Band structure

1. Bloch's theorem
2. Nearly free electron theory
3. Tight binding approach
4. Effective mass
5. Holes

1. Bloch's theorem

$$\begin{cases} \psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}}\, u_{\vec{k}}(\vec{r}) \\ u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}+\vec{R}) \end{cases} \qquad (1)$$

$$\vec{R} = n\vec{a} + m\vec{b} + p\vec{c}$$

Proof

1D

$$\psi(x+a) = C\,\psi(x) \qquad (2)$$

$$\psi(x+Na) \underset{(2)}{=} C^N \psi(x) = \psi(x) \qquad (3)$$

periodical condition

$$C^N \underset{(3)}{=} 1 \qquad (4)$$

$$C \underset{(4)}{=} e^{i\underbrace{\frac{2\pi}{N} m}_{ka}} \qquad k = \frac{2\pi}{a}\frac{m}{N} \qquad (5)$$

$$\psi(x+a) \underset{(5)}{=} e^{ika}\,\psi(x) \qquad (6)$$

3D

$$\psi_{\vec{k}}(\vec{r}+\vec{R}) \underset{\substack{\text{Similar}\\ \text{to (6)}}}{=} e^{i\vec{k}\cdot\vec{R}}\,\psi_{\vec{k}}(\vec{r}) \quad (7)$$

$$\left\{\begin{array}{ll}
\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}}\,u_{\vec{k}}(\vec{r}) & (8) \\
e^{i\vec{k}(\vec{r}+\vec{R})}\,u_{\vec{k}}(\bar{r}+\bar{R}) \underset{(7,8)}{=} e^{i\bar{k}\bar{R}}\,e^{i\bar{k}\bar{r}}\,u_k(\vec{r}) & (9) \\
u_k(\bar{r}+\bar{R}) \underset{(9)}{=} u_k(\vec{r}) & (10)
\end{array}\right.$$

Comp. (1,2)

$$\psi_{\vec{k}+\vec{K}}(\vec{r}+\vec{R}) = \underbrace{e^{i(\vec{k}+\vec{K})\cdot\vec{R}}}_{e^{i\vec{k}\cdot\vec{R}}}\,\psi_{\vec{k}+\vec{K}}(r) \quad (11)$$

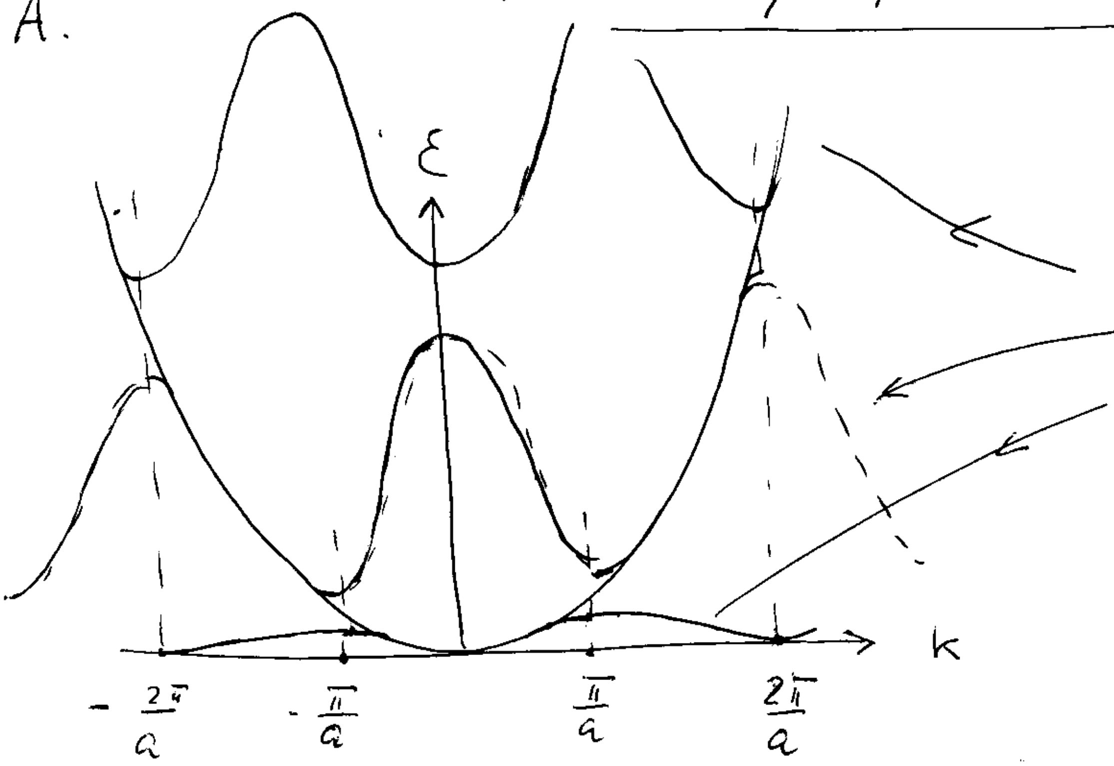
$$\left\{\begin{array}{ll}
\psi_{\vec{k}+\vec{K}}(\vec{r}) \underset{(11)}{\equiv} \psi_{\vec{k}}(\vec{r}) & (12) \\
\varepsilon_{\vec{k}+\vec{K}} \underset{(12)}{=} \varepsilon_{\vec{k}} & (13)
\end{array}\right.$$

