LECTURE #16

Note Title 10/27/2008

Chapt 4 - 5 - 6

~~Chap 7~~

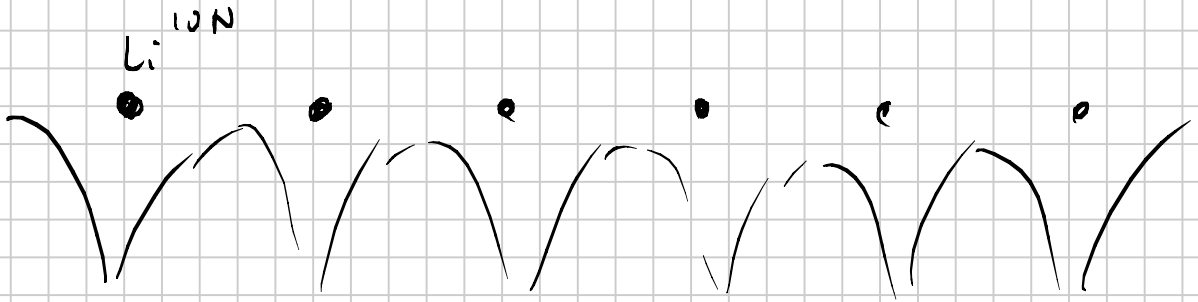
Chap 8

Li METAL BCC STRUCTURE

ELECTRONIC PROPERTIES

Li → $(1s)^2 (2s)$

V_{ION} POTENTIAL ON 2S È DUE TO 3 PROTONS + 2 1S ELECTRONS



→ PERIODIC POTENTIAL

I WANT TO SOLVE THE PROBLEM OF 1 ELECTRON MOVING IN THE POTENTIAL OF THE IONS $\Rightarrow$ ELECTRONIC STRUCTURE PROBLEM

SCHROEDINGER EQUATION FOR 1 ELECTRON

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

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

DESCRIBING BRAVAIS LATTICE

V_{ION} IS PERIODIC

$\psi_m \quad E_m$

MOST IMPORTANT THEOREM IN CONDENSED MATTER PHYSICS

BLOCH'S THEOREM

GIVEN ELECTRON MOVING IN THE PERIODIC POTENTIAL $V_{ION}(\vec{r})$

EIGENSTATES ARE ALWAYS OF THE FORM

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r}) \qquad \text{WITH}$$

$$u_{n\vec{k}}(\vec{r}+\vec{R}_i) = u_{n\vec{k}}(\vec{r}) \quad \forall\ R_i$$

(I.E. u IS A PERIODIC FUNCTION)

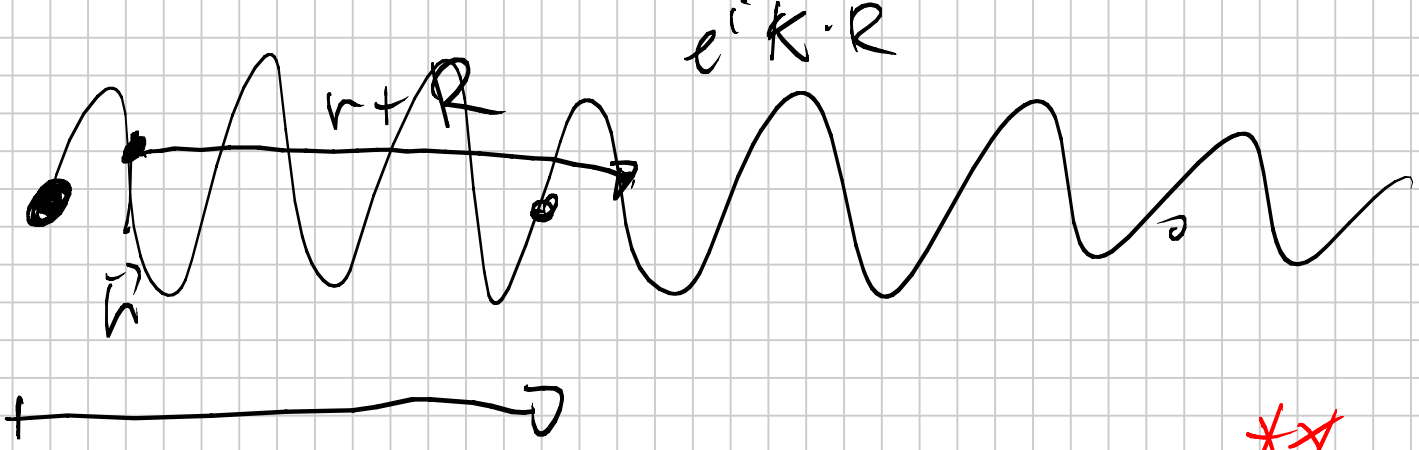
$\vec{k} = (k_x, k_y, k_z)$ IS A QUANTUM NUMBER CALLED "CRYSTAL MOMENTUM".

