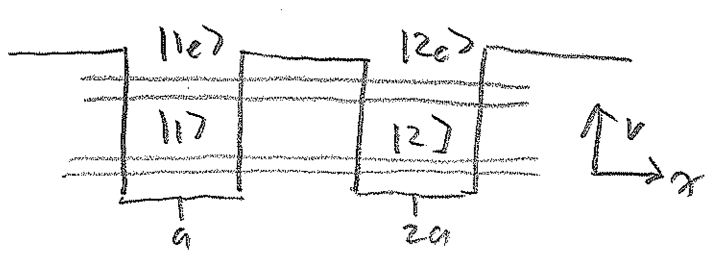
Day 13

Last time: $m^* = \hbar^2 \left[\frac{d^2E}{dk^2}\Big|_{k=k_0} \right]^{-1}$

$$m^*_{qwell} = \hbar^2 \left([-2\beta a^2 \cos ka] \Big|_{k=0} \right)^{-1}$$

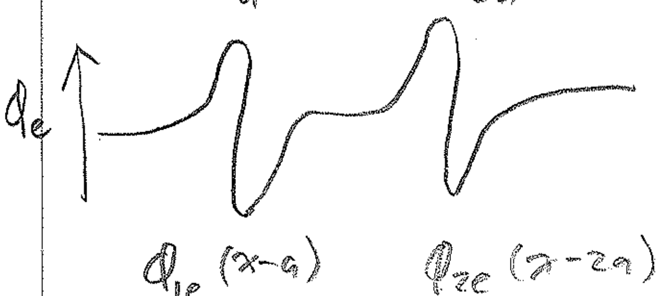
$$= -\frac{\hbar^2}{2\beta a^2}, \quad \text{recall } \beta < 0$$

Conduction band is a LCAO of excited states, $|1e\rangle, |2e\rangle, \ldots$



excited state w.f. are odd functions

$$\phi_e(-x) = -\phi_e(x)$$



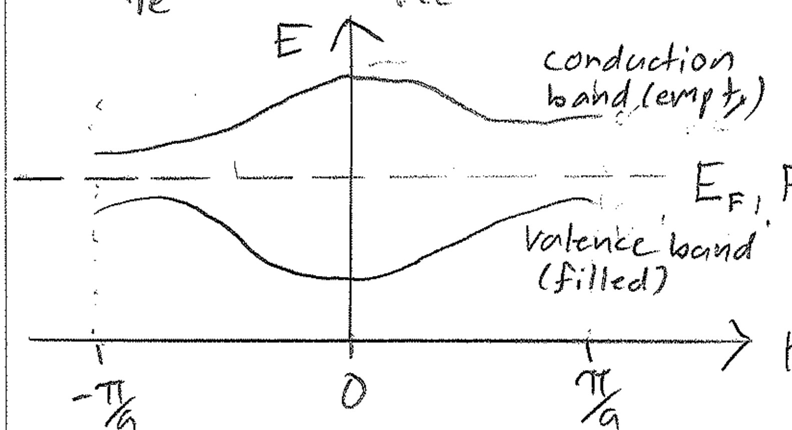
$$\Rightarrow \beta_e = \langle 2_e | \hat{H} | 1e \rangle$$

$$= \langle 2e | \hat{V}(x-a) | 1e \rangle$$

$$+ \langle 2e | \hat{V}(x-2a) | 1e \rangle$$

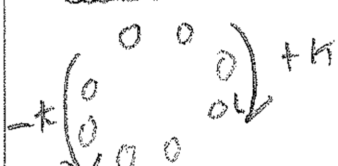
→ even

$$> 0$$



$$E_{gap} = (\alpha_e - 2\beta_e) - (\alpha - 2\beta)$$

Periodic boundar conditions: N sites $\Rightarrow c_1 = c_{N+1}$



$$\Rightarrow e^{ikNa} = 1$$

$$Nka = q\, 2\pi$$

$$\text{or } k_q = \frac{q}{N} \frac{2\pi}{a}$$

$\Rightarrow$ 1st Brillouin zone with periodic conditions is $-\frac{\pi}{a} \ldots \frac{\pi}{a}$

E_F **Fermi Energy**: the maximum occupied energy at $T = 0\,K$.

