LECTURE # 14

Note Title 10/24/2007

LATTICE $\vec{R}_i$

$$V_{ions}(\vec{r} + \vec{R}_i) = V_{ions}(\vec{r}) \quad \forall \vec{R}_i$$

due to protons & core electrons

Solve 1 electron problem

$$\left(-\frac{\hbar^2 \vec{\nabla}^2}{2m} + V_{ions}(r)\right)\psi(\vec{r}) = E\psi(\vec{r})$$

BLOCH'S THEOREM

$$\psi_{nk}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{nk}(r)$$

$$u_{nk}(\vec{r} + \vec{R}_i) = u_{nk}(\vec{r})$$

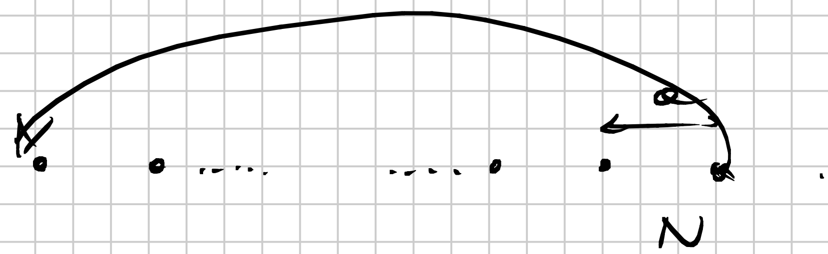
$$\Longleftrightarrow$$

$$\psi_{nk}(\vec{r} + \vec{R}_i) = e^{i\vec{k}\cdot\vec{R}_i}\psi_{nk}(\vec{r})$$

PROOFS NOT REQUIRED

POSSIBLE VALUES FOR K!

BORN VON KARMANN BOUNDARY CONDITION



N total # of unit cells

$$\psi_{mk}(x+Na) \equiv \psi_{mk}(x)$$

$$e^{ikNa}\,\psi_{mk}(x) \Rightarrow e^{ikNa} = 1$$

$$K = \overset{b_1}{\frac{2\pi}{a}}\,\frac{m}{N} \qquad 0 \le m < N$$

m integer

3D

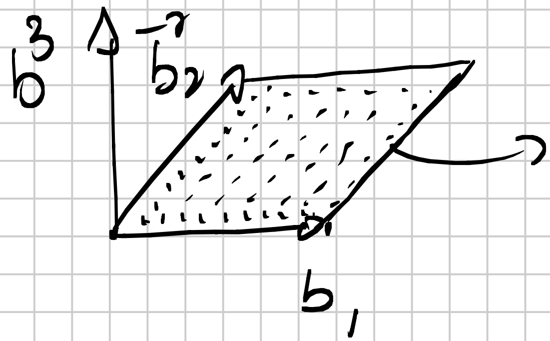
$$\psi_{m\vec{k}}(\vec{r} + N\vec{a}_i) = \psi_{mk}(\vec{r})$$

$$\vec{a}_i \left\{ \begin{array}{l} \vec{a}_1 \\ \vec{a}_2 \\ \vec{a}_3 \end{array} \right.$$

PRIMITIVE VECTORS

$$\vec{k} = \frac{m_1}{N}\vec{b}_1 + \frac{m_2}{N}\vec{b}_2 + \frac{m_3}{N}\vec{b}_3$$

$$\left.\begin{array}{l} b_1 \\ b_2 \\ b_3 \end{array}\right\}$$ PRIMITIVE VECTORS OF REC LATTICE



N^3 possible values for k

$$\boxed{\#\ \text{K POINTS} \equiv \#\ \text{UNIT CELLS}}$$

What is $\vec{k}$?

Good quantum number

$$\boxed{\psi_k(r+\underline{\vec{R}}) \to e^{ik\cdot \underline{R}}\,\psi_k(\vec{r})}$$

In the free space:

p good quantum number

$$\psi_p(\vec{r}+\underline{\underline{\vec{r}'}}) \to e^{ip\cdot\vec{r}'}\psi_p(\vec{r})$$