$\psi_{n\vec{k}}(\vec{r})$ IS NOT PERIODIC

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

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

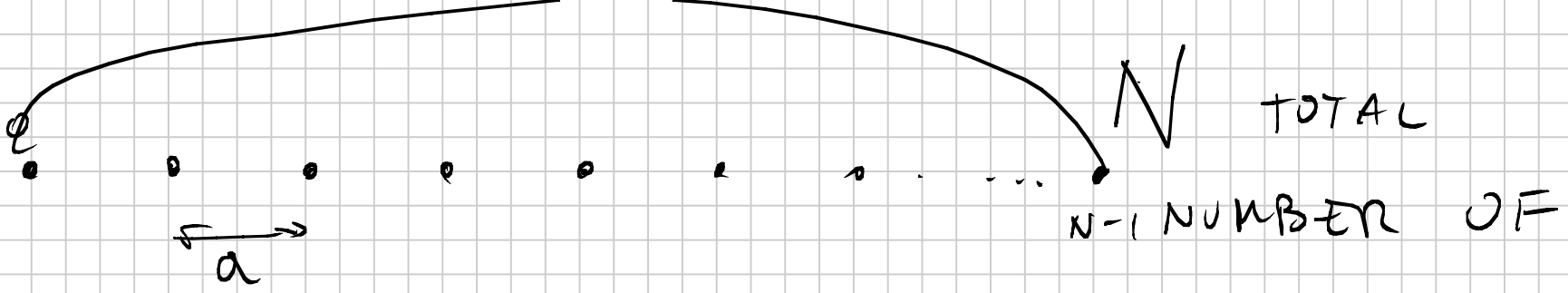
$\vec{k}$ TELLS ME HOW WAVEFUNCTION CHANGE UNDER A TRANSLATION OF $\vec{R}$.

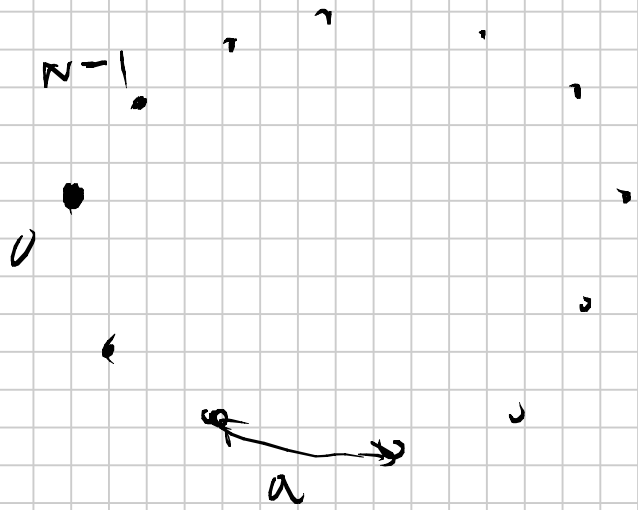


$$\psi_{m\vec{K}}(\vec{r}+\vec{R}) = e^{i\vec{K}\cdot\vec{R}}\,\psi_{m\vec{K}}(\vec{r}) \quad **$$

POSSIBLE VALUES FOR $\vec{K}$?