$$\Downarrow$$

It suffices to consider the B zone (14)

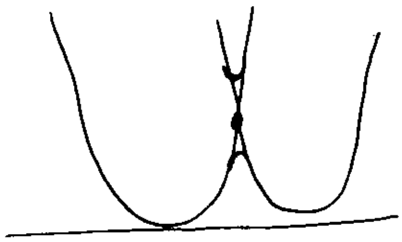
2. Nearly free electron theory

A.



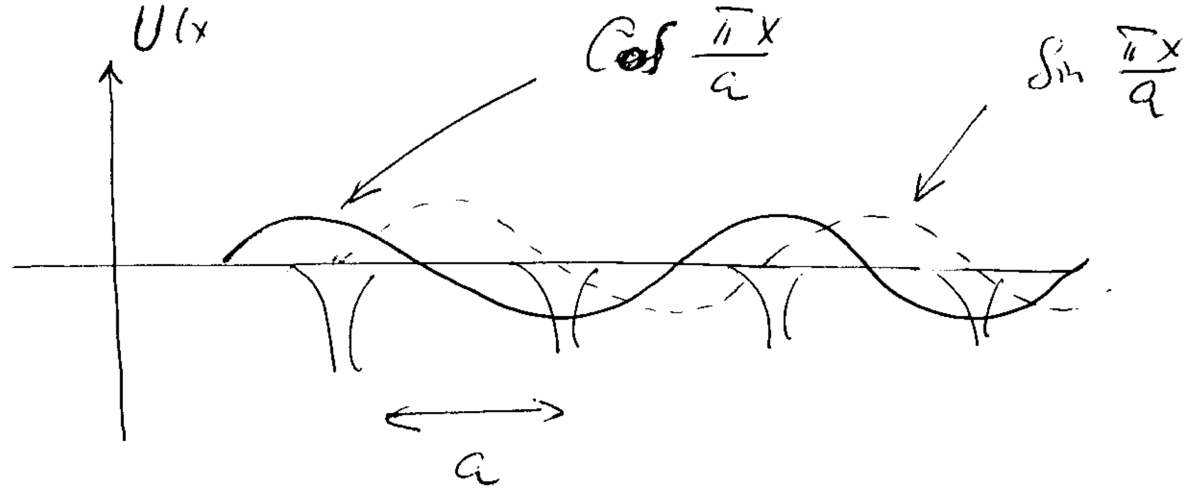
Repeated zone cheme

Reduced Zone cheme

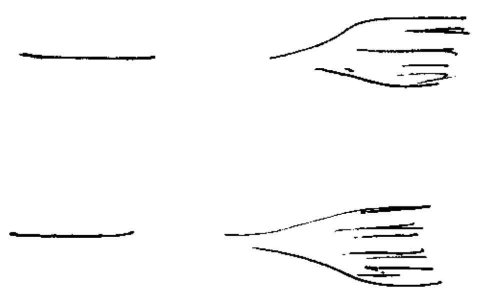


B. Compare Bragg reflection

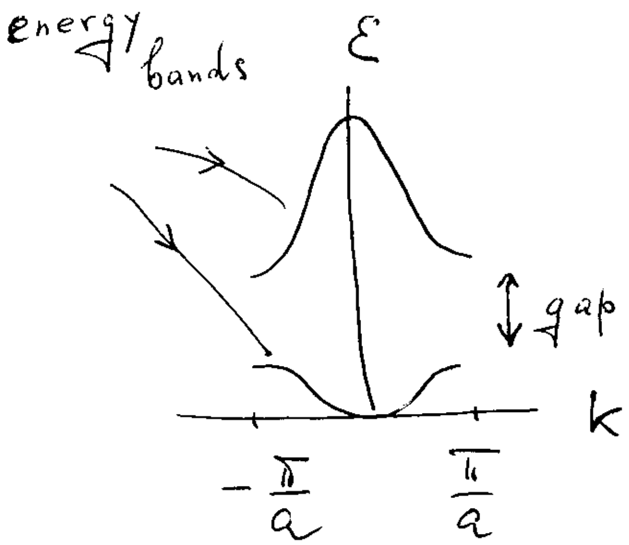
C.



D



Metals, insulators, semiconductors



gap $\gtrsim 5$ eV $\Rightarrow$ insulator

gap $\lesssim 2$ eV $\Rightarrow$ semiconductor

gap $= 0$ metal

Number of states

$$2 \sum_{k \in BZ} \Rightarrow 2 \int_{BZ} \frac{L\,dk}{2\pi} = 2 \frac{L}{2\pi} \frac{2\pi}{a} = \frac{L}{a} 2 = 2N$$

spin

In 1D

1. Odd number of electrons per cell – metal
2. Even number – insulator semiconductor

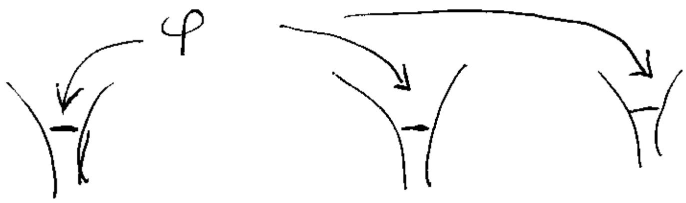
In 3D

1. Odd number of electrons in a primitive cell – metallic behaviour

2. Even – metal, insulator, semiconductor

