Reciprocal lattices

$n(\vec{r})$: density of electrons / atom

$\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$: primitive trans. vectors

$\vec{T} = \mu_1 \vec{a}_1 + \mu_2 \vec{a}_2 + \mu_3 \vec{a}_3$, $\mu_1, \mu_2, \mu_3 \in \mathbb{Z}$

$\vec{T}$: translation vector $\Rightarrow$ general

If $\vec{r}_0$ is the position of a lattice point

$\mapsto$ $\vec{r}\,' = \vec{r}_0 + \vec{T}$ is also a lattice point

$n(\vec{r}) = n(\vec{r} + \vec{T})$: symmetries of the lattice

$n(\vec{r})$ is a periodic function with period $\vec{T}$

Any periodic function can be expanded through a Fourier series of sines and cosines

Example: $n(x)$ of a 1D crystal with periodicity a

$$n(x) = n_0 + \sum_{p \geq 0} \left[C_p \cos\left(\frac{2\pi p x}{a}\right) + S_p \sin\left(\frac{2\pi p x}{a}\right) \right]$$

p: positive integer

$C_p, S_p \in \mathbb{R}$ are the weight of the pth harmonic

$\frac{2\pi}{a}$: guarrantee that the function is periodic in a

$\frac{2\pi}{a} p$: position of the p-th point of the reciprocal lattice

$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2} \qquad \sin(x) = \frac{e^{ix} - e^{-ix}}{2i} \qquad \frac{1}{i} = -i$$

$$\sin(x) = -\frac{i}{2}\left(e^{ix} - e^{-ix}\right)$$

$$C_p \cos\left(\frac{2\pi p x}{a}\right) + S_p \sin\left(\frac{2\pi p x}{a}\right) = \frac{C_p}{2}\left[\exp\left(\frac{i2\pi p x}{a}\right) + \exp\left(\frac{-2\pi p x}{a}\right)\right]$$

$$- \frac{iS_p}{2}\left[\exp\left(\frac{i2\pi p x}{a}\right) - \exp\left(\frac{-2\pi p x}{a}\right)\right]$$

$$= \frac{C_p - iS_p}{2} \exp\left(\frac{i2\pi p x}{a}\right) + \frac{C_p + iS_p}{2} \exp\left(\frac{-i2\pi p x}{a}\right)$$

$$= n_p \exp\left(\frac{i2\pi p x}{a}\right) + n_{-p} \exp\left(\frac{-i2\pi p x}{a}\right)$$

$$n_p = \frac{C_p - iS_p}{2} \qquad n_{-p} = \frac{C_p + iS_p}{2}$$

$n_p = n_{-p}^*$ Cond. Satisfied

$$n(x) = n_0 + \sum_p n_p \exp\left(\frac{i2\pi p x}{a}\right)$$

$$n_p = \frac{1}{a}\int_0^a n(x) \exp\left(\frac{-i2\pi p x}{a}\right) dx$$

$$n(x) = n_0 + \sum_k n_k \exp\left(\frac{i2\pi k x}{a}\right)$$

$$\int_0^a \left[n_0 + \sum_k n_k \exp\left(\frac{i2\pi k x}{a}\right)\right] \exp\left(\frac{-i2\pi p x}{a}\right) dx =$$

$$= n_0 \int_0^a \exp\left(\frac{-i2\pi p x}{a}\right) dx + \sum_k n_k \int_0^a \exp\left(\frac{i2\pi k x}{a}\right) \exp\left(\frac{-i2\pi p x}{a}\right) dx$$

- $$\int_0^a \exp\left(\frac{-i2\pi p x}{a}\right) dx = \frac{a}{-i2\pi p}\left[\exp\left(\frac{-i2\pi p a}{a}\right) - 1\right]$$

$$= \frac{a}{-i2\pi p}\left[1-1\right] = 0$$

$$\frac{2\pi p a}{a} = 2\pi p \qquad \exp\left(-i2\pi p\right) = 1$$ for p an integer number

