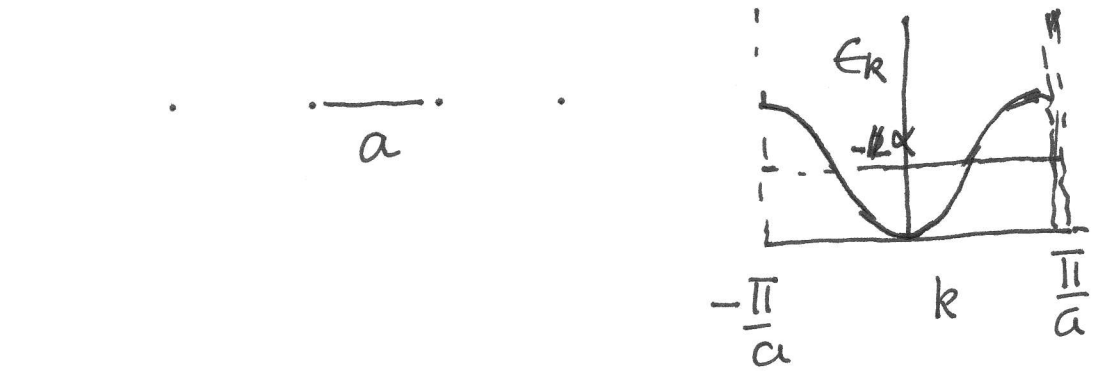
Effective mass of electrons in Tight Binding model

1. dimension

$$\epsilon_k = -\alpha - 2\gamma \cos ka$$



$-\alpha$ = Average energy.

γ = Hopping energy or tunneling matrix element.

$k \simeq 0$, $\quad \epsilon_k \cong -\alpha - 2\gamma\left(1 - \frac{k^2a^2}{2}\right)$

$$= (-\alpha - 2\gamma) + (\gamma a^2)k^2 = \epsilon_0 + \frac{\hbar^2}{2m^*}k^2$$

$$\frac{\hbar^2}{2m^*} = \gamma a^2 \Rightarrow m^* = \frac{\hbar^2}{2\gamma a^2} \Rightarrow m^* \propto \frac{1}{\gamma}$$

For a given a $\quad m^* \to \infty$ as $\gamma \to 0$ (no hopping)

Estimate of m^*/m_e

$$\frac{m^*}{m_e} = \frac{1}{2}\left(\frac{\hbar^2}{m_e a_B^2}\right)\cdot\left(\frac{a_B}{a}\right)^2 \cdot \frac{1}{\gamma} \qquad \text{Ryd.} \; \frac{\hbar^2}{2m_e a_B^2}$$

$$= \left(\frac{R}{\gamma}\right)\cdot\left(\frac{a_B}{a}\right)^2$$

$R = 13.6$ ev

$\gamma = 1$ ev

$a = 3\,A^0 \Rightarrow a/a_B = 6$

$$\frac{m^*}{m_e} = 13.6 \times \frac{1}{6^2} = 0.38$$ Medium

If $\gamma = 0.1$ ev : $m^*/m = 3.8$ (heavy fermion)

$\gamma = 0.01$, $m^*/m = 38$ (heavy fermions)

For $k \lesssim \pi/a$, $\tilde{K} = (\pi/a - k) \approx 0$

$$\epsilon_k = -\alpha - 2\gamma \cos ka = -\alpha - 2\gamma \cos(\pi - \tilde{K}a)$$
$$= -\alpha + 2\gamma \cos(\tilde{K}a)$$

$$\epsilon_k = -\alpha + 2\gamma\left(1 - \frac{\tilde{K}^2 a^2}{2}\right) = -\alpha + 2\gamma - \gamma a^2 \tilde{K}^2$$
$$= \epsilon_{\pi/a} + \frac{\hbar^2 \tilde{K}^2}{2m^*}$$

$$\hbar^2/2m^* = -\gamma a^2$$
$$\Rightarrow \quad m^* = -\frac{\hbar^2}{2\gamma a^2} < 0$$

Negative mass near the band maximum.

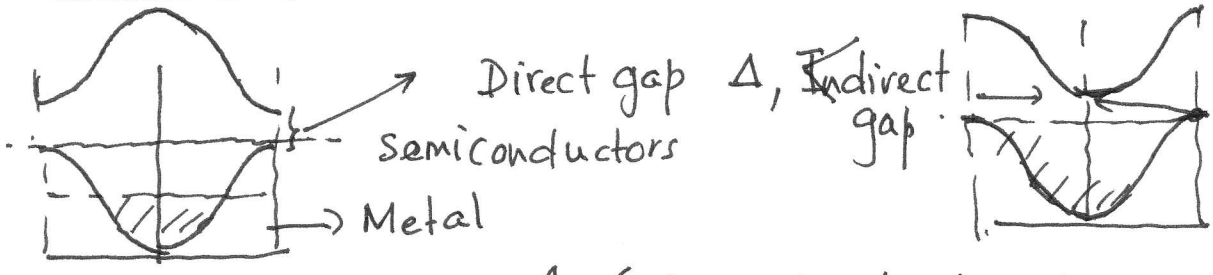
What does negative mass mean ?

$$\vec{F} = m^* \ddot{\vec{x}} = -e\vec{E}$$ $-e$ = electron charge

$$\ddot{x} = -\frac{e}{m^*} E = +\frac{e}{|m^*|} E$$

Dynamics of these electrons with $m^* < 0$, can be treated as positive mass particle with positve charge.

