9/4

Homework:

Weisong Tu - Office Hours
Wed 2 to 3 PM
@ Tutoring Center
Room 201 Nielsen.

Sep 4-2:06 PM

Vectors and Covectors.

Solid State Physics:

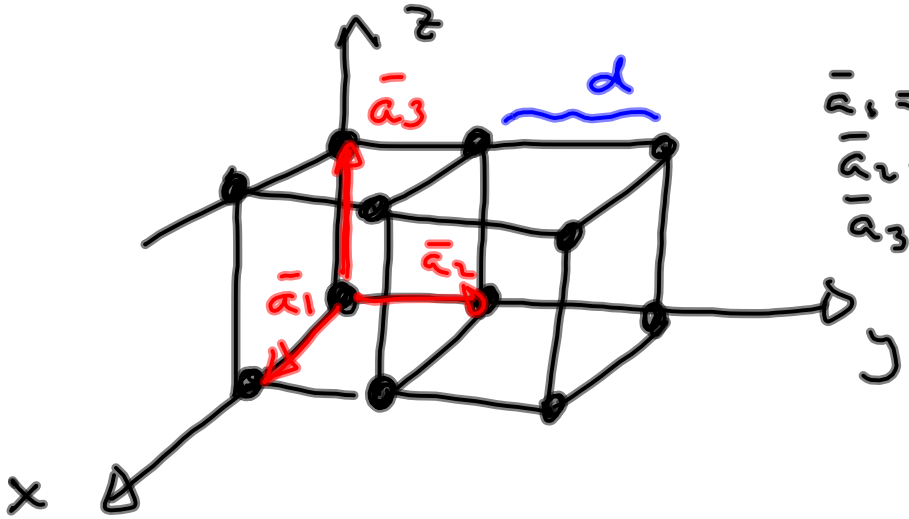
A crystal is formed by an orderly array of ions that form a lattice in real space. The lattice is called Bravais lattice and there is a small number of this lattices such as cubic, face centered cubic, body center cubic, etc.

Sep 4-2:14 PM

To define the position of a ion in the lattice we define a basis:

Ex: cubic lattice

d : lattice spacing



$\bar{a}_1 = d\hat{x}$

$\bar{a}_2 = d\hat{y}$

$\bar{a}_3 = d\hat{z}$

$\bar{a}_i$: are vectors of length d that connect the ion chosen as the origine with a nearest neighbor

$\{\bar{a}_i\}$ are linearly independent.

Now the position of any ion at site $\bar{R}$ can be written as:

Sep 4-2:23 PM

$\bar{R} = n_1 \bar{a}_1 + n_2 \bar{a}_2 + n_3 \bar{a}_3$ with n_i integers

We can use the vectors $\bar{R}$ to define our lattice but we also can define the lattice using families of planes perpendicular to the vectors $\bar{R}$.

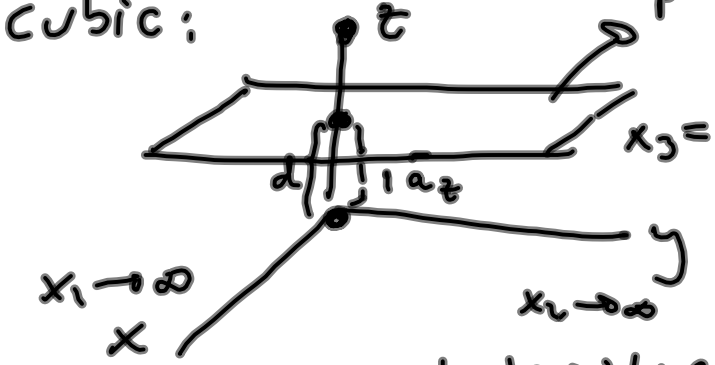
For example: in the cubic lattice we can use the families of planes perpendicular to $\hat{x}$, $\hat{y}$ and $\hat{z}$.

Sep 4-2:28 PM

Miller indices: are used by crystalographers to identify the families of planes in a system.

Planes are defined by 3 points in a Bravais lattice and the collection of all planes parallel to each other expands the crystal.

Cubic:



$(h,k,l)=(0,0,1)$

x_i: point where plane cuts the axis.

