right)u_{no}(\vec{r})\,d\tau \equiv \vec{p}_{nn} = \langle\vec{p}\rangle_n$$

expectation value

$$\vec{p}_{nn'} = \frac{1}{V}\int u_{no}^*(\vec{r})\left(\frac{\hbar}{i}\vec{\nabla}\right)u_{n'o}(\vec{r})\,d\tau$$

"momentum matrix elements"

different bands (at $\vec{k}=0$)

Still quite general, because all information $\{E_n(0)\}$, $\{u_{no}(\vec{r})\}$ for all n is used!

$\vec{k}\approx 0$ is needed so that we can stop at 2nd order

- See the physics in Eq.(8): $\vec{k}$-dependence enters
  - a linear k term (related to $\vec{p}_{nn}\equiv\langle\vec{p}\rangle_n$; may vanish (depending on situation)) ($\vec{v}_n = \langle\vec{p}\rangle_n/m$)
  - $\hbar^2k^2/2m$ term as in free electron
  - $|\vec{k}\cdot\vec{p}_{nn'}|^2/(E_n(0)-E_{n'}(0))$ terms $\equiv$ ($\vec{p}_{nn'}$ is important (do 2 bands couple?); $|E_n(0)-E_{n'}(0)|$ (closer bands matter))

- A "cheap" but important result: $k \to 0$ (ignore k^2 terms)

$$E_n(\vec{k}) \approx E_n(0) + \frac{\hbar}{m}\vec{k}\cdot\vec{p}_{nn} \qquad (9)$$

But taking $E_n(\vec{k})$ as continuous function† in $\vec{k}$, we have

$$E_n(\vec{k}) \approx E_n(0) + \left(\vec{\nabla}_{\vec{k}} E_n(\vec{k})\Big|_{\vec{k}=0}\right)\cdot\vec{k} \qquad (10)$$ (Taylor expansion, 1st term)

Comparing Eq.(9) and Eq.(10): gradient of $E(\vec{k})$ at $\vec{k}=0$ (the point of expansion)

$$\frac{\hbar}{m}\vec{p}_{nn} = \hbar\frac{\langle\vec{p}\rangle_n}{m} = \vec{\nabla}_{\vec{k}} E_n(\vec{k})\Big|_{\vec{k}=0} \qquad (11a)$$

OR $$\boxed{\langle\vec{v}\rangle_n = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}} E_n(\vec{k})\Big|_{\vec{k}=0}} \qquad (11b)$$

$\langle\vec{v}\rangle_n$: the velocity for an electron in the state $\psi_{n0}(\vec{r})$ [at $\vec{k}=0$]

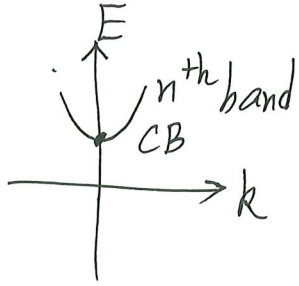
"$\frac{1}{\hbar}\times$ Gradient (slope) of $E_n(\vec{k})$ at $\vec{k}=0$"

† There are N ($\sim 10^{23}$) $\vec{k}$-values in 1st B.Z. for a $\sim 1\text{cm}^3$ crystal. Thus, $\vec{k}$-values are densely spaced in 1st B.Z.

- Eq. (11b) is a general result even for other values of $\vec{k}$:

$$\vec{v}_{n\vec{k}} = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}} E_n(\vec{k}) \qquad (12)$$

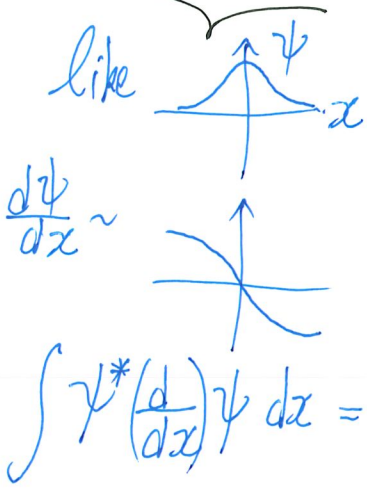
- Back to Eq. (11b), if the n^{th} band has an extreme at $\vec{k}=0$, e.g.



