LECTURE #16

Note Title 2/18/2009

ANNOUNCEMENT : MON FEB 23RD NO - CLASS

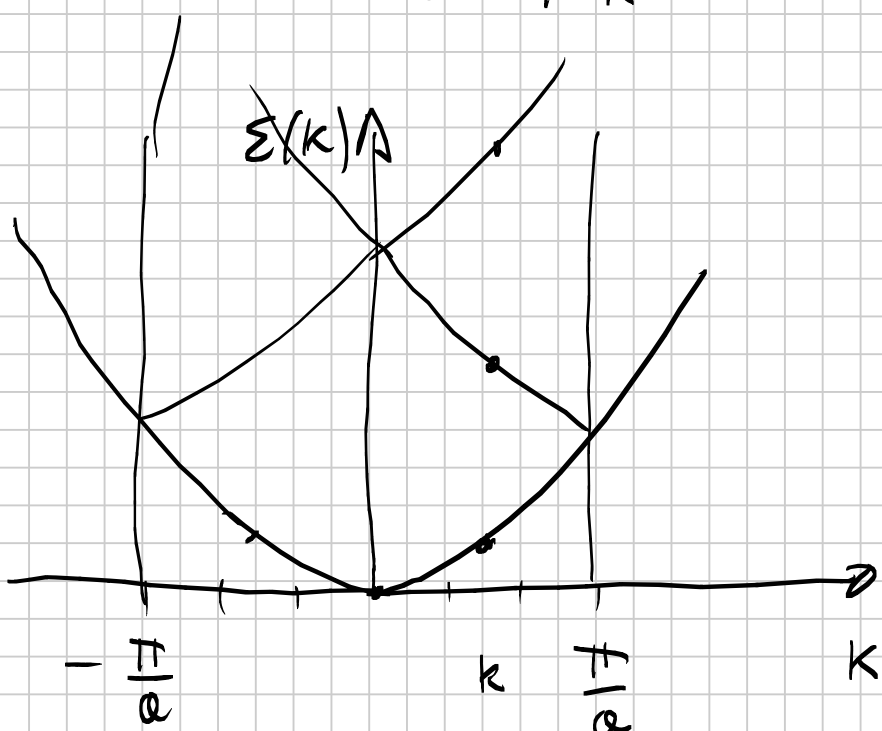
ELECTRONIC STATES IN SOLIDS

NEARLY - FREE ELECTRONS APPROX

PERIODIC

K CRYSTAL MOMENTUM → MANY $\psi_{nK} = e^{iK \cdot r} u_{nK}(\vec{r})$

BAND FOLDING



PERTURBATION THEORY

$\tilde{V}$ IS THE FOURIER T OF THE ION POTENTIAL

FIX K

$$\varepsilon(k) = \underbrace{\frac{\hbar^2 k^2}{2m}}_{\varepsilon^{(0)}(k)} + C + \sum_{G_m} \frac{|\tilde{V}(G_m)|^2}{\varepsilon^{0}(k) - \varepsilon^{(0)}(k+G_m)} + O(V^3)$$

MARTIN'S QUESTION : WHAT ABOUT $-k$?

$$\Delta\varepsilon^{(2)}(k) \sim \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{\varepsilon - \varepsilon'}$$

$\langle k|V|k'\rangle \neq 0$ ONLY IF $k - k' = G_m$

IF I HAD $-K$

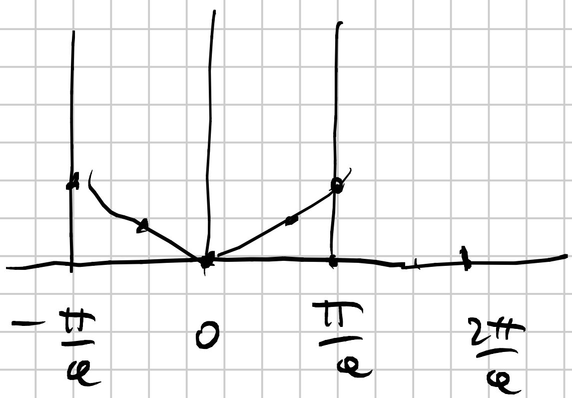
$$\sum_{k} \langle k|V|k'\rangle\langle k'|V|-k\rangle$$