- The family is composed by planes parallel to x-y and separated a distance d from each other.
- Find the plane in the family closer to the origin.
- define $(h,k,l)=\left(\frac{1}{x_1},\frac{1}{x_2},\frac{1}{x_3}\right)$

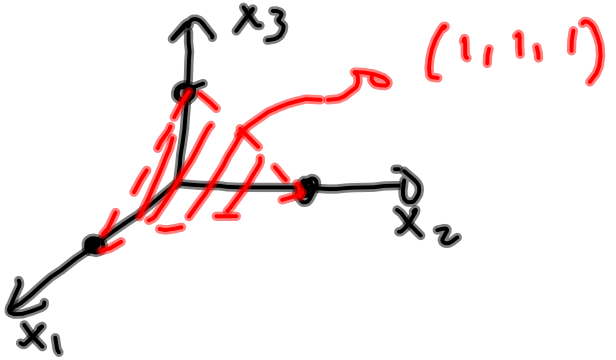
Sep 4-2:37 PM

(1,0,0) defines the family of planes ⊥ to $\bar{a}_1$

(0,1,0) " " " " " " " " $\bar{a}_2$

(0,0,1) " " " " " " " " $\bar{a}_3$

Notice that in some lattices we also can define families of planes that are NOT perpendicular to any basis vector.



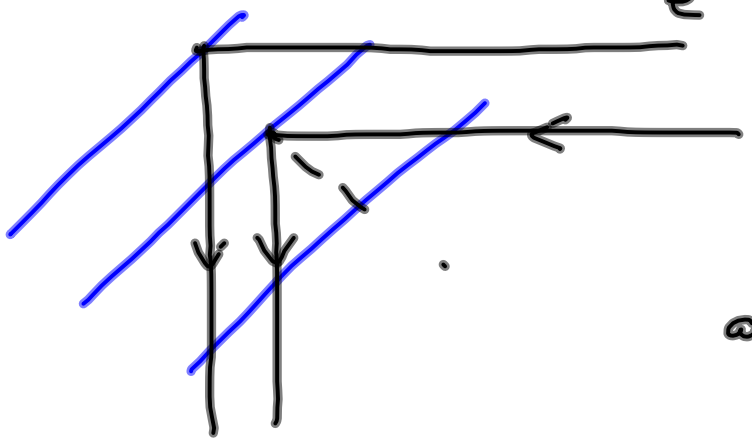
orthogonal to

$\bar{R} = \bar{a}_1 + \bar{a}_2 + \bar{a}_3$

Sep 4-2:45 PM

Why are planes important?

Lattice structure is studied by looking at the interference pattern obtained when x-rays are reflected on the lattice. The properties of the lattice planes determined this pattern.



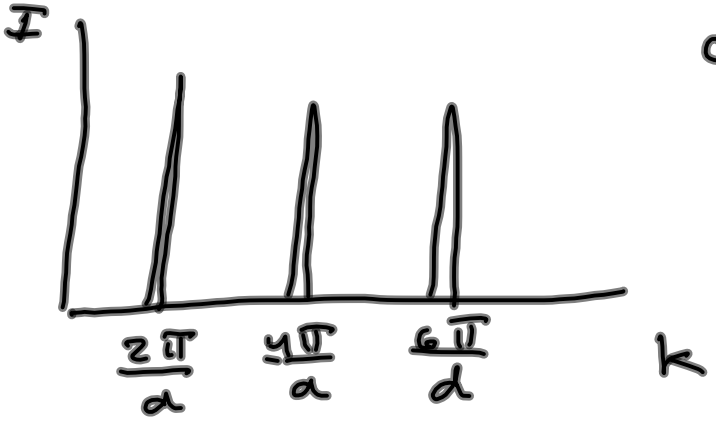
$e^{i\bar{k}\cdot\bar{r}}$ plane wave with wave vector $\bar{k}$

$\bar{k}\cdot\bar{r} = k_i r^i$ (as tensors)

and $[\bar{r}]$ = length then $[\bar{k}]$ = length^{-1}.

Sep 4-2:49 PM

Experimentalists can vary $\bar{k}$ by controlling the energy (wave length) of the electromagnetic wave - They find that the reflected intensity is a function of $\bar{k}$.



The reflected light has the form:

$e^{i \bar{k} (\bar{r}+\bar{R})}$

where $\bar{R}$ is the position of the scatterer (ion) and $\bar{r}$ is a general position in space.