then $\nabla_{\vec{k}} E_n(\vec{k})\big|_{\vec{k}=0} = 0$, then $\sim k$ term in Eq. (8) vanishes

or $\vec{p}_{nn} = 0$ by symmetry reason (e.g. Bottom of CB $\sim$ s-character)

then $\sim k$ term in Eq. (8) also vanishes



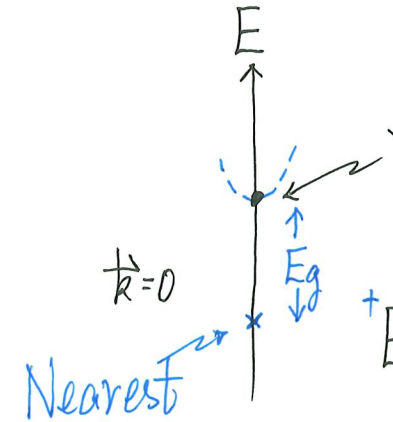
Remark: Educational to contrast

Free Electron	Electron in Bloch state (solid)
$\vec{p} = \hbar\vec{k}$	$\langle \vec{p} \rangle_n = \vec{p}_{nn} = \frac{m}{\hbar}\vec{\nabla}_{\vec{k}} E_n(\vec{k})$ (not $\hbar\vec{k}$)

Back to Eq. (8): $E_n(\vec{k}) \cong (\text{constant}) + \text{linear } k + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2}\sum_{n'(\neq n)} \frac{|\vec{k}\cdot\vec{P}_{nn'}|^2}{E_n(0)-E_{n'}(0)}$

just like free electron (nothing new)

physical reason for curvature AND thus also gives the physical reason for m^*



$^+E_c(k) \sim E_g + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2}\frac{|P_{cv}|^2}{E_g}k^2$

$\sim E_g + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 k^2}{2m}\left(\frac{2|P_{cv}|^2}{mE_g}\right)$

an energy

the most important term

$\frac{1}{m_c^*} = \frac{1}{m} + \frac{1}{m}\left(\frac{2|P_{cv}|^2}{m}\right)\frac{1}{E_g}$

OR $\frac{m}{m_c^*} = 1 + \frac{2|P_{cv}|^2}{m}\cdot\frac{1}{E_g}$

This is the physical picture

- States of lower energies (at $\vec{k}=0$) want to curl $E_n(\vec{k})$ up (nearby state(s) is(are) most important)
- States of higher energies (at $\vec{k}=0$) want to bend $E_n(\vec{k})$ down
- $\vec{P}_{nn'}$ OR $\frac{2|\vec{P}_{nn'}|^2}{m}$ vs $|E_n(0)-E_{n'}(0)|$ is crucial!

$^+$ Not been careful about vector nature (see later)

