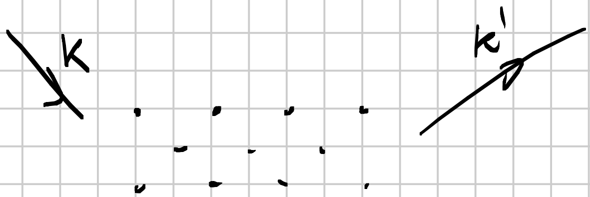
LECTURE #13

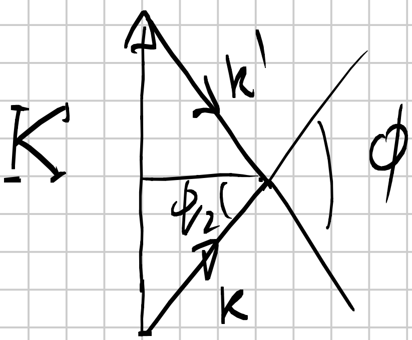
Note Title 2/11/2009

RECIPROCAL LATTICE $\{\vec{K}_i\}$



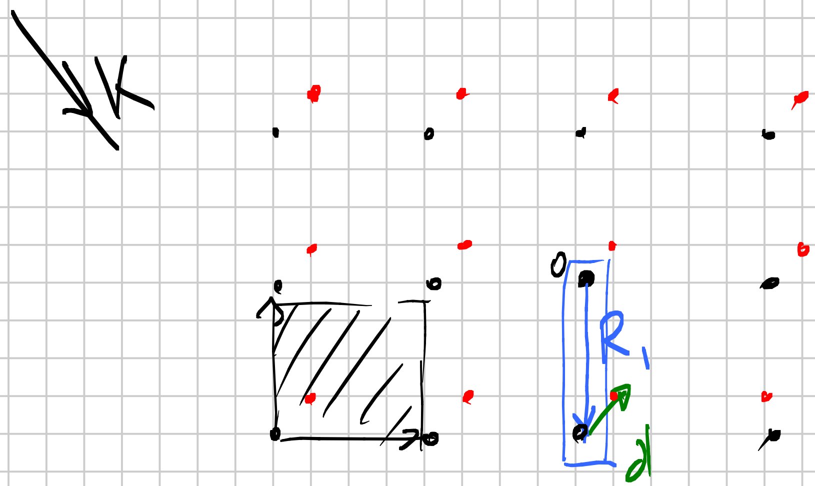
CONSTRUCTIVE INTERFERENCE OF LIGHT FROM __ALL__ ATOMS

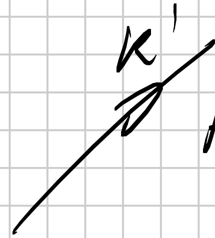
$$\iff \quad \vec{k}-\vec{k}' = \vec{K}_i$$



$$\frac{|K|}{2} = |k| \sin\frac{\phi}{2}$$

WHAT HAPPENS IF THERE IS A BASIS?





$$A = e^{\underbrace{i(k-k')\cdot R_1}_{}} \to \text{DIFFERENCE OF OPTICAL PATH}$$