$\langle k | V | k' \rangle \neq 0 \qquad k - k' = G_m$

$\langle k' | V | -k \rangle \neq 0 \qquad k' + k = G_m'$

$2k = G_m'' \qquad k = \dfrac{G_m}{2}$

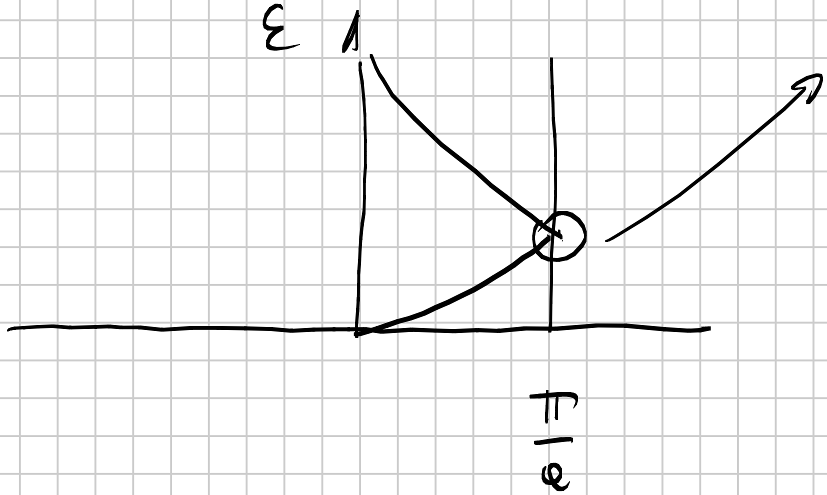
$\Downarrow$



$$\boxed{\text{THIS HAPPENS ONLY AT THE BZ BOUNDARIES}}$$

DEGENERATE STATES AT BZ BOUNDARIES

1° ORDER DEGENERATE PERTURBATION THEORY



$$\psi_1 = \frac{1}{\sqrt{L}} e^{i\frac{\pi}{a}x}$$

$$\psi_2 = \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{a}x}$$

V IONS

1° ORDER PT

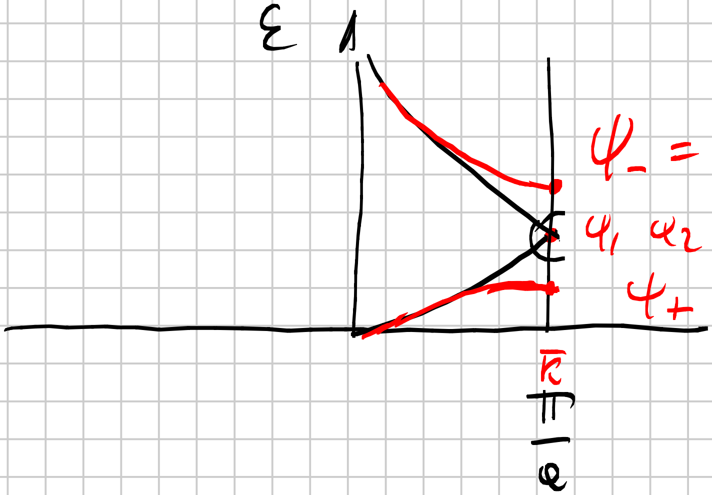
$$\begin{vmatrix} \langle \psi_1 | V | \psi_1 \rangle & \langle \psi_1 | V | \psi_2 \rangle \\ \langle \psi_2 | V | \psi_1 \rangle & \langle \psi_2 | V | \psi_2 \end{vmatrix} \xrightarrow{\text{DIAGONALIZE}} \Delta E^{(1)}$$

$$\langle \psi_1 | V | \psi_1 \rangle = \frac{1}{L} \int e^{\cancel{-i\frac{\pi}{a}x}} V(x)\, e^{\cancel{i\frac{\pi}{a}x}} \, dx = C$$

$$= \langle \psi_2 | V | \psi_2 \rangle$$

$$\langle \psi_1 | V | \psi_2 \rangle = \frac{1}{L} \int e^{-i\frac{2\pi}{a}x} V(x)\, dx = \tilde{V}\left(k = \frac{2\pi}{a}\right)$$

$$\Delta E = \begin{bmatrix} c & \tilde{V}\left(\frac{2\pi}{a}\right) \\ \tilde{V}\left(\frac{2\pi}{a}\right) & c \end{bmatrix} \to c \pm \tilde{V}\left(\frac{2\pi}{a}\right)$$