$$\frac{m}{m_c^*} = 1 + \frac{2|p_{cv}|^2}{m}\cdot\frac{1}{E_g} \quad (13)$$

conduction band effective mass

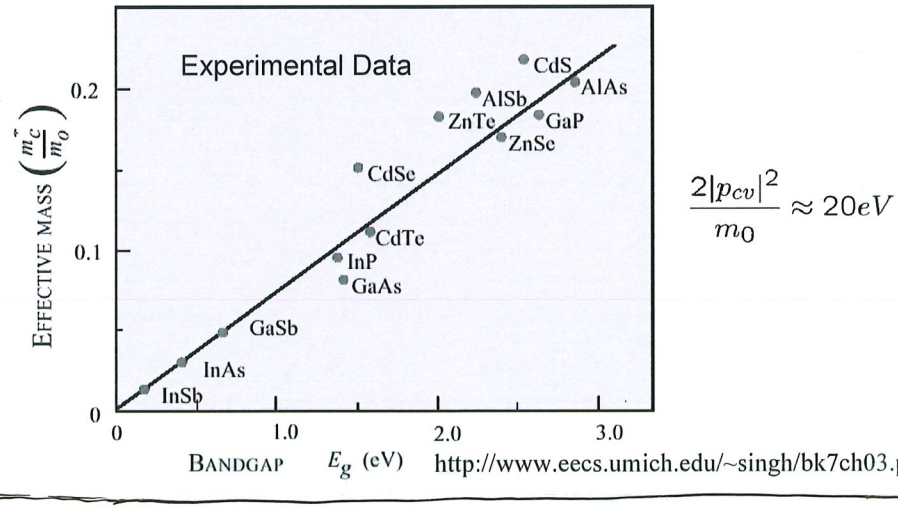
(13) is an important and handy result

- can regard $\frac{2|p_{cv}|^2}{m}$ as a material parameter (turns out to be even more than that!)
- $\frac{m}{m_c^*} \propto \frac{1}{E_g}$ (bigger gap, bigger m^*(CB); smaller gap, smaller m^*)

CB curling up rapidly with k

Momentum Matrix Elements and k.p Effective Mass

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2}\frac{|p_{cv}|^2}{E_g} \quad (13)$$



$\frac{2|p_{cv}|^2}{m_0} \approx 20eV$

http://www.eecs.umich.edu/~singh/bk7ch03.pdf

It works!

$\frac{2}{m}|p_{cv}|^2 \approx 20$ eV (nearly a constant) for a wide range of materials! (14)

(Handy number to carry around)

$$\vec{P}_{cv} = \frac{1}{V}\int u^*_{CB,0}(\vec{r})\left(\frac{\hbar}{i}\vec{\nabla}\right)u_{VB,0}(\vec{r})\,d\tau \sim \int (s\text{-like})\left(\frac{\hbar}{i}\vec{\nabla}\right)(p\text{-like})\,d\tau \neq 0 \quad (15)$$

$\vec{P}_{cv}$: Momentum Matrix element OR "Optical matrix element"

$u_{CB,0}$: Bottom of CB

$u_{VB,0}$: Top of VB

same $\vec{P}_{cv}$ is crucial for whether there will be optical transitions from VB maximum to CB minimum by absorbing light

$$\left|\frac{-e}{m}\int \psi^*_{final}\,(\vec{A}\cdot\hat{\vec{p}})\,\psi_{initial}\,d\tau\right|^2$$

$\vec{A}$: vector potential; $\hat{\vec{p}}$: momentum

a QM way of representing electron-photon interaction

determines transition rate and absorption coefficient

∴ $\vec{P}_{cv}$ (OR $\vec{P}_{nn'}$) also determines selection rules

Formal expression for $1/m^*$ from Eq. (8)

Eq. (8) is $E_n(\vec{k}) \cong E_n(0) + \frac{\hbar}{m}\vec{k}\cdot\langle u_{n0}|\hat{\vec{p}}|u_{n0}\rangle + \frac{\hbar^2}{m^2}\sum_{\alpha\beta} k_\alpha k_\beta \sum_{n'(\neq n)} \frac{P_{\alpha,nn'}\,P_{\beta,n'n}}{E_n(0) - E_{n'}(0)}$ (16)

(write out $|\vec{k}\cdot\vec{p}_{nn'}|^2$)

$$\left(\frac{1}{m^*}\right)_{\alpha\beta} = \frac{1}{\hbar^2}\frac{\partial E_n(\vec{k})}{\partial k_\alpha \partial k_\beta} = \frac{1}{m}\delta_{\alpha\beta} + \frac{1}{m^2}\sum_{n'(\neq n)} \frac{P_{\alpha,nn'}\,P_{\beta n'n} + P_{\beta,nn'}\,P_{\alpha,n'n}}{E_n(0) - E_{n'}(0)} \qquad (17)$$

