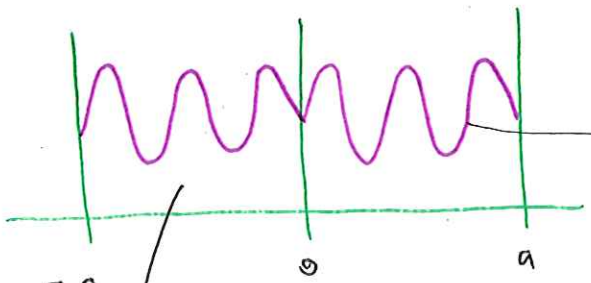
Physics 410/510 - Solid State Physics
Spring 2015
Wednesday, Week 9:

Review:

Application of Bloch's theorem: $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$

$\downarrow$

periodic in crystal.

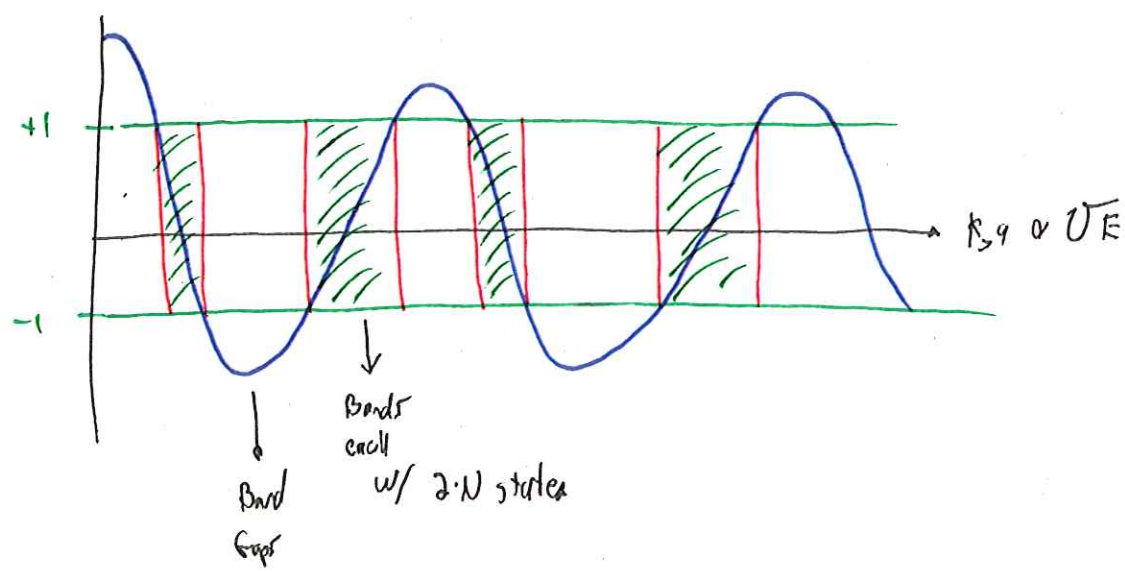


$$\psi_k(x) = e^{ikx}\left(A\sin(k_0 x) + B\cos(k_0 x)\right) \qquad x \in [0,a]$$

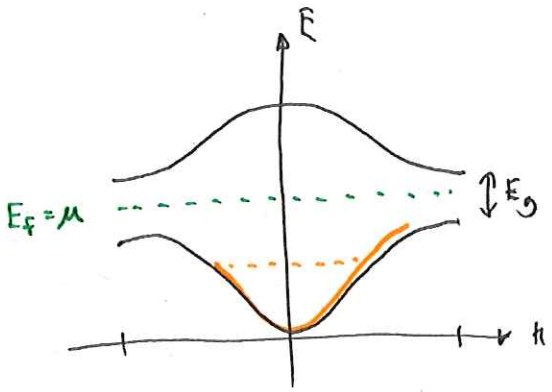
$$V(x) = \alpha \sum_j \delta(x - ja)$$

$$\psi_k(x) = e^{+ik(x-a)}\left(A\sin(k_0(x+a)) + B\cos(k_0(x+a))\right) \qquad x \in [-a,0]$$

$$\Rightarrow \quad \cos(ka) = \cos(k_0 a) + \frac{m\alpha a}{\hbar^2}\frac{\sin(k_0 a)}{k_0 a}$$

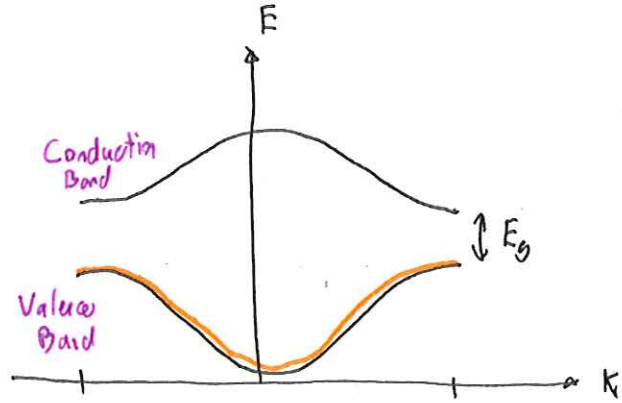


Energy Bands in 1D:



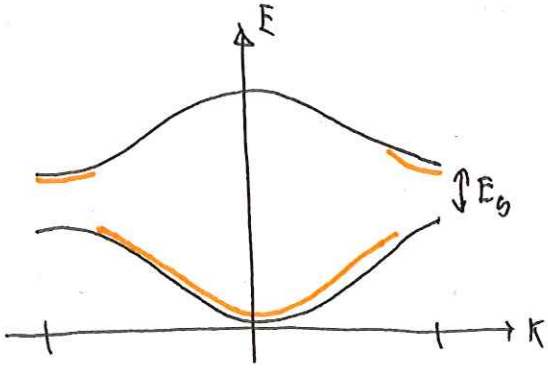
Electric Currents in Metals

Odd # e^-'s per unit cell



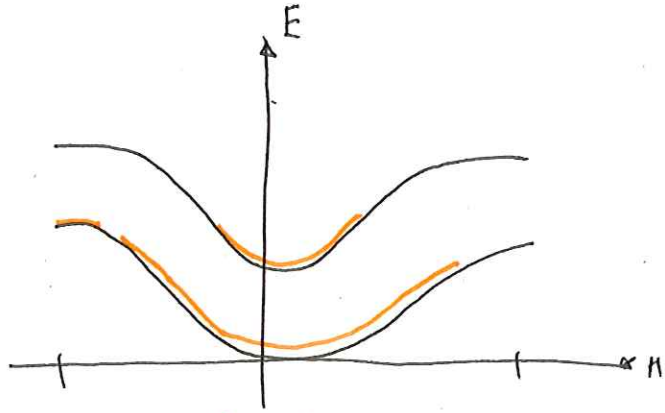
Band insulator

Even # e^-'s per unit cell



Thermally activated charge carriers

=) Some charge carriers!!



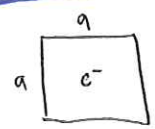
Band overlap

=) charge carriers

The case of band overlap can be quite common in real materials because they live in 3D.

Energy Bands in 2D & 3D:

Monovalent atoms

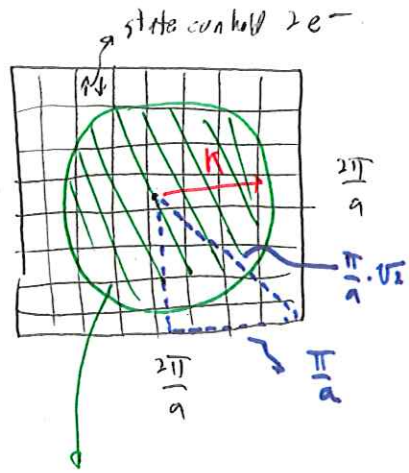


=>

Monovalent

↓

Can fill half of the 1st BZ



What is the radius of the disk?

Radius of disk:

$$\pi k^2 = \frac{1}{2}\left(\frac{2\pi}{a}\right)^2 = \frac{2\pi^2}{a^2}$$

$$K = \frac{\sqrt{2}\pi}{a} \approx \frac{2.5}{a} < \frac{\pi}{a}$$

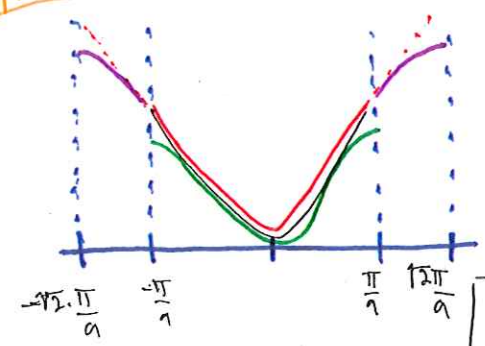
☆ Show PPT.

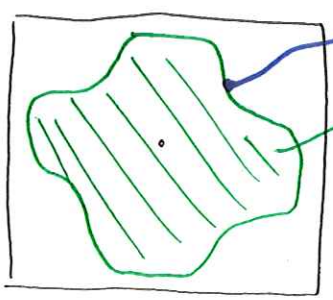
Fermi Sea forms a disk: area $= \frac{1}{2}\left(\frac{2\pi}{a}\right)^2 = \frac{1}{2}$ 1st BZ.

☆ Sec 3.1

- Adding a periodic potential: ① States close to zone boundary get moved down in energy (from opening of band gap.)

② Electrons preferentially fill states close to BZ edge.



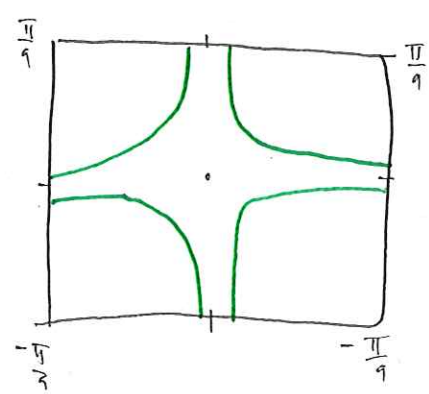


Fermi surface

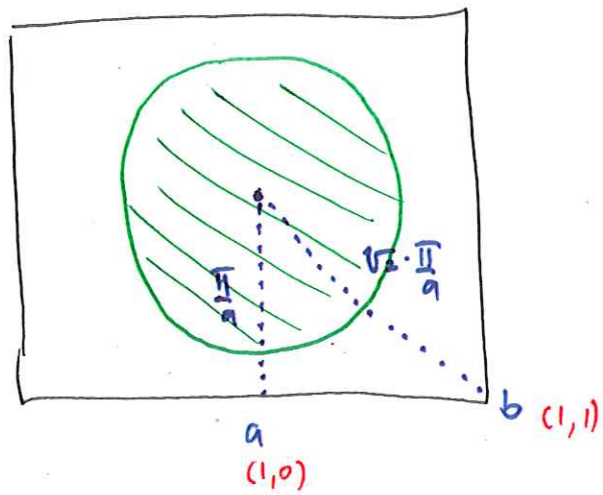
Fermi sea still fill ½ 1st BZ.