BORN - VON KARMANN BOUNDARY CONDITIONS





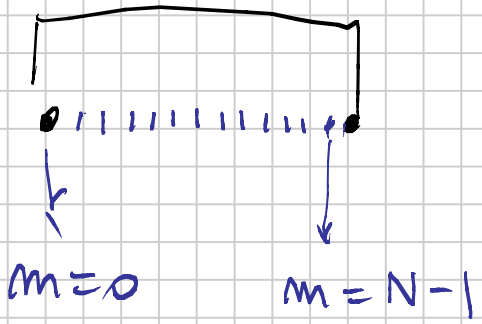
RING

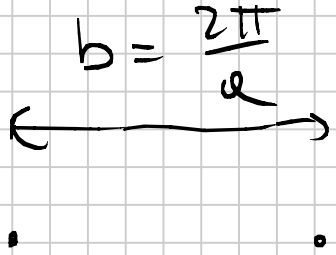
$$\psi_{nk}(x + Na) = \psi_{nk}(x) \qquad \text{USING } (**) \Rightarrow$$

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

$$kNa = 2\pi m$$

$$K = \left(\frac{2\pi}{a}\right)\frac{m}{N}, \qquad K = b\,\frac{m}{N}$$





ON EACH UNIT CELL OF THE RECIPROCAL LATTICE I HAVE THE SAME NUMBER OF K POINTS WHICH IS EQUAL TO N

(TOTAL NUMBER OF UNIT CELLS IN CRYSTAL)

3 DIMENSIONS $\vec{a}_1, \vec{a}_2, \vec{a}_3$

BORN VON KARMANN BOUNDARY CONDITION

FOR EACH OF 3 DIRECTIONS DEFINED BY

$\vec{a}_1, \vec{a}_2, \vec{a}_3$ TOTAL # UNIT CELLS N^3

$$\psi_{m\vec{k}}(\vec{r} + N\vec{a}_1) = \psi_{m\vec{k}}(\vec{r})$$

$\vec{b}_1, \vec{b}_2, \vec{b}_3$ PRIMITIVE VECTORS RECIPROCAL LATTICE

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

K POINTS IN A UNIT CELL OF THE REC LATICE $=$ TOTAL # OF UNIT CELLS (N^3)

WHAT IS $\vec{k}$? CRYSTAL MOMENTUM

IN THE FREE SPACE

P IS A GOOD QUANTUM NUMBER

$$\psi_p(\vec{r} + \vec{r}') = e^{i\frac{p}{\hbar}\cdot\vec{r}'}\,\psi_p(\vec{r})$$

IN A CRYSTAL

$$\psi_k(\vec{r} + \vec{R}_i) = e^{ik\cdot R_i}\,\psi_k(\vec{r})$$

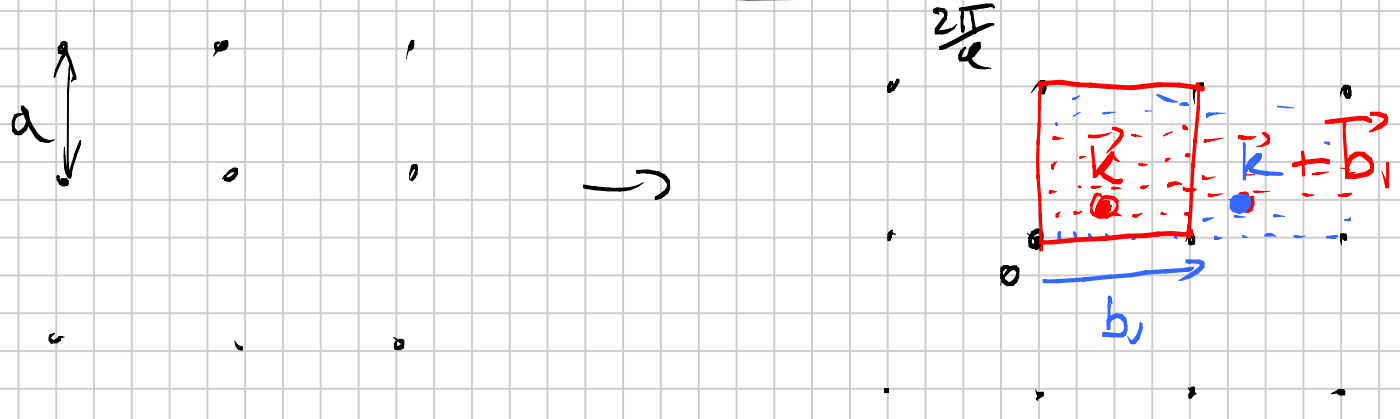
$\vec{k}$ IS NOT THE LINEAR MOMENTUM OF THE ELECTON