- also work for $(1/m^*)_{\alpha\beta}$ around other $\vec{k}$-point
- Express how electron in a solid [with $V(\vec{r})$ accounted for] will respond to "external forces" [meaning forces beyond $V(\vec{r})$ [the jungle of ions plus mean-field electron-electron interaction]

  e.g. lattice vibrations (phonons)
  impurities / defects
  external applied $\vec{\mathcal{E}}$-field / $\vec{\mathcal{B}}$-field

What we just did in the simplest approach falls into:

- $\vec{k} \cdot \vec{p}$ ("k dot p") theory (most important for semiconductors)
- Kane Model (usually 4 bands: 1 CB + 3 VBs)
- Effective Mass Approximation (stay tuned, more to follow)
- Luttinger basis (Luttinger-Kohn-basis) functions
- Effective Mass Representation (EMR)

(b) Looking Closer : 2-band Model and extensions/applications

Eq.(7c): $$\left(\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right] + \left(\frac{\hbar}{m}\vec{k}\cdot\hat{\vec{p}} + \frac{\hbar^2k^2}{2m}\right)\right) u_{n\vec{k}}(\vec{r}) = E_n(\vec{k})\, u_{n\vec{k}}(\vec{r})$$

{ after moving $e^{i\vec{k}\cdot\vec{r}}$ through $\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})$

Formally, $\{u_{n0}(\vec{r})\}$ are knowns (all n), we can expand

$$u_{n\vec{k}}(\vec{r}) = \sum_{n'} C_{nn'}(\vec{k})\, u_{n'0}(\vec{r}) \qquad (18)$$

(this is exact)

unknowns — periodic

using all $u_{n'0}(\vec{r})$ at $\vec{k}=0$ (all periodic) ← (Key idea in the approach)

OR

$\vec{k}\neq 0$ (where we look for the solution)

$$e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r}) = \sum_{n'} C_{nn'}(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}\, u_{n',\vec{k}=0}(\vec{r}) \qquad (18a)$$

↑ where we know all the solutions

OR

$$\psi_{n\vec{k}}(\vec{r}) = \sum_{n'} C_{nn'}(\vec{k}) \underbrace{\frac{1}{\sqrt{V}}\, e^{i\vec{k}\cdot\vec{r}}\, u_{n',\vec{k}=0}(\vec{r})}_{\text{Luttinger basis functions}} \qquad (18b)$$

Aside: Luttinger & Kohn, Phys. Rev. 97, 869 (1955)

Showed that $\chi_{n\vec{k}}(\vec{r}) \equiv e^{i\vec{k}\cdot\vec{r}} u_{n,\vec{k}=0}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n0}(\vec{r})$ (different)

form a complete set (using all $\vec{k}$ and all n) and can be used to expand other functions (e.g. unknown ψ when external field is applied).

The idea is that unknown $u_{n\vec{k}}(\vec{r})$ can be expanded using $u_{n'0}(\vec{r})$ of all n'; or generally $u_{n'\vec{k}_0}(\vec{r})$ for all n' if solutions are known at $\vec{k}_0$.

Using the Luttinger basis functions is (sometimes) referred to as the Effective Mass Representation. (EMR).

$$u_{n\vec{k}}(\vec{r}) = \sum_{n'} C_{nn'}(\vec{k})\, u_{n'0}(\vec{r}) \Rightarrow \infty \times \infty \text{ Matrix problem for } C_{nn'} \quad \text{(formal, exact)}$$

- Now, focus only on <u>Two Bands</u> (c, v) (thus (2×2) part of a huge matrix)

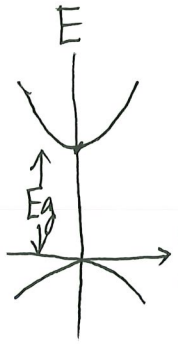
$$\underbrace{\begin{pmatrix} E_g + \frac{\hbar^2 k^2}{2m} & \frac{\hbar}{m}\vec{k}\cdot\vec{p}_{cv} \\ \frac{\hbar}{m}\vec{k}\cdot\vec{p}_{vc} & 0 + \frac{\hbar^2 k^2}{2m} \end{pmatrix}}_{\text{want eigenvalues of } 2\times 2 \text{ matrix (can do it exactly}^+)} \begin{pmatrix} C_{CB} \\ C_{VB} \end{pmatrix} = E(\vec{k}) \begin{pmatrix} C_{CB} \\ C_{VB} \end{pmatrix} \quad (19)$$

Approximation (but more useful)

(Ex.)