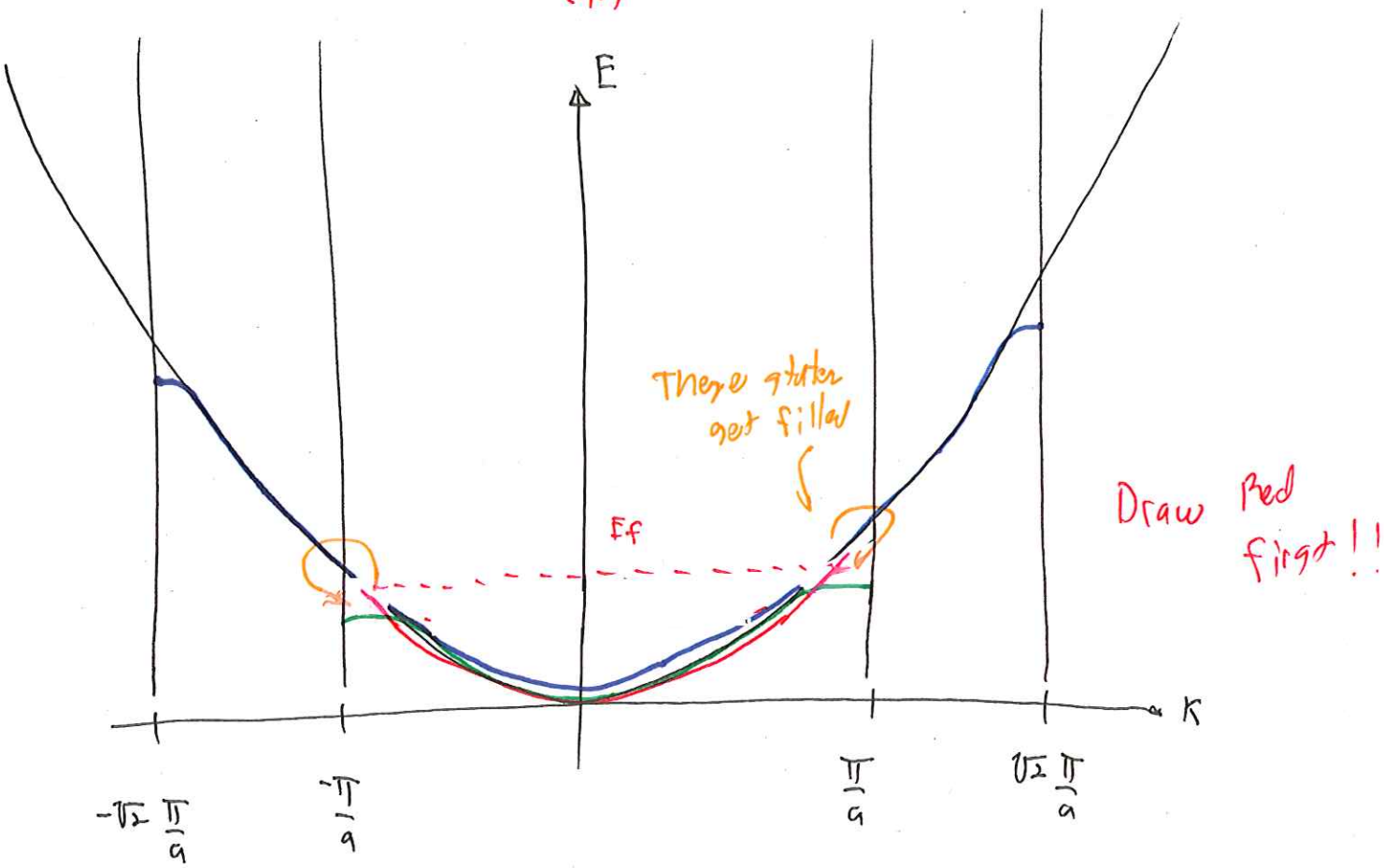
③ Increasing strength of $V(\vec{r})$ ⇒ $|V_{\vec{G}}|$ get larger & band gap grows so electronic energy state @ boundary get smaller.

$$E = E_0 - 2t\cos(k_x a) - 2t\cos(k_y a)$$

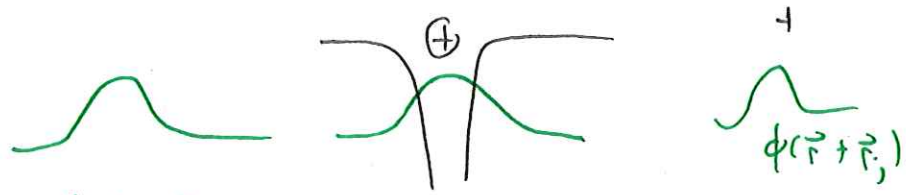


An illustration of band bending at the BZ edge:





The shape of the fermi sea is obtained via tight-binding:



$\phi(\vec{r})$ is groundstate s-orbital (spherically symmetric)

& form

$$\psi_{\vec{k}}(\vec{r}) \equiv \frac{1}{\sqrt{N}} \sum_j \exp(i\vec{k}\cdot\vec{R}_j)\,\phi(\vec{r}-\vec{R}_j) = |\vec{k}\rangle$$

$\vec{R}_j \in$ [Lattice Vectors]

labled w/ $\vec{k}$ since it is a Bloch function:

$\psi_{\vec{k}}(\vec{r})$ is a Bloch function

$$\psi_{\vec{k}}(\vec{r}+\vec{R}) = \frac{1}{\sqrt{N}} \sum_j \exp(i\vec{k}\cdot\vec{R}_j)\,\phi(\vec{r}+\vec{R}-\vec{R}_j)$$

$$= e^{i\vec{k}\cdot\vec{R}} \frac{1}{\sqrt{N}} \sum_j \exp(i\vec{k}\cdot(\vec{R}_j-\vec{R}))\,\phi(\vec{r}-(\vec{R}_j-\vec{R}))$$

$$= e^{i\vec{k}\cdot\vec{R}}\,\psi_{\vec{k}}(\vec{r}) \quad \blacksquare$$

$\vec{R}$ = Lattice Vector

Then we can calculate then energies directly:

$$E_{\vec{k}} = \langle\vec{k}|H|\vec{k}\rangle = \frac{1}{N}\sum_j\sum_m \int e^{-i\vec{k}\cdot\vec{R}_m}\phi^*(\vec{r}-\vec{R}_m)\,H\,e^{i\vec{k}\cdot\vec{R}_j}\phi(\vec{r}-\vec{R}_j)\,d\vec{r}$$

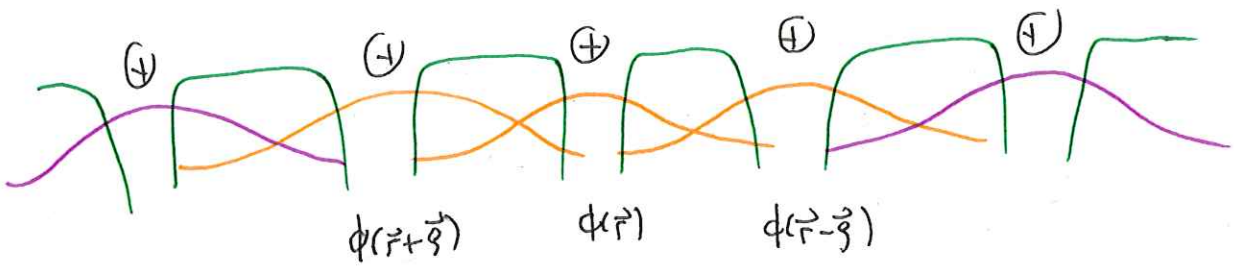
$$= \frac{1}{N}\sum_{j,m} e^{i\vec{k}\cdot(\vec{R}_j-\vec{R}_m)} \int \phi^*(\vec{r}-\vec{R}_m)\,H\,\phi(\vec{r}-\vec{R}_j)\,d\vec{r}$$

& $\vec{\rho}_m \equiv \vec{R}_m - \vec{R}_j$ $\quad \vec{r}-\vec{R}_j \to \vec{r}$ $\Rightarrow$ $\vec{r}-(\vec{R}_m-\vec{R}_j)$ $\quad \vec{r}$ $\quad d\vec{r}$

$$= \frac{1}{N}\sum_{j,m} e^{-i\vec{k}\cdot\vec{\rho}_m} \int \phi^*(\vec{r}-\vec{\rho}_m)\,H\,\phi(\vec{r})\,d\vec{r}$$

There are N copies of this from j sum, so,

$$\langle \vec{k}|H|\vec{k}\rangle = \sum_m e^{-i\vec{k}\cdot\vec{\rho}_m} \underbrace{\int \phi^*(\vec{r}-\vec{\rho}_m)\, H\, \phi(\vec{r})\, d\vec{r}}$$



We only keep $\vec{\rho}_m = \begin{cases} 0 \\ \pm\vec{\rho} \end{cases}$ Nearest Neighbors

So,

$$E_{\vec{k}} = \langle \vec{k}|H|\vec{k}\rangle = \overbrace{\int \phi^*(\vec{r})\, H\, \phi(\vec{r})\, d\vec{r}}^{-\alpha} + \sum_m e^{-i\vec{k}\cdot\vec{\rho}_m} \overbrace{\int \phi^*(\vec{r}-\vec{\rho})\, H\, \phi(\vec{r})\, d\vec{r}}^{-\gamma}$$

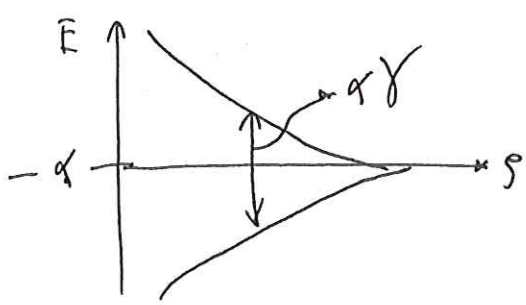
Main tight-binding result.