3. Tight binding approach

1 D



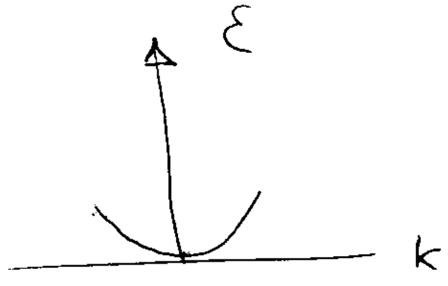
$$i\hbar \frac{d\psi_n}{dt} = E_0 \psi_n - V\psi_{n-1} - V\psi_{n+1}$$

$$\psi_n = C e^{i(k x_n - \omega t)}$$

$$x_n = na$$

$$\underbrace{\hbar\omega}_{\varepsilon} = E_0 - 2V \cos ka$$

4. Effective mass



$$\varepsilon = \frac{\hbar^2 k^2}{2m^*} = \frac{p^2}{2m^*} \qquad p = \hbar k$$

$$\frac{dv}{dt} = \frac{d}{dt}\left(\frac{d\varepsilon}{dp}\right) = \underbrace{\frac{d^2\varepsilon}{dp^2}}_{\frac{1}{m^*}} \frac{dp}{dt} = \frac{1}{m^*}(-eE)$$

$$\left.\begin{aligned} \delta\varepsilon &= -eE\,\delta x \\ \delta p &= \frac{dp}{d\varepsilon}\,\delta\varepsilon = \frac{1}{v}\,\delta\varepsilon \\ \frac{dp}{dt} &= \frac{1}{v}(-eE\,v) \end{aligned}\right\} \Rightarrow \frac{dp}{dt} = -eE$$

$$\boxed{m^* \frac{dv}{dt} = -eE}$$

5. Electrons, holes in semiconductors