Metals, Semiconductors, Insulators.

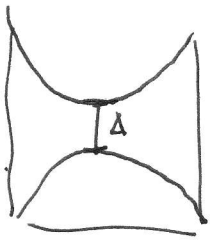


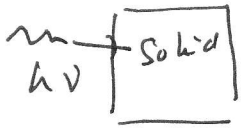
$\Delta \lesssim 1\text{-}2$ eV Semicond.

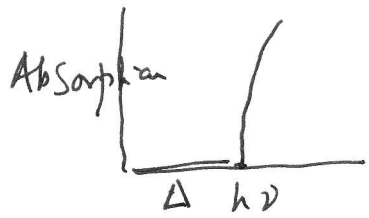
> 2 eV Insulator

How do you check band structure Experimentally

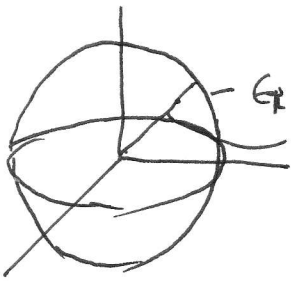
1. Band gaps (Semiconductors / Insulators)
   Optical absorption







2. Energy band dispersion $\epsilon_{\vec{k}}$
   Constant energy surfaces $\epsilon_{\vec{k}} = \epsilon$



$\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} = \epsilon$ (free electrons)

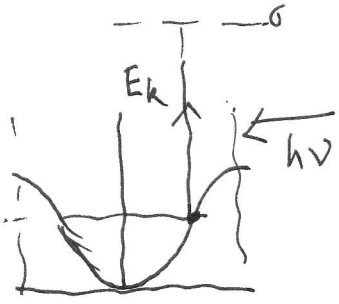
$\epsilon = \epsilon_F$, $k = k_F$: Fermi Surface

Sphere : 3d
Circle : 2d
Points : 1d

Expts:

① Cyclotron resonance
de Haas - van Alphen oscillations } Apply ext. $\vec{B}$

② Angle resolved photo-emission (ARPES)



$h\nu = E_{\vec{k}} + KE$ (+ work fn)

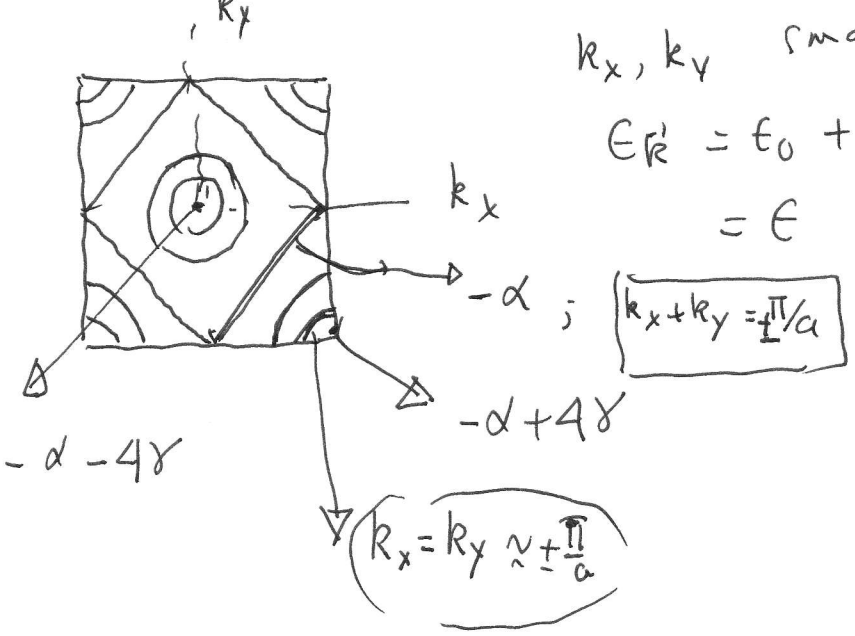
Picks up $\vec{k}$ → $\epsilon_{\vec{k}}$

Has become extremely powerful technique.

Constant Energy surfaces are NOT Spheres/circles in general (3d, 2d)

2d: Tight binding model / Square lattice

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



k_x, k_y small

$$\epsilon_{\vec{k}} = \epsilon_0 + \frac{\hbar^2 k^2}{2m^*}$$

$= \epsilon \Rightarrow$ Circles

Turns out $\boxed{\epsilon_F = -\alpha}$

Band is $\frac{1}{2}$-full.