- $$\int_0^a \exp\left(\frac{i2\pi k x}{a}\right)\exp\left(\frac{-i2\pi p x}{a}\right)dx = \int_0^a \exp\left[\frac{i2\pi x}{a}(k-p)\right]dx$$

$$= \frac{a}{i2\pi(k-p)}\left\{\exp\left[\frac{i2\pi a}{a}(k-p)\right]-1\right\} = 0$$

k and p are integers

unless $k=p$:

$$= \int_0^a \exp\left[\frac{i2\pi x}{a}\underbrace{(k-p)}_{=0}\right]dx = \int_0^a 1\,dx = a$$

$$n_p = \frac{1}{a}\sum_k n_k\, a\, \delta_{kp} \qquad \delta_{kp} = \begin{cases} 1 & k=p \\ 0 & \text{otherwise} \end{cases}$$

$$= \frac{a}{a}\sum_k \delta_{kp} n_k = n_p. \checkmark$$

$$n(x) = n_0 + \sum_p n_p \exp\left(\frac{i2\pi p x}{a}\right)$$

$$n_p = \frac{1}{a}\int_0^a n(x)\exp\left(\frac{-i2\pi p x}{a}\right)dx$$

we could do the same for $n(\vec{r})$

$$\vec{G} = 2\pi\left(\frac{p_x}{a_x}, \frac{p_y}{a_y}, \frac{p_z}{a_z}\right) \qquad \vec{G}\cdot\vec{r} = \frac{2\pi p_x x}{a_x} + \frac{2\pi p_y y}{a_y} + \frac{2\pi p_z z}{a_z}$$

$$n(\vec{r}) \sum_{p_x,p_y,p_z} n_{\vec{G}} \exp\left(i\vec{G}\cdot\vec{r}\right) = \sum_{\vec{G}}' n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}$$

$$n_{\vec{G}} = \frac{1}{V_c} \int_{V_c} n(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, d\vec{r}$$

V_c: Volume of the cell.

$$n(\vec{r}) = n(\vec{r}+\vec{T})$$

$$\sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}} = \sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot(\vec{r}+\vec{T})}$$

$$= \sum_{\vec{G}} n_{\vec{G}}\, e^{i(\vec{G}\cdot\vec{r} + \vec{G}\cdot\vec{T})}$$

$$\sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}} = \sum_{\vec{G}} n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}\, e^{i\vec{G}\cdot\vec{T}}$$

$$n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}} = n_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}\, e^{i\vec{G}\cdot\vec{T}}$$

$$1 = e^{i\vec{G}\cdot\vec{T}}$$

$\vec{G}\cdot\vec{T} = 2\pi n$

n an integer

We know $\vec{T}$!

$$\vec{T} = \mu_1 \vec{a}_1 + \mu_2 \vec{a}_2 + \mu_3 \vec{a}_3$$

$\vec{G} = \nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3$: General Trans. vector in reciprocal space

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2 \times \vec{a}_3)}$$

$\{\vec{b}_1, \vec{b}_2, \vec{b}_3\}$: primitive trans. vectors of the reciprocal lattice

$$\vec{b}_i \cdot \vec{a}_j = 2\pi\,\delta_{ij} = \begin{cases} 2\pi & i = j \\ 0 & i \neq j \end{cases}$$

Homework: find $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$

Cubic lattice:

$\vec{a}_1 = a\,\hat{\imath}$ $\qquad \vec{a}_2 = a\,\hat{\jmath}$ $\qquad \vec{a}_3 = a\,\hat{k}$

Body-centered lattice:

$\vec{a}_1 = \frac{a}{2}(-\hat{\imath} + \hat{\jmath} + \hat{k})$ $\qquad \vec{a}_2 = \frac{a}{2}(\hat{\imath} - \hat{\jmath} + \hat{k})$

$\vec{a}_3 = \frac{a}{2}(\hat{\imath} + \hat{\jmath} - \hat{k})$