Sep 4-2:56 PM

The maximum intensity (the peaks) occur when $\bar{k}$ is such that

$e^{i\bar{k}\cdot\bar{R}} = 1$ then $\bar{k}\cdot\bar{R} = 2\pi n$ → integer

The values of $\bar{k}$ such that $\bar{k}\cdot\bar{R} = 2\pi n$ will be called $\bar{K}$ so that $\bar{K}\cdot\bar{R} = 2\pi n$.

It can be shown that the vectors $\bar{K}$ also form a periodic lattice. This lattice is in k-space or reciprocal space. The reciprocal space is called <u>dual</u> space by mathematicians.

Sep 4-3:00 PM

Reciprocal basis:

In dual space (or reciprocal space) we can define a basis $\{\bar{b}_i\}$ that will generate all the vectors $\bar{K}$ that form the reciprocal lattice (in tensor notation we will see that $\bar{b}_i = \hat{b}^i$)

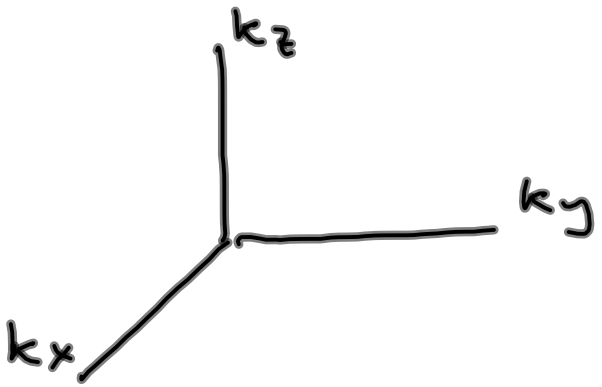
Sep 4-3:05 PM

Example: Find the dual basis for the cubic lattice.

$$\bar{K} = m_1 \bar{b}_1 + m_2 \bar{b}_2 + m_3 \bar{b}_3$$

m_i are integers

$\bar{K}$ point in reciprocal lattice.



If $\bar{K} \cdot \bar{R} = K_i R^i = 2\pi n$ $\bar{K}$ belongs to reciprocal lattice.

Then

$$\bar{K} \cdot \bar{R} = m_1 n_1 \bar{a}_1 \cdot \bar{b}_1 + m_2 n_2 \bar{a}_2 \cdot \bar{b}_2 + m_3 n_3 \bar{a}_3 \cdot \bar{b}_3 + n_1 m_2 \bar{a}_1 \cdot \bar{b}_2 + n_1 m_3 \bar{a}_1 \cdot \bar{b}_3 + n_2 m_3 \bar{a}_2 \cdot \bar{b}_3 + \cdots = 2\pi h$$

This is true if:

$\bar{a}_i \cdot \bar{b}_i = 2\pi$ and $\bar{a}_i \cdot \bar{b}_j = 0$ if $i \neq j$.

Sep 4-3:10 PM

In general to find the reciprocal basis we require:

$$a_i \cdot b^j = \delta_i{}^j 2\pi$$

for physicists

Mathematicians use:

$$a_i \cdot b^j = \delta_i{}^j$$

This works in any dimension.

Sep 4-3:17 PM

For 3D you can use:

$$\bar{b}_i = 2\pi \frac{\bar{a}_j \times \bar{a}_k}{\bar{a}_i \cdot (\bar{a}_j \times \bar{a}_k)}$$

i, j, k in cyclic order.

$\bar{a}_i \cdot (\bar{a}_j \times \bar{a}_k)$: volume of unit cell in real space

Clearly

$\bar{a}_i \cdot \bar{b}_i = 2\pi$

$\bar{a}_j \cdot \bar{b}_i = 0$ if $i \neq j$.

Ex: cubic lattice:

$$\bar{b}_1 = 2\pi \frac{\bar{a}_2 \times \bar{a}_3}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)} = \frac{2\pi d^2 \hat{x}}{d^3} = \frac{2\pi}{d}\hat{x}$$

($\bar{a}_2 \times \bar{a}_3 = d^2 \hat{x}$; $\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3) = d^3$)

$\bar{b}_i = \frac{2\pi}{d}\bar{x}_i$ cubic lattice of size $\frac{2\pi}{d}$ (volume $\frac{(2\pi)^3}{d^3}$).

Sep 4-3:19 PM