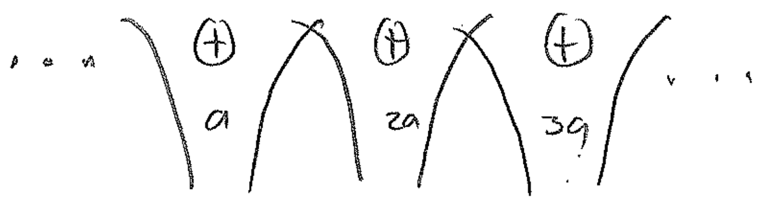
If E_F is in the band gap at $T = 0\,K$, the material is a semiconductor or insulator.

If if E_F lies within a band, it is a metal.

for $T > 0$, occupancy of given energy, E is given by Fermi-Dirac statistics:

$$\langle n_e \rangle = \frac{1}{e^{E/k_BT} + 1}$$

Example: consider a 1D system of hydrogen.



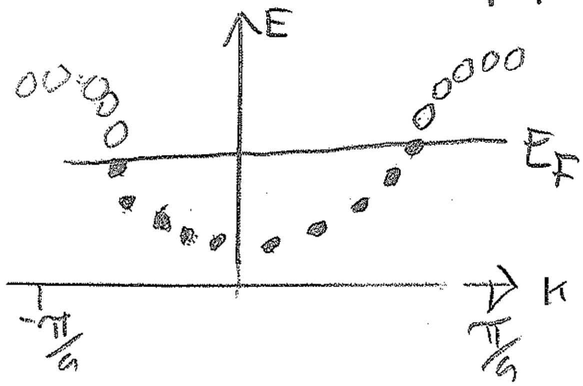
$$E = \alpha + 2\beta \cos ka$$

$$\psi_k = \sum_n e^{ikna}\, \varphi(\vec{r} - na)$$

↳ H wavefunc

$$\alpha = \langle 1_{1s} | \hat{H} | 1_{1s} \rangle$$
$$\simeq -13.6\ eV$$

Each hydrogen has only 1 electron, but $2e^-$ are allowed per site (1 spin up, 1 spin down) if hydrogen was a solid of 20 atoms, only 10 k modes would be populated.



Therefore 1D hydrogen is a metal, the Fermi energy lies in the band.

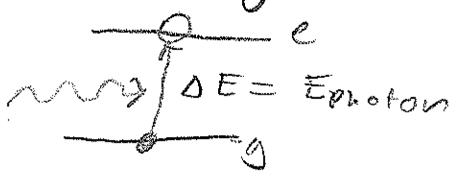
What about 1D helium?

each He has 2 electrons per atom, so 20 Helium atoms fill 20 k-modes, so the valence band is filled.

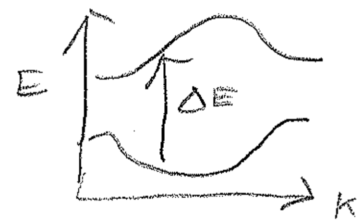
∴ 1D helium is an insulator.

Semiconductors are insulators with smaller band-gap where $E_{gap} \simeq$ energy of visible light, and can be thermally populated at room temperature to conduct electricity.

Atomic gas



Periodic system



ΔE must match an occupied and unoccupied eigenstate and conserve k, (i.e. photon momentum, $p = \hbar k$)

Semiconductors are further classified as direct vs. indirect. A <u>Direct Gap</u> occurs when the lowest point in the conduction band occurs at same k-value as the highest energy in the valence band.

Worksheet: within a band are the energies equally spaced? (100 atom handout)