$$\boxed{E_{\vec{k}} = -\alpha - \gamma \sum e^{-i\vec{k}\cdot\vec{\rho}_m}} \qquad \vec{k} \in 1^{\circ}\ BZ$$

The factor γ is what opens up the band bands!! for Hydrogenic $|100\rangle$ states as $\phi(\vec{r})$:

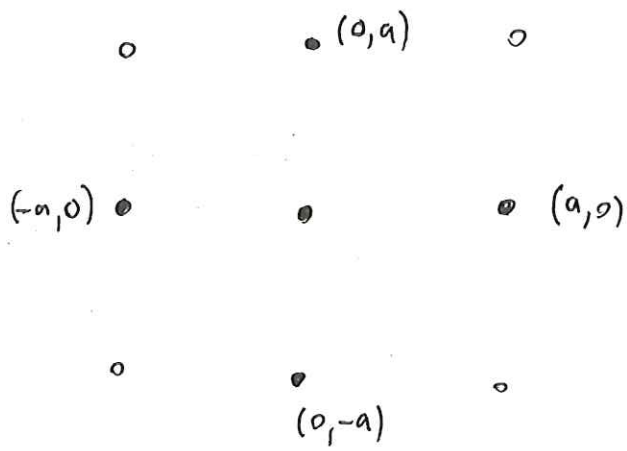
$$\gamma \propto e^{-\rho/a_0}$$

$$\text{i.e.} \quad \gamma \to 0 \quad \rho \gg a_0 \approx 0.5\ \text{Å}$$



Band gets wider with larger γ.

Back to the 2D square example:

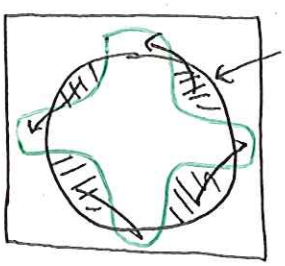


$$\vec{g}_m = \begin{pmatrix} \pm a \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \pm a \end{pmatrix}$$

$$E(\vec{k}) = -\alpha - \gamma\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right)$$

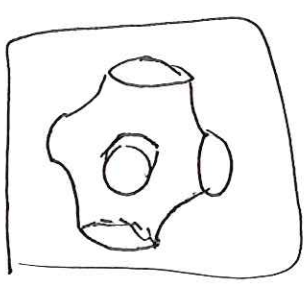
☆ Show PPT

$$= \boxed{-\alpha - 2\gamma\left[\cos(k_x a) + \cos(k_y a)\right]}$$



Those electrons move to fill lower energy states.

☆ Show PPT of SC Fermi surface:



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Spring 2015
Friday, Week 9:

Review:

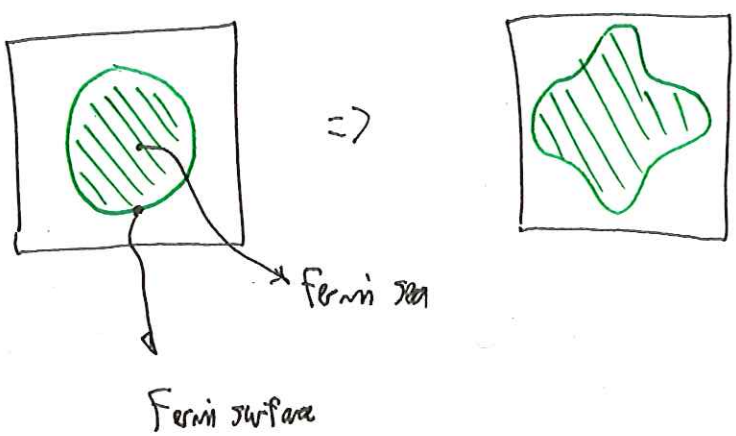
$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_j \exp(i\vec{k}\cdot\vec{R}_j)\,\phi(\vec{r}-\vec{R}_j)$$

Tight-binding Bloch Function

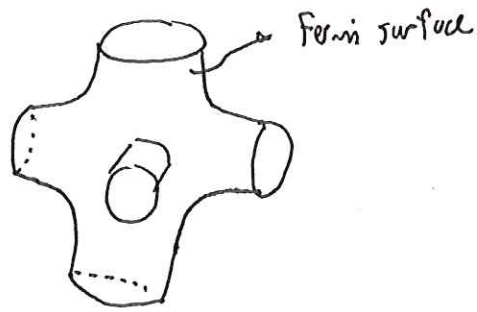
$$E(\vec{k}) = -\alpha - \gamma \sum_m e^{-i\vec{k}\cdot\vec{g}_m}$$