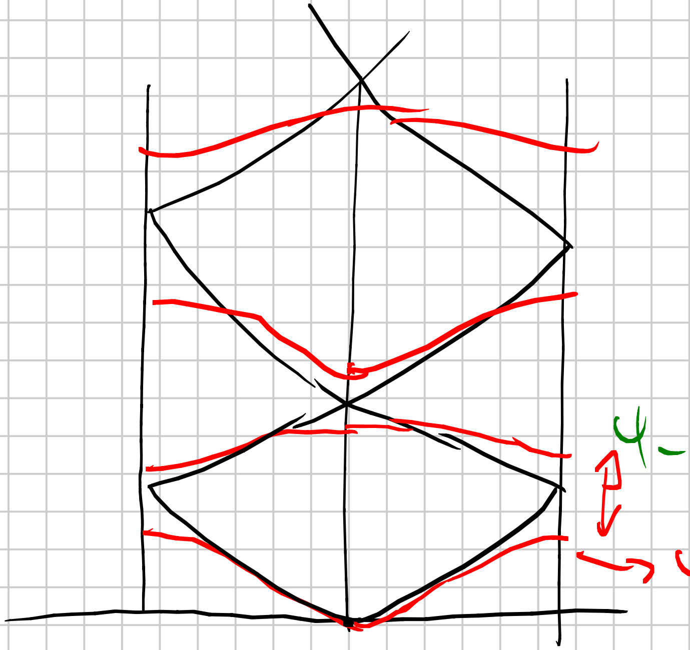


$$\psi_- = (\psi_1 - \psi_2) \frac{1}{\sqrt{2}}$$

$$\psi_+ = (\psi_1 + \psi_2)/\sqrt{2}$$

$$2\tilde{V}\left(\frac{2\pi}{a}\right)$$

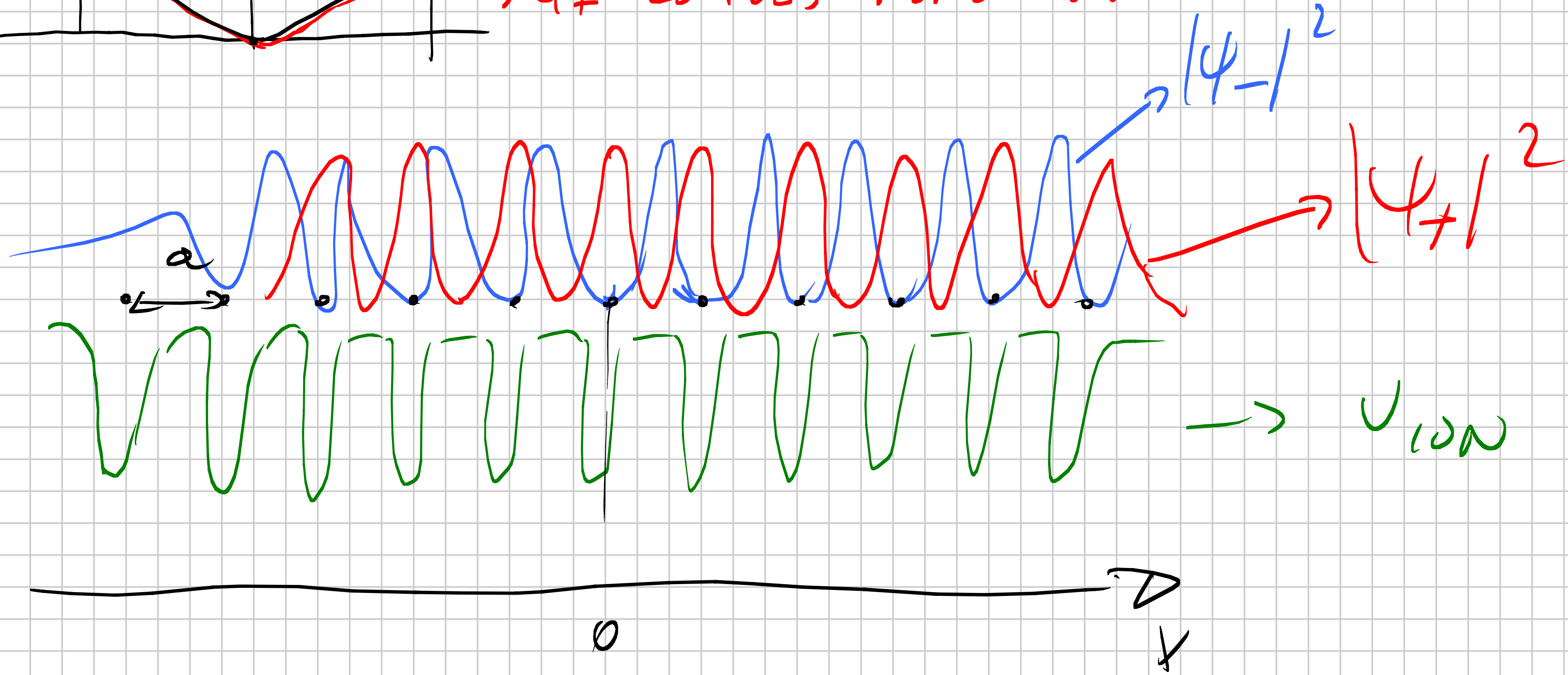