$$+ e^{i(k-k')\cdot(R_1+d)}$$

$$A = e^{i(k-k')R_1}\left(f_1 \cdot 1 + f_2 e^{i(k-k')\vec{d}}\right)$$

$f_1 \quad f_2$ ATOMIC STRUCTURE FACTORS

$$\left[f_1 + f_2 e^{i(k-k')\cdot\vec{d}}\right] \to \text{STRUCTURE FACTOR}$$

$$e^{i(k-k')\cdot R_i} = 1 \quad \forall R_i \Rightarrow \text{PEAK}$$

$$\vec{k} - \vec{k}' = \vec{K}_i$$

$$S(\vec{K}) = \left[f_1 + f_2 e^{i\vec{K}\cdot d}\right]$$

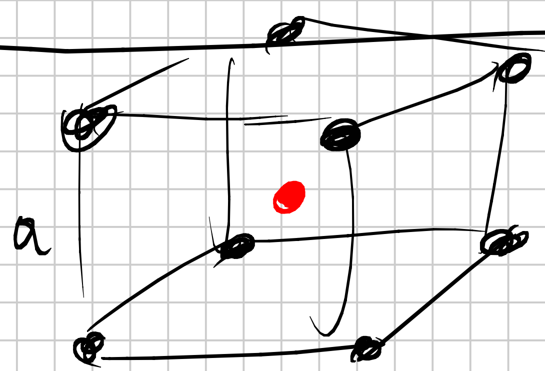
UNIT CELL MANY ATOMS d_i

$$S(\vec{K}) = \sum_i f_i(K) e^{i\vec{K}\cdot\vec{d}_i}$$

ATOMS UNIT CELL

$$f_i \sim \int d^3r\, \rho(r)\, e^{ikr}$$

$$f_i(K) \sim f_i(K=0)$$



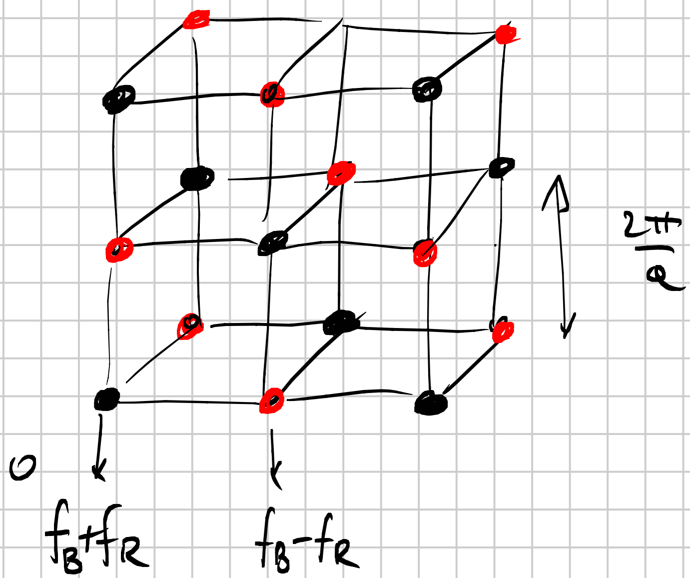
SIMPLE CUBIC WITH 2 ATOM BASIS

$$\vec{K} = m_1 \frac{2\pi}{a}\hat{x} + m_2 \frac{2\pi}{a}\hat{y} + m_3 \frac{2\pi}{a}\hat{z}$$

$$\vec{d}_{RED} = \frac{a}{2}(1\ 1\ 1)$$

$$S(\vec{K}) = \left(f_B + f_R\, e^{i\vec{K}\cdot\vec{d}_{RED}}\right) = \left(f_B + f_R\, e^{i\pi(m_1+m_2+m_3)}\right) = \begin{cases} f_B + f_R & m_1+m_2+m_3 \text{ EVEN} \\ f_B - f_R & m_1+m_2+m_3 \text{ ODD} \end{cases}$$

RECIPROCAL LATTICE



CENTRAL ONE SAME AS VERTEX

$f_B = f_R \Rightarrow$ S=0 RED POINTS IN REC SPACE

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CHAP 8

SYMMETRY OF LATTICE $\Longleftrightarrow$ ELECTRONIC STATES

BORN- OPPENHEIMER APPROXIMATION

e + IONS

e DYNAMIC
FOR IONS IN
A <u>FIXED</u> POSITION

LATTICE DYNAMICS

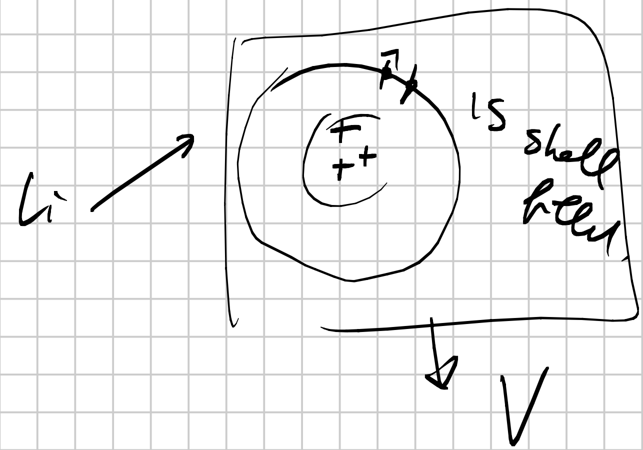
ELECTRONS NOT <u>FREE</u> BUT NO e-e INTERACTION

SINGLE ELECTRONS

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(r)\right)\psi_e(r) = E\,\psi_e(r) \qquad (I)$$

$V(r)$ HAS THE SYMMETRY OF THE LATTICE

$$V(\vec{r} + \vec{R}_i) = V(\vec{r}) \qquad (\mathrm{II})$$



Li $\to (1s)^2 (2s)$

Li Li Li

PSEUDOPOTENTIALS $V(\vec{r})$ (INCLUDE CORE ELECTRONIC STATES IN THE $V(r)$

BLOCH THEOREM

SOLUTIONS OF PROBLEM (I) WITH $V(\vec{r})$ HAVING PROPERTY II

$$\psi_{mk}(\vec{r}) = e^{ik\cdot r} u_{mk}(\vec{r})$$

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

u_{mk} HAS THE PERIODICITY OF LATTICE

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

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

K QUANTUM # $\Longleftrightarrow$ HOW STATES TRANSFORM WHEN I MAKE TRANSLATION IN THE LATTICE

FREE PARTICLE

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

CONTINUOUS TRANSLATION SYMMETRY

DISCRETE TRANSLATION SYMMETRY

LATTICE

$$\psi_k(r + R_i) \to e^{ik\cdot R_i}\,\psi_k(r)$$

$\boxed{k \quad \text{CRYSTAL MOMENTUM}}$