K is "similar" to particle momentum but not exactly the same

$-i\hbar\vec{\nabla} = \hat{p}$ real momentum

$e^{i\vec{k}\cdot\vec{r}}\, u_{nn}(\vec{r})$ is not eigenstate of $\hat{p}$

$\vec{K}$ is crystal momentum $\neq$ momentum p

$$-i\hbar\vec{\nabla}\Big(\underbrace{e^{i\vec{k}\cdot\vec{r}}\,u(r)}_{\psi_{km}}\Big) \to \hbar k\,\psi_{km}\ \underbrace{-i\hbar\,e^{i\vec{k}\cdot\vec{r}}\,\vec{\nabla}u(r)}$$

$\Rightarrow$ ψ_{mk} not eigenstate of $\hat{p}$

$\vec{k} + \vec{K}$ ADD Reciprocal lattice vector

$\parallel$

$\vec{k}$

$$\underbrace{\psi_{m\,k+K}(\vec{r}+\vec{R}_i)} = e^{i\vec{k}\cdot\vec{R}_i}\ \overset{=1}{\boxed{e^{i\vec{K}\cdot\vec{R}_i}}}\ \underbrace{\psi_{m\,k+K}(\vec{r})}$$

$$\psi_{mk}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}_i}\ \psi_{mk}(\vec{r})$$

$$\Rightarrow \boxed{\psi_{m\,k+K} = \psi_{mk}}$$

$k \rightarrow k + K$ SAME STATE

$\Rightarrow \boxed{E(k + K) = E(k)}$ ENERGY

1 e^- Energy is PERIODIC in the Reciprocal lattice

Restrict k only in 1 unit cell of reciprocal lattice $\Rightarrow$ 1° Brillouin Zone

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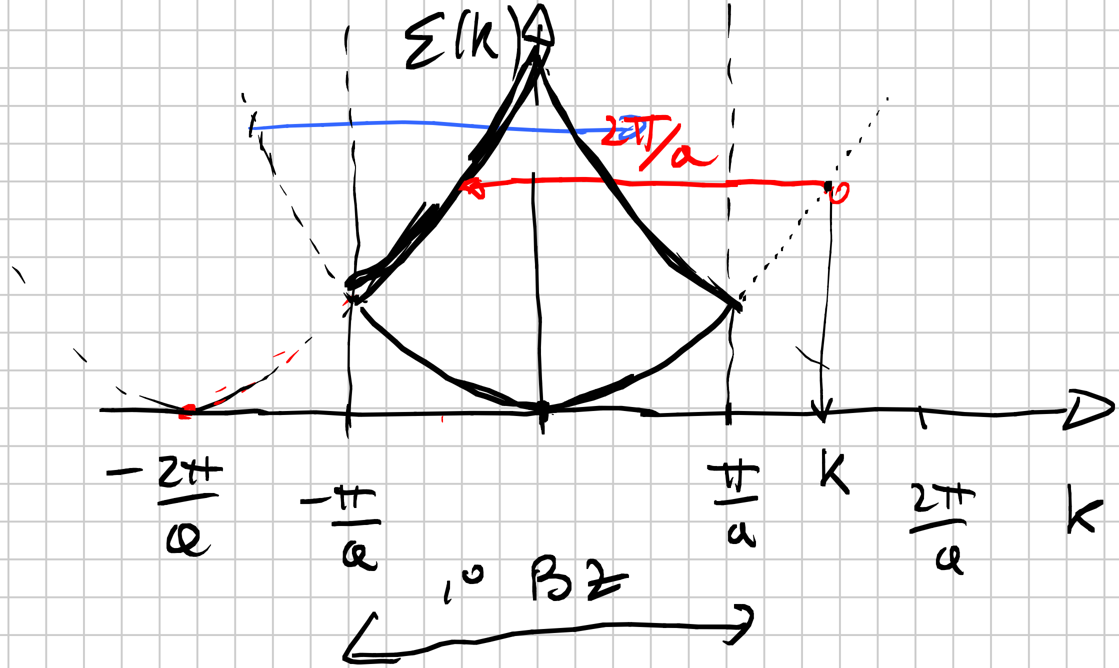
$E(K)$ ASSUME V_{ions} VERY SMALL