(i) <u>if E_g is not so small</u> ($E_g \gg \left|\frac{\hbar}{m}\vec{k}\cdot\vec{p}_{cv}\right|$), then perturbation works

$$\boxed{E_c(\vec{k}) \cong E_g + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2}\frac{|\vec{k}\cdot\vec{p}_{cv}|^2}{E_g}} \quad (20) \quad \text{(as before)}$$



$$E_v(\vec{k}) \cong \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2}{m^2}\frac{|\vec{k}\cdot\vec{p}_{cv}|^2}{E_g}$$

(but be careful, there are other VB's with nearly the same energy)

2-band model

+ Will then see non-parabolic behavior

(ii) When we include into n' three VB states (degenerate, ignore spin-orbit interaction)

then we will encounter

$$\int u^{*}_{CB,0}(\vec{r})\ \hat{\vec{p}}\ u^{(1)}_{VB,0}(\vec{r})\ d\tau$$

"s" $\sim\vec{\nabla}$ "p_x" (along x-direction, say)

CB (s)

VB ~ p_x-state, p_y-state, p_z-state

LCAO picture, e.g. all mostly p-character (such as p_x, p_y, p_z states)

with $\langle s0|\hat{p}_x|x0\rangle \neq 0$ [but $\langle s0|\hat{p}_y|x0\rangle = 0$, $\langle s0|\hat{p}_x|y0\rangle = 0$, etc.]

$\hat{p}_x \sim \frac{d}{dx}$

Similarly, $\int u^{*}_{CB,0}(\vec{r})\ \hat{p}_y\ u^{(2)}_{VB,0}(\vec{r})\ d\tau = \langle s0|\hat{p}_y|y0\rangle \neq 0$ [but $\langle s0|\hat{p}_y|z0\rangle = 0$, etc.]

"p_y" state

Also, $\langle s0|\hat{p}_z|z0\rangle \neq 0$

p_z state

By crystal's symmetry,

$$\langle s0|\hat{p}_x|x0\rangle = \langle s0|\hat{p}_y|y0\rangle = \langle s0|\hat{p}_z|z0\rangle \neq 0 = p_{cv} \quad (21)$$

Then, we should focus on a (4×4) part of a huge matrix

Schematically,[†]

	$\lvert C\rangle$ ($u_{CB,0}$)	$\lvert V^{(1)}\rangle$ ($u^{(1)}_{VB,0}\sim p_x$)	$\lvert V^{(2)}\rangle$ ($u^{(2)}_{VB,0}\sim p_y$)	$\lvert V^{(3)}\rangle$ ($u^{(3)}_{VB,0}\sim p_z$)
$\langle C\rvert$	$E_g+\frac{\hbar^2\lvert k\rvert^2}{2m}$	$\frac{\hbar}{m}k_x p_{cv}$	$\frac{\hbar}{m}k_y p_{cv}$	$\frac{\hbar}{m}k_z p_{cv}$
$\langle V^{(1)}\rvert$	$\frac{\hbar}{m}k_x p^*_{cv}$	$\frac{\hbar^2\lvert k\rvert^2}{2m}$ ← degenerate	complicated terms	"
$\langle V^{(2)}\rvert$	$\frac{\hbar}{m}k_y p^*_{cv}$	complicated terms	$\frac{\hbar^2\lvert k\rvert^2}{2m}$	"
$\langle V^{(3)}\rvert$	$\frac{\hbar}{m}k_z p^*_{cv}$	"	"	$\frac{\hbar^2\lvert k\rvert^2}{2m}$

(22)

← This Valence Band 3×3 part is complicated (Kane Model) [6×6 including spin]