$$2\bar{k} = G_m$$



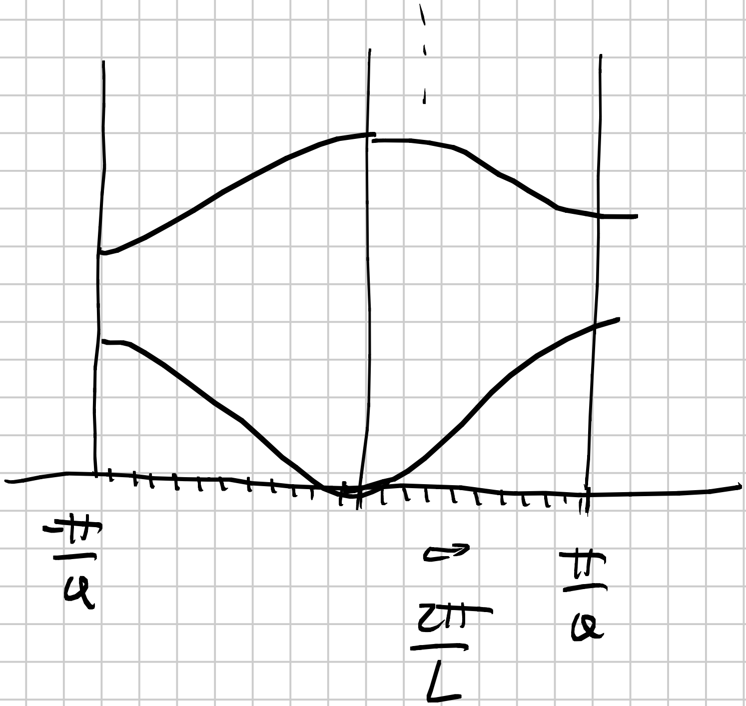
$$\psi_- \sim e^{i\frac{\pi}{a}x} - e^{-i\frac{\pi}{a}x} \sim \sin\frac{\pi}{a}x$$

$$\psi_+ \sim e^{i\frac{\pi}{a}x} + e^{-i\frac{\pi}{a}x} \sim \cos\frac{\pi}{a}x$$