1D System

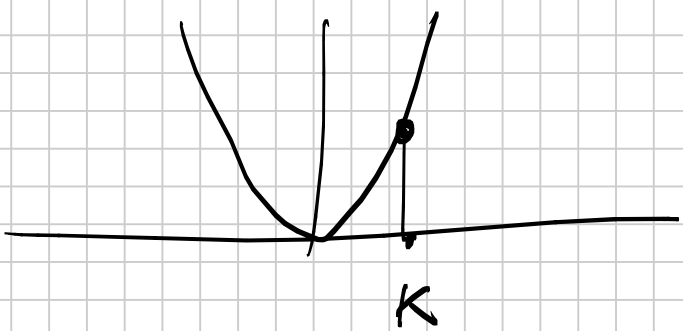
$\psi_{nk} \sim e^{i\vec{k}\cdot\vec{r}}$ $E(k) \sim \frac{\hbar^2 k^2}{2m}$



$K = \frac{2\pi}{a}$

$\mathcal{E}(k) = \mathcal{E}\left(k + \frac{2\pi}{a}\right)$

Free case

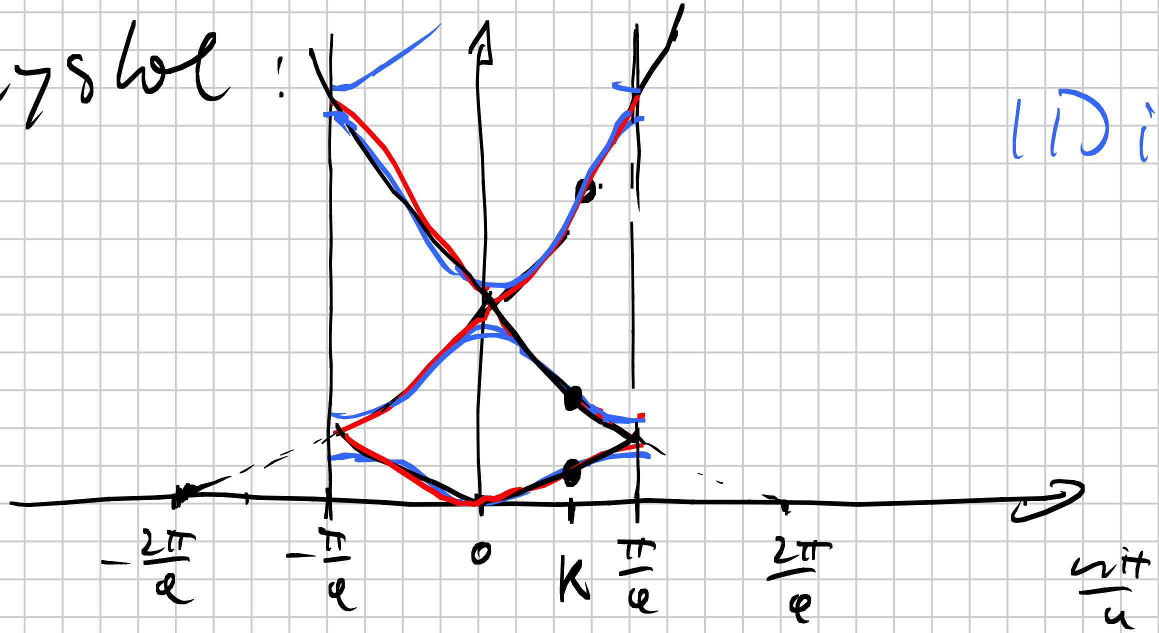


$k \rightarrow \frac{\hbar^2 k^2}{2m}$ | Energy.

$\downarrow$

$\hbar k$ momentum

Crystal :