For conduction band,

$$E_c(\vec{k}) \underset{\text{around } \vec{k}=0}{=} E_g+\frac{\hbar^2\lvert k\rvert^2}{2m}+\frac{\hbar^2}{m^2}\frac{\lvert P_{cv}\rvert^2}{E_g}\left(k_x^2+k_y^2+k_z^2\right)=E_g+\frac{\hbar^2\lvert k\rvert^2}{2m}+\underbrace{\frac{\hbar^2}{2m}k^2}\left(\frac{2}{m}\lvert P_{cv}\rvert^2\cdot\frac{1}{E_g}\right) \quad (20)$$

isotropic CB around minimum! (same as before)

[†] Even so, may need to fold the effects from other n' beyond the 4×4

(iii) Kane Model (E.O. Kane, J. Phys. Chem. Solids 1, 249 (1957)) [a classic]

(just the idea here) ↑ InSb bands using $\vec{k}\cdot\vec{p}$ method

- 1 CB + VB, including spin-orbit interaction (8 bands)
- Use $|j, m_j\rangle$ states for VB's instead of $|\ell=1, s=\tfrac{1}{2}, m_\ell, m_s\rangle$

$j=3/2$, $j=1/2$

$(m_j = 3/2, 1/2, -1/2, -3/2)$ $(m_j = 1/2, -1/2)$ ← these become the split-off band as $j=1/2$ states have lower energy (due to H_{SO})

6 VB states ($u^{(i)}_{VB,\vec{k}=0}(\vec{r})$)

- Write down 8 × 8 matrix [CB↑, CB↓, 6 VB's with $|j, m_j\rangle$]

$$\begin{pmatrix} (4\times4) & 0 \\ 0 & (4\times4) \end{pmatrix} \quad \text{(same)}$$

$$\text{with } (4\times4) = \begin{pmatrix} E_s & 0 & \frac{\hbar}{m}kp & 0 \\ 0 & E_p - \frac{\Delta}{3} & \frac{\sqrt{2}}{3}\Delta & 0 \\ \frac{\hbar}{m}kp^* & \frac{\sqrt{2}}{3}\Delta & E_p & 0 \\ 0 & 0 & 0 & E_p + \frac{\Delta}{3} \end{pmatrix}$$

apart from $\frac{\hbar^2k^2}{2m}$ terms

$\Delta = \Delta_{SO}$

E_s, E_p are s, p band energies without H_{SO}

This gives 4 bands (each degenerate due to spin (m_j))

$$E_c(\vec{k}) = E_g + \frac{\hbar^2 k^2}{2m}\left[1 + \frac{2P^2}{3m}\left(\frac{2}{E_g} + \frac{1}{E_g+\Delta}\right)\right]$$

pushing up by 2 bands at energy 0

pushing up by 1 band at energy $-\Delta$ (the split off band)

heavy hole ⇝ $E_{hh} = \frac{\hbar^2 k^2}{2m}$ ← curling up! (need other bands to bend it down)

$$E_{eh} = \frac{\hbar^2 k^2}{2m}\left(1 - \frac{4P^2}{3mE_g}\right) \qquad (23)$$

bending down by CB

$$E_{so} = -\Delta + \frac{\hbar^2 k^2}{2m}\left[1 - \frac{2P^2}{3m(E_g+\Delta)}\right]$$

bending down by CB

Recall: $\frac{2P^2}{m} \sim 20$ eV for many materials

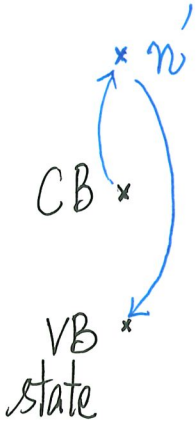
This 4-band model is popular for many III-V compounds. It is very popular in recent years because it is needed for models of topological materials.

Kane went further to include effects of other bands, by folding effects back to the 4×4 part.