$\to \psi_+$ COUPLES MORE WITH V_{ION}



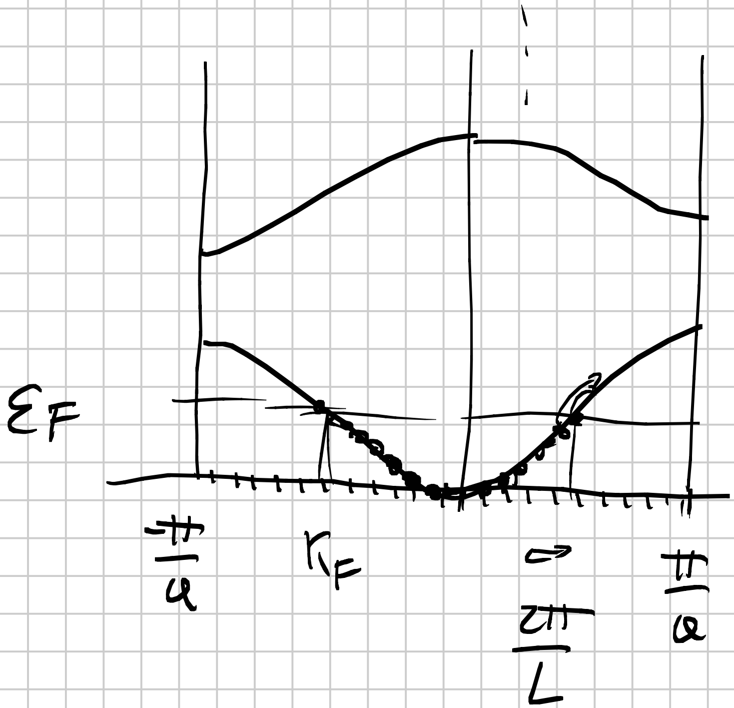
TOTAL LENGTH L



NUMBER OF K STATES IS THE SAME AS # OF IONS

$$\# \text{ K STATES} = \frac{\frac{2\pi}{a}}{\frac{2\pi}{L}} = \frac{L}{a} = \# \text{ IONS}$$

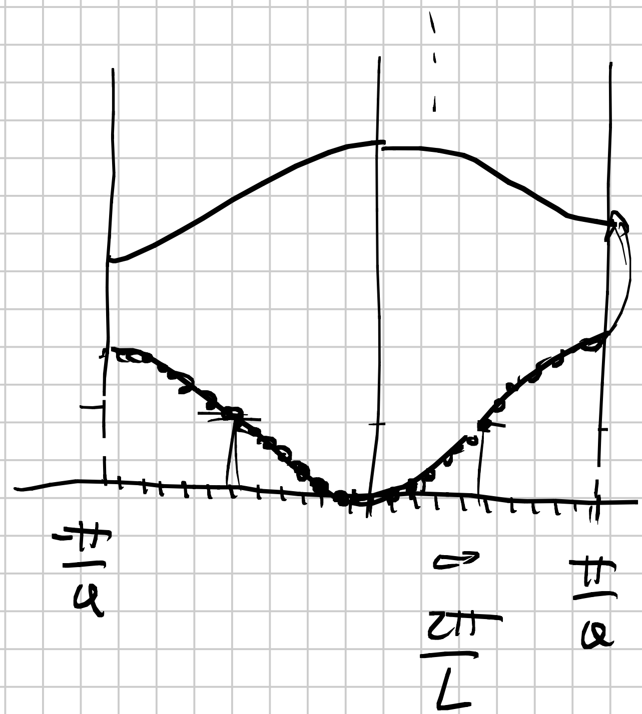
CASE 1 $\quad \# e = \# \text{ IONS} \quad$ 1e PER ATOM



METAL (BAND PARTIALLY FILLED WITH ELECTRONS)