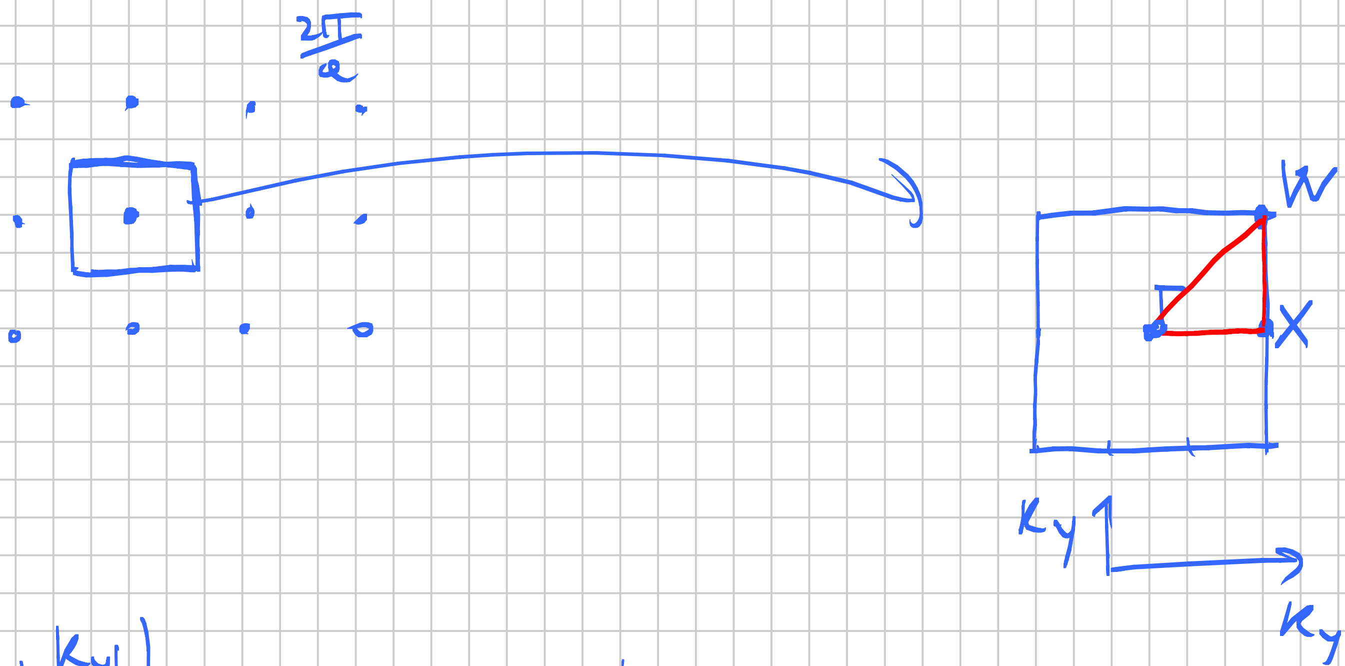
1Dimensional system.

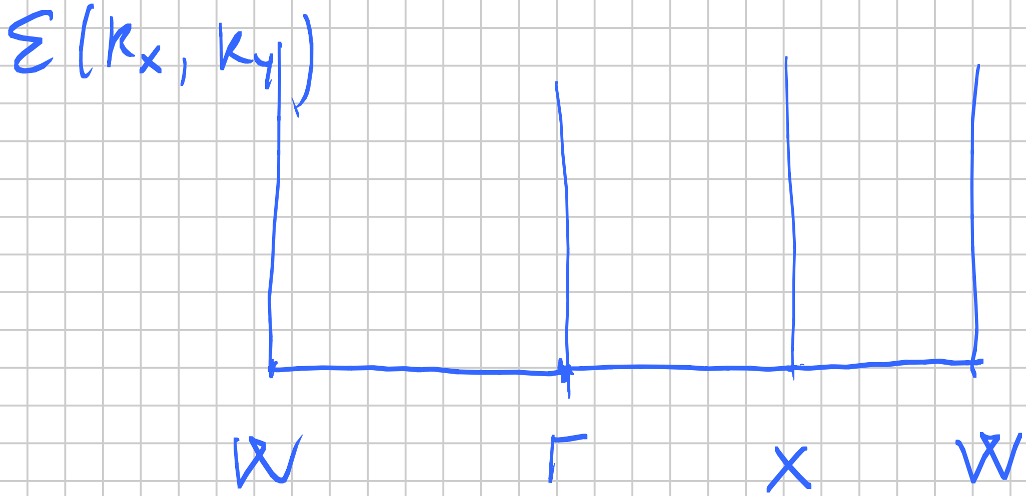
$$k \to \underset{\varepsilon_1}{\frac{\hbar^2 k^2}{2m}}, \quad \underset{\varepsilon_2}{\frac{\hbar^2 \left(k - \frac{2\pi}{a}\right)^2}{2m}}, \quad \underset{\varepsilon_3}{\frac{\hbar^2 \left(k + \frac{2\pi}{a}\right)^2}{2m}}, \ \dots$$

ε_1 ε_2 ε_3 MAKE THE

BANDS OF THE CRYSTAL

$\boxed{\text{2 D System}}$ NEARLY FREE ELECTRON





$$\varepsilon^0(k_x,k_y) = \frac{\hbar^2 (k_x^2+k_y^2)}{2m}$$