Ex) 2D square lattice w/ monovalent atoms

$$E(\vec{k}) = -\alpha - 2\gamma\left[\cos(k_x a) + \cos(k_y a)\right]$$



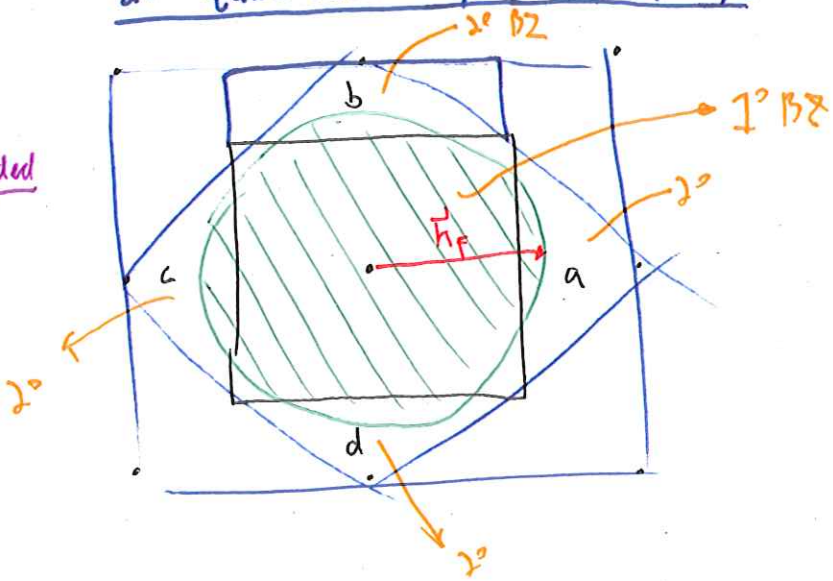
In 3D,



2D Square Lattice w/ Divalent Atoms:

Free:

Extended



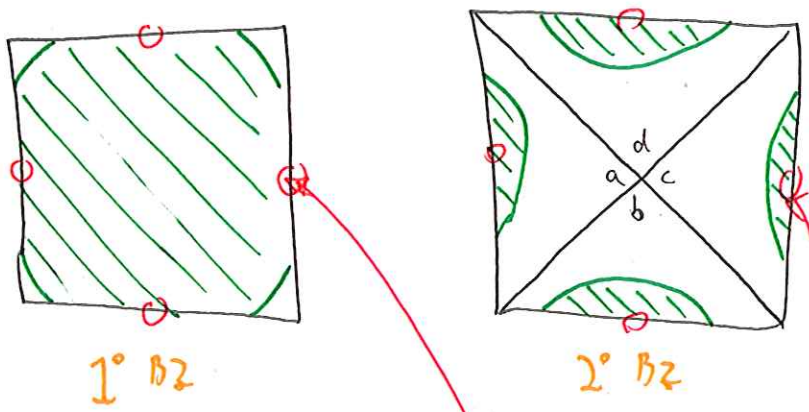
all 1° BZ

$$\pi k_F^2 = \left(\frac{2\pi}{a}\right)^2$$

$$k_F = \frac{2}{a}\sqrt{\pi}$$

$$\approx \frac{3.55}{a} > \frac{\pi}{a}$$

Reduced



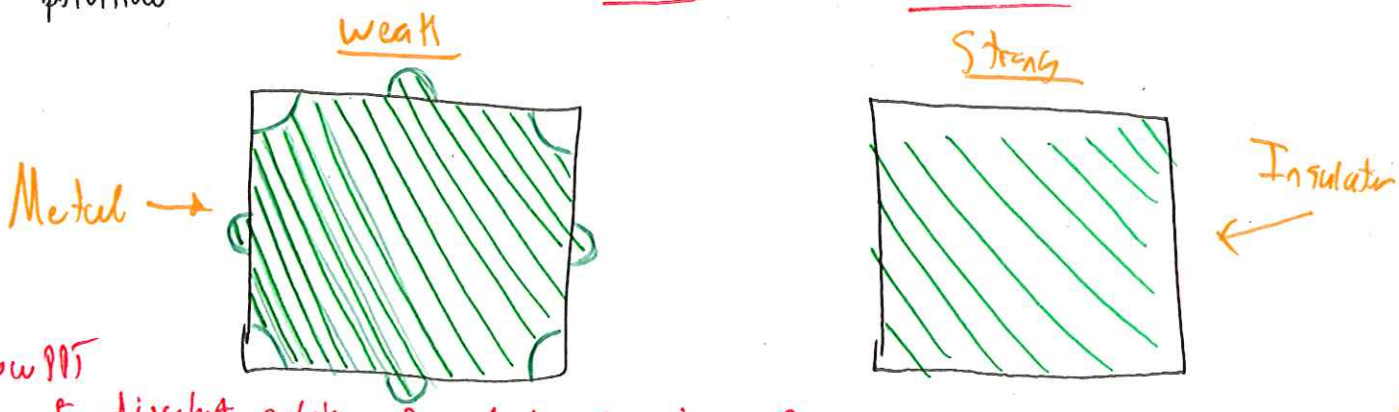
N.B. Top of section b will take up such to center of 1° BZ for neighboring cell.

Nearly Free:

Applying a potential will lower energy here & raise it here, so for a weak potential we have:

Lower band

Upper band



Show PPT of divalent calcium free electron fermi surface.

Take-home: A weak potential can allow for band overlap & a metallic state even when # e^- is even.