E.g. $\frac{\hbar}{m}\vec{k}\cdot\hat{\vec{p}}$ term

["11" element]

$$\frac{\hbar^2}{m^2}\frac{\langle c|\vec{k}\cdot\hat{\vec{p}}|n'0\rangle\langle n'0|\vec{k}\cdot\hat{\vec{p}}|c\rangle}{(E_c(0)-E_{n'}(0))} \text{ in "11" element}$$



["12" element]

$$\frac{\hbar^2}{m^2}\frac{\langle c|\vec{k}\cdot\hat{\vec{p}}|n'0\rangle\langle n'0|\vec{k}\cdot\vec{p}|VB^{(1)}\rangle}{(E_c(0)-E_{n'}(0))} \text{ contributes to "12" element}$$

∴ quadratic terms in elements

This folding back the effects of other bands in especially important for the description of the top of Valence bands

the "complicated 3×3" part

(iv) Top of Valence Bands[†] at $\vec{k}=0$ (Si, Ge) (just the idea here)

" Fold effects of other (beyond 3×3) bands into 3×3

$$\begin{vmatrix} L k_x^2 + M(k_y^2+k_z^2) + \frac{\hbar^2 k^2}{2m} - E & N k_x k_y & N k_x k_z \\ N k_x k_y & L k_y^2 + M(k_x^2+k_z^2) + \frac{\hbar^2 k^2}{2m} - E & N k_y k_z \\ N k_x k_z & N k_y k_z & L k_z^2 + M(k_x^2+k_y^2) + \frac{\hbar^2 k^2}{2m} - E \end{vmatrix} = 0 \qquad (24)$$

where $L, M, N \sim \sum_{n' \neq 3 \text{ bands}} \frac{\langle v|\hat{p}_\alpha|n'\rangle\langle n'|\hat{p}_\beta|v'\rangle}{E_v(0) - E_{n'}(0)}$ effects on other bands

(v, v' for 3×3 elements)

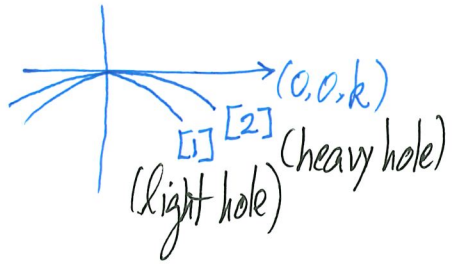
Can solve for three $E(\vec{k})$'s (3 VB's)

[†] Dresselhaus, Phys. Rev. 100, 580 (1955)
Dresselhaus, Kip, Kittel, Phys. Rev. 98, 368 (1955)

E.g. For $\vec{k}$ in $(0,0,k)$ (or equivalent)

$$E_{v1}(k) = Lk^2, \quad E_{v2}(k) = Mk^2, \quad E_{v3} = Mk^2$$

(E_{v2}, E_{v3}: degenerate)



For $\vec{k}$ in $\frac{1}{\sqrt{3}}(k,k,k)$ direction

(E_{v2}, E_{v3}: degenerate)

$$E_{v1}(k) = \frac{L+2M-2N}{3}k^2, \quad E_{v2}(k) = \frac{L+2M+N}{3}k^2, \quad E_{v3}(k) = \frac{L+2M+N}{3}k^2$$

- Anisotropic (so called "surfaces of constant energy are warped") ("deformed")
- Degenerate ones are "heavy hole" bands [v2 and v3]
  Non-generate one is "light hole" band [v1]

> spin-orbit interaction is ignored

Dresselhaus, Kip, Kittel included spin-orbit interaction (6×6 with $|j, m_j\rangle$)

$$A = \frac{1}{3}(L+2M) + \frac{\hbar^2}{2m} \; ; \quad B = \frac{1}{3}(L-M) \; ; \quad C^2 = \frac{1}{3}\left[N^2 - (L-M)^2\right]$$

$|6\times 6| = 0$ gives

$$E_{3/2}(\vec{k}) = Ak^2 \pm \left[B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_y^2)\right]^{1/2}$$

each doubly degenerate (two bands "±" non-parabolic terms)