2 e PER ION

INSULATOR

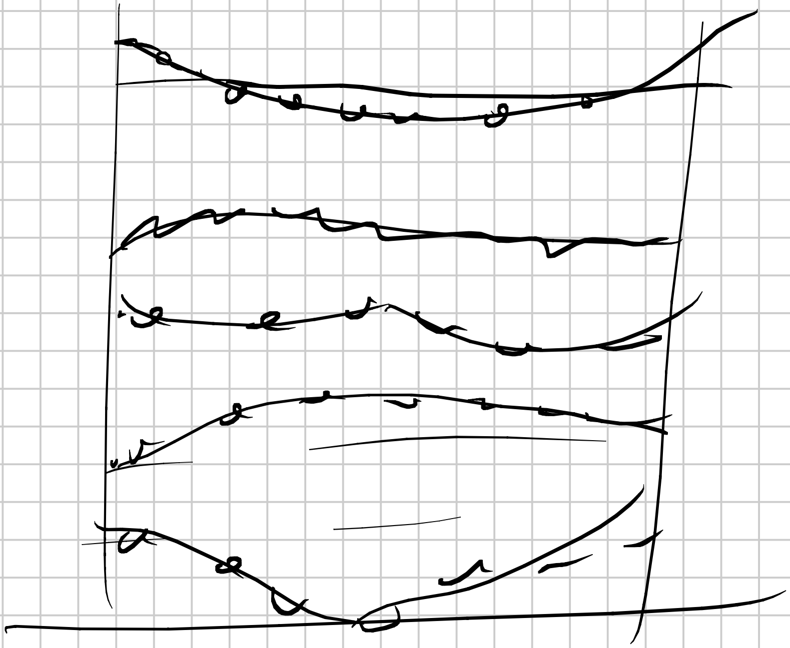


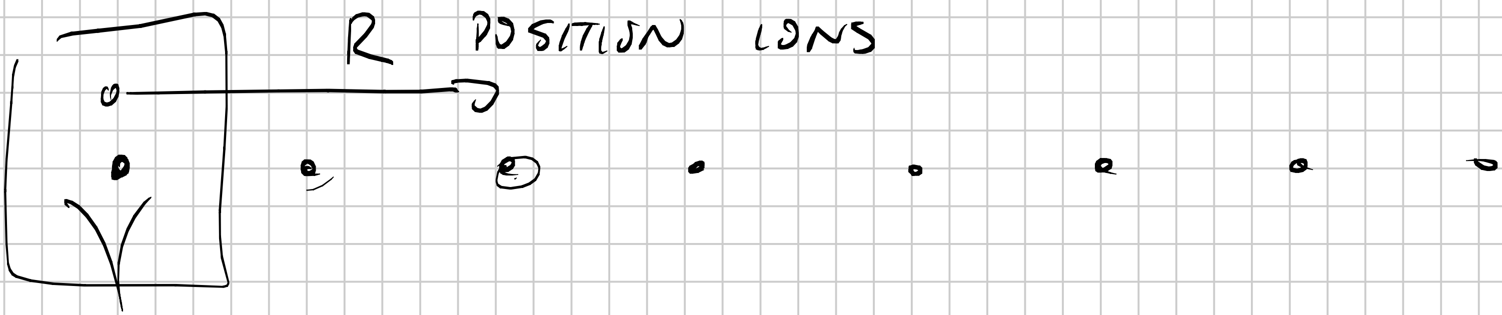
$V \gg k_B T$

INSULATOR

$V \sim k_B T$

SEMICONDUCTOR



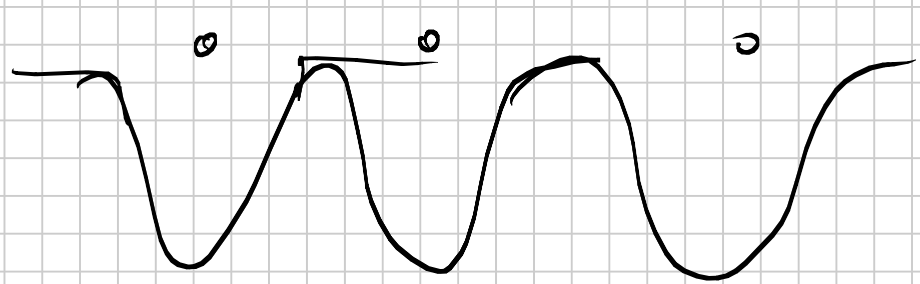


SINGLE ATOM

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{AT}(\vec{r})\right)\varphi_n(\vec{r}) = \varepsilon_n(\vec{r})$$

FULL CRYSTAL POTENTIAL V

$$V = \sum_{\vec{R}} V_{AT}(\vec{r} - \vec{R})$$



BASIS:

$$\psi_{Km} = \sum_{R} e^{iK\cdot\vec{R}} \underbrace{\varphi_m(\vec{r} - \vec{R})}$$

BLOCH FUNCTIONS