Other places where Band Theory (as we've presented it) fails in predicting metal-insulator states

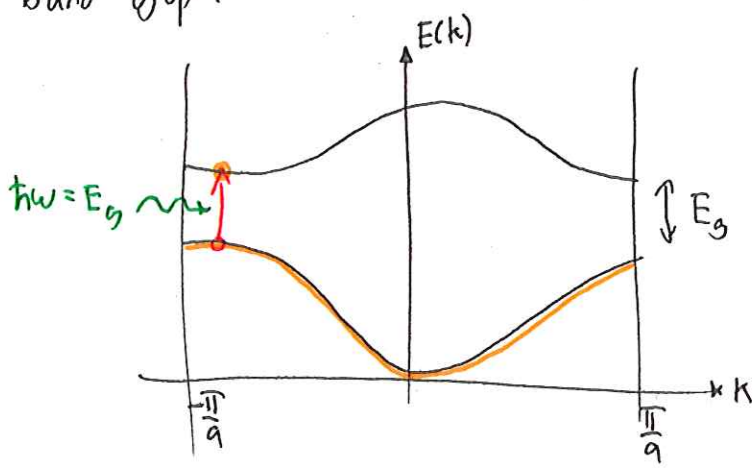
- Magnets: spin-spin interaction strong ⇒ filling ↑↓ doesn't work.
- Mott Insulators: (NiO, CoO)

  strong $e^- - e^-$ interaction, so even w/ monovalent atoms, only 1 e^- sits at each atom (no ↑↓) & the system is insulating!!

Optical Properties & Band structure:

- Insulators & Semiconductors:

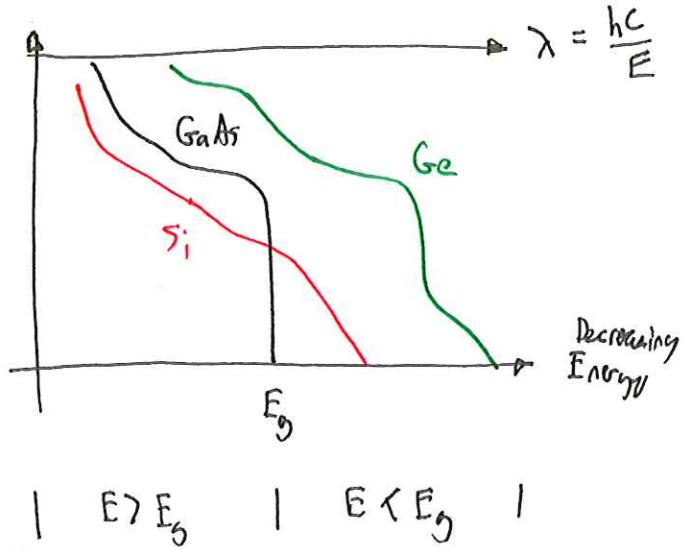
  Band insulators cannot absorb photons w/ energy less than their band gap:



Show POT of light absorption spectra. There is a strong drop in the absorption for wavelengths greater than band gap wavelength.

- If $E_g \gtrsim 3.2$ eV, the crystal will be optically transparent.

Optical Absorption Spectra

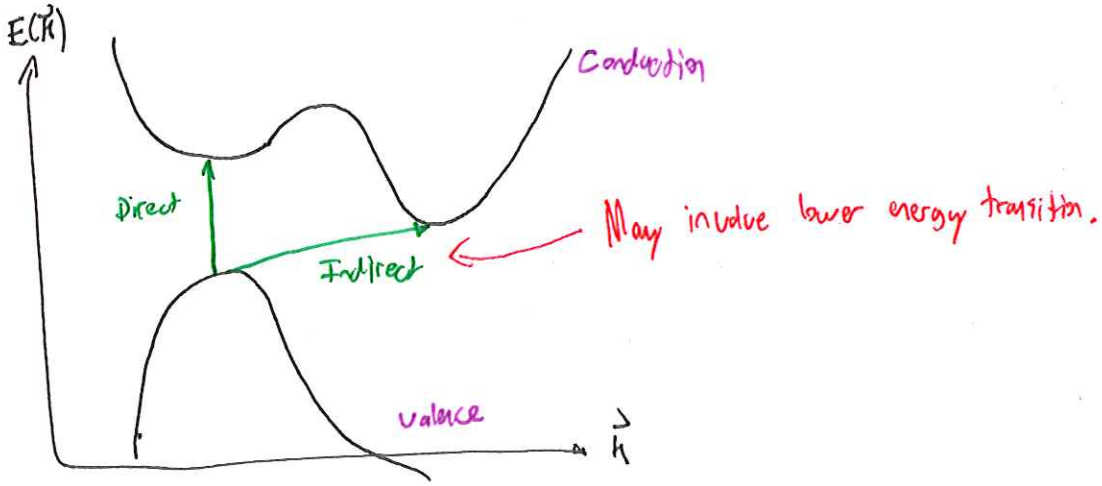


Show POT of semiconductors

Color:

- CdS has $E_g \sim 2.6\,eV$ so blue & violet opt absorbed & red & green
- Small band gap semiconductor such as Si, Ge, GaAs have $E_g < 1.5\,eV$, so the absorb most visible & look black.
- Quartz, Diamond, Aluminum oxide, BN have $E_g > 3.2\,eV$ so they are transparent.

The onset for absorption of photons can be sharp or gradual. This has to do w/ the indirect or direct bandgap nature.