$j = 3/2$

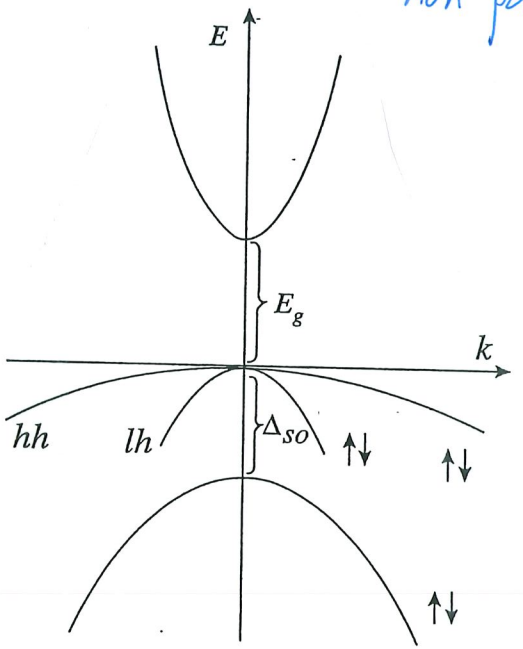
$$E_{1/2}(\vec{k}) = -\Delta_{so} + Ak^2$$

(split-off band) (doubly degenerate)

$j = 1/2$

Valence band parameters for silicon and germanium in units of $\hbar^2/2m$

	A	$\lvert B\rvert$	$\lvert C\rvert$
Si	−4.29	0.68	4.87
Ge	−13.38	8.48	13.15



Heavy hole (*hh*), light hole (*lh*), and split-off (*so*) energy bands for diamond structure semiconductors. The Kramers degeneracy is indicated by the up and down arrows.

← Typical VB structure for Si, Ge

(v) What for?

- $\vec{k}\cdot\vec{p}$, Kane Model, ... want to parameterize semiconductor VB's + CB (a few important band)
- m^* or $\left(\frac{1}{m^*}\right)_{\alpha\beta}$ affects transport (response to applied external fields) and optical (response to EM fields) properties (affect density of states) ($\vec{p}_{nn'}$)
- heterostructures

Semiconductor A	Semiconductor B
need to know when electrons live in A, they see	when electrons live in B, they see
$\begin{pmatrix} 3\times 3 \end{pmatrix}_A$	$\begin{pmatrix} 3\times 3 \end{pmatrix}_B$
valence bands	valence bands
$\hat{H}_A$	$\hat{H}_B$

$\hat{H}(z)$ describes the A/B heterostructure

$z \in A : \hat{H}_A$

$z \in B : \hat{H}_B$

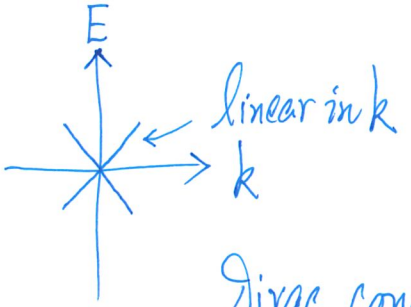
(vi) By-product : linear dispersion from 2-band model

Back to $\begin{pmatrix} E_g + \frac{\hbar^2 k^2}{2m} & \frac{\hbar}{m}\vec{k}\cdot\vec{p}_{cv} \\ \frac{\hbar}{m}\vec{k}\cdot\vec{p}_{vc} & \frac{\hbar^2 k^2}{2m} \end{pmatrix}$ solve it exactly (Ex.)

When $E_g = 0$ (the two bands touch at $\vec{k}=0$),

$$E_\pm = \pm \frac{\hbar}{m}|\vec{k}\cdot\vec{p}_{cv}| + \frac{\hbar^2 k^2}{2m} \quad (25)$$

linear k term; negligible for ($k \approx 0$)



Dirac cone structure [Graphene at K-points]

For $E_g \approx 0$ (small gap), still see linear part adding into quadratic part

∴ When two bands cross and open up a gap (by tuning some parameters), there will be linear dispersion at the $\vec{k}$-point the bands cross.

Remark: Experiments on topological materials often work on such systems