$$\vec{p} = -i\hbar\vec{\nabla}_r \qquad \text{LINEAR MOMENTUM}$$

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

IS $\psi_{n\vec{k}}(\vec{r})$ EIGENSTATE OF $-i\hbar\vec{\nabla}$?

$$-i\hbar\vec{\nabla}\left(e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r})\right) = \hbar k\, \psi_{km} - i\hbar e^{i\vec{k}\cdot\vec{r}}\vec{\nabla} u$$



WHAT HAPPENS TO THE QUANTUM # $\vec{K}$ WHEN I ADD A RECIPROCAL LATTICE VECTOR $\vec{K}$?

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

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

(1) $\vec{k}$ AND $\vec{k}+\vec{K}_j$ DEFINE THE SAME QUANTUM #

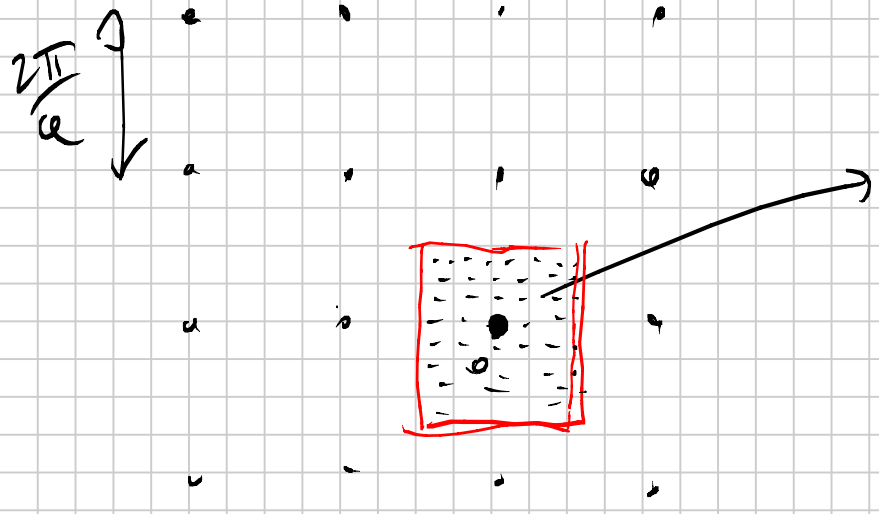
(2) $\psi_{m\,\vec{k}+\vec{K}_j} = \psi_{m\vec{k}}$ $\forall \vec{K}_j$ IN RECIPROCAL LATTICE