- <u>Direct</u>: $\Delta\vec{k} \approx 0$

  <u>Indirect</u>: $\Delta\vec{k} \neq 0$

Indirect processes involve a non-zero $\vec{k}$, but the $\vec{k}$ of a photon is small:

$$\hbar|\vec{k}|\cdot c = E$$
$$= |\vec{p}|c$$

$$\Rightarrow \quad |\vec{k}| = \frac{E}{\hbar}\cdot\frac{1}{c} \approx \frac{1\,eV}{4\times10^{-15}\,eV\cdot s}\,\frac{1}{3\times10^{8}} = 10^{6}\,m^{-1}$$

Compared to phonons:

$$|\vec{k}| = \frac{E}{\hbar}\cdot\frac{1}{v_s} \qquad \underline{c \gg v_s} \qquad \approx \frac{1}{a} = 10^{10}\,m^{-1}$$

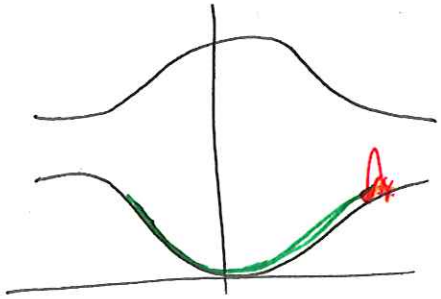
$$\Rightarrow \quad \boxed{|\vec{k}|_{photon} \ll |\vec{k}|_{phonon}}$$

Because energy & momentum must be conserved, indirect transitions often involve complicated phonon absorption/emission processes that are <u>not efficient</u>:

But indirect absorption can still occur & does occur; just much less efficiently.

Optical Properties of Metals

What gives metals their color?

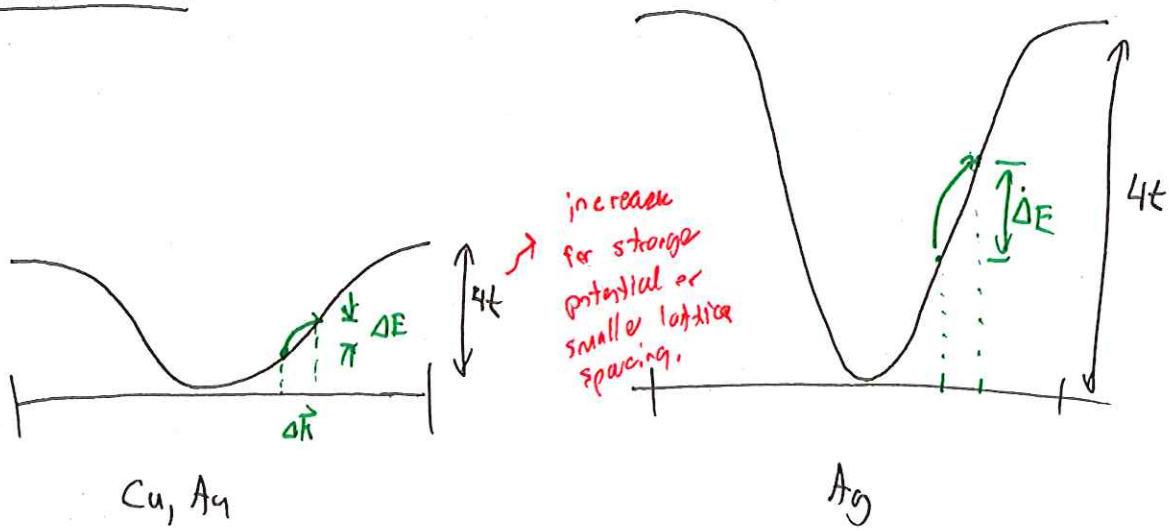


Intraband transitions dominate.

Metals absorb & re-emit light very efficiently & is why they are shiny. The re-emission process occurs very quickly.

Metals that do not form surface oxides look shinier, such as Ag, Au, Pt.

Color of metals: Intraband Transitions



$\Delta E_{Ag} >> \Delta E_{Cu}$ so Ag can absorb & re-emit higher energy photons, as well as lower energy photons, so Ag looks more mirror-like. Cu only absorbs-re-emits Red → Green so looks coppery.

Impurities:

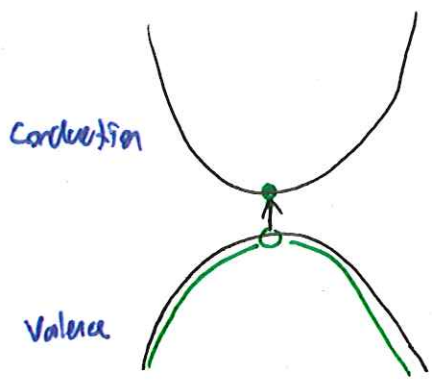
Small levels of impurities can transform optical & electronic properties.

Show PPT

Ex) B in Diamond.

Semiconductor Physics:

Consider a filled valence band & exciting a single electron from the valence to the conduction band:



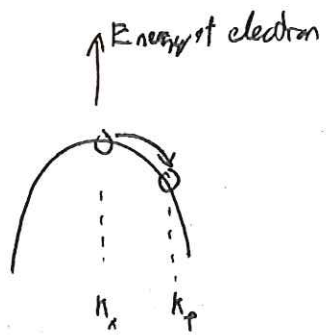
An absence of an electron from the valence band is called a "hole"

- We keep track of holes & treat them as individual elementary particles.

The charge of an electron $= -e$

The charge of an absence of an electron $= +e$

Energy of a hole?



- To move electron down takes negative energy (spontaneous)
- To move a hole from $k_i \to k_f$ takes positive energy (work).

Like pushing balloon under water!!