(3) $E_m(\vec{k}+\vec{K}) = E(\vec{k})$

ENERGY IS PERIODIC IN THE RECIPROCAL LATTICE

LOOK ONLY AT K IN ONE UNIT CELL OF THE RECIPROCAL

LATTICE

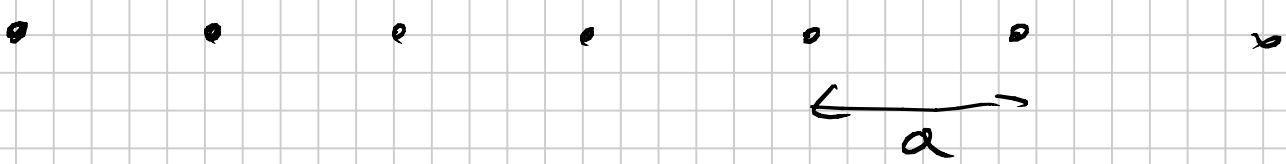


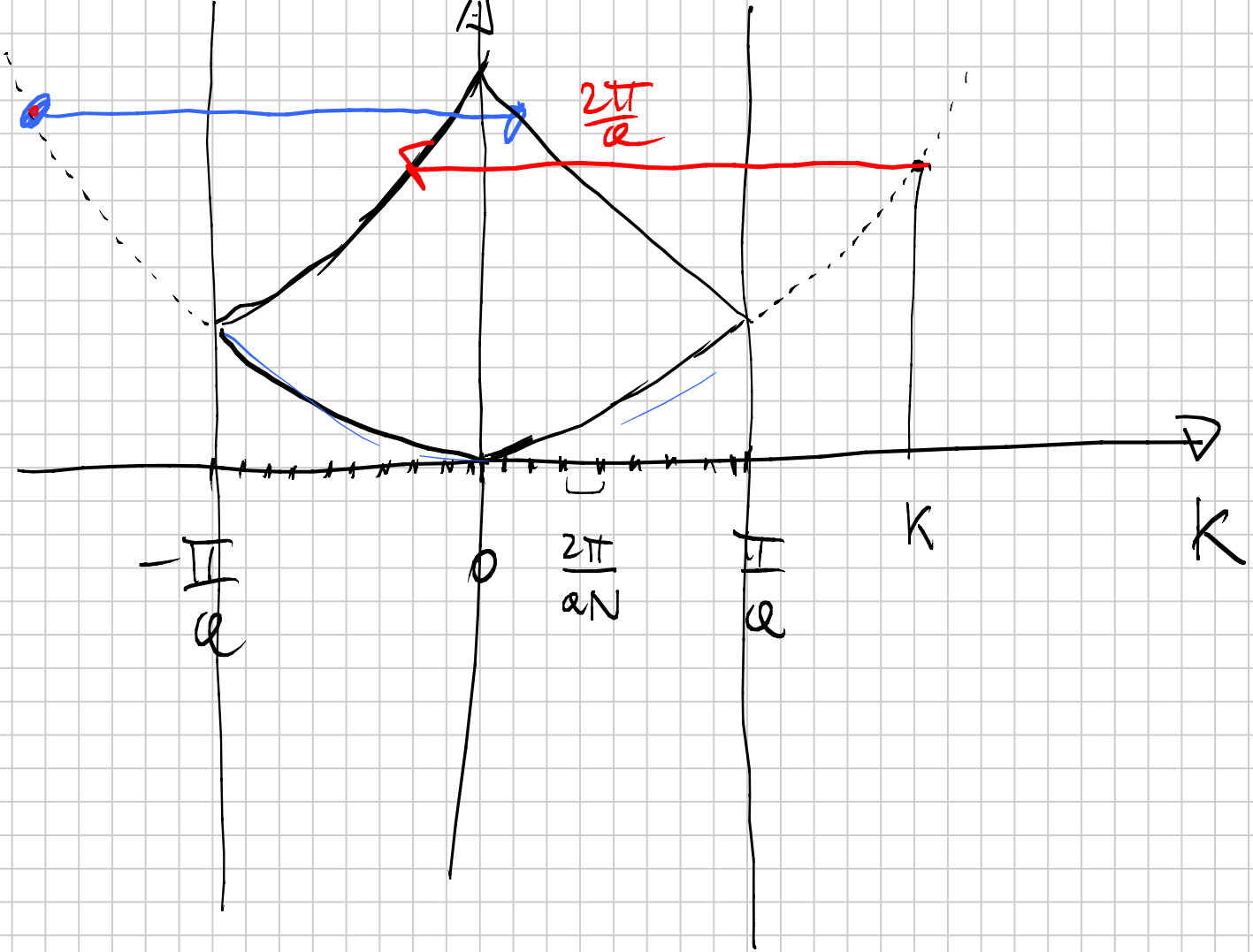
RESTRICT DESCRIPTION OF ELECTRONIC STATES ONLY TO 1° BRILLOUIN ZONE

V_{ION} VERY WEAK

$\psi_{nk} \sim e^{ikx}$

$E \sim \frac{\hbar^2 k^2}{2m}$




$\frac{2\pi}{a}$
$-\frac{\pi}{a}$
0
$\frac{2\pi}{aN}$
$\frac{\pi}{a}$
K
K