Last time: Real Fourier Expansion

$$n(x) = \frac{A_0}{2} + \sum_{p=1}^{\infty}\left[A_p \cos(k_p x) + B_p \sin(k_p x)\right]$$

$k_p = \frac{2\pi p}{a}$ like wave vector

$$A_p = \langle \cos(k_p x) | n(x) \rangle$$

$$= \frac{2}{a}\int_{x=0}^{a} \cos(k_p x)\, n(x)\, dx$$

$$= \frac{2}{a}\int_{x=0}^{a} \cos\left(\frac{2\pi p x}{a}\right) n(x)\, dx$$

B_p ... sin —.—.—

Euler: $e^{i\theta} = \cos\theta + i\sin\theta$

$$(e^{i\theta})^* = e^{-i\theta} = \cos\theta - i\sin\theta$$

$$\cos\theta = \frac{e^{i\theta}+e^{-i\theta}}{2} \qquad \sin = \frac{e^{i\theta}-e^{-i\theta}}{2i}$$

$$n(x) = \sum_{p=-\infty}^{\infty} C_p e^{ik_p x}$$

complex Fourier series

$\{C_p\}$ - fourier coefficients, complex

$\{e^{ik_p x}\}$ - basis functions

$$C_p = \langle e^{ik_p x} | n(x) \rangle$$

$$= \frac{1}{a}\int_{x=0}^{a} e^{-ik_p x} n(x)\, dx = \frac{1}{a}\int_{x=0}^{a} e^{\frac{-i2\pi p x}{a}} n(x)\, dx$$

$$C_{-p} = \frac{1}{a}\int_{x=0}^{a} e^{\frac{-i2\pi(-p)x}{a}} n(x)\, dx = \frac{1}{a}\int_{x=0}^{a} e^{\frac{+i2\pi p x}{a}} n(x)\, dx$$

$$= (C_p)^*$$

$C_{-p} = C_p^*$ only if $n(x)$ real

$$C_p = \frac{1}{2}(A_p - iB_p)$$

$$C_{-p} = \frac{1}{2}(A_p + iB_p) = C_p^*$$

$$C_0 = \frac{1}{2}A_0$$

One final complication
→ 3 dimensions

$$n(\vec{r}) = n(x, y, z)$$

$$n(x) = \sum_{p=-\infty}^{+\infty} C_p e^{ik_p x} = \sum_{p=-\infty}^{+\infty} C_p e^{i\vec{k}_p \cdot \vec{x}}$$

$$n(\vec{r}) = \sum_{p_1}\sum_{p_2}\sum_{p_3 = -\infty}^{+\infty} \tilde{n}_{\vec{p}}\, e^{i\vec{k}_{p_1}\cdot\vec{x}}\, e^{i\vec{k}_{p_2}\cdot\vec{y}}\, e^{i\vec{k}_{p_3}\cdot\vec{z}}$$

$$= \sum_{\vec{p}} \tilde{n}_{\vec{p}}\, e^{i\vec{G}\cdot\vec{r}}$$

$$\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \qquad \vec{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

Direct Lattice vector

$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

$\{\vec{a}_i\} \rightarrow$ primitive translation vectors for direct lattice.

$\vec{T}$ moves from one lattice site to another.

$\vec{G}$ = Reciprocal lattice vector (Fourier Transform Lattice Vector)

$$\vec{G} = \underbrace{\nu_1 \vec{b}_1}_{\text{like } T_{P_1}} + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3$$

$\{\vec{b}_i\} \rightarrow$ primitive translation vectors for the reciprocal lattice

Condition : $\{\vec{b}_i\}_3$ $\vec{G}$

$n(\vec{r})$ is periodic

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

$$\| $$

$$\sum_{\vec{p}} \tilde{n}_{\vec{p}}\, e^{i\vec{G}\cdot(\vec{r}+\vec{T})} = \underbrace{\sum_{\vec{p}} \hat{n}_{\vec{p}}\, e^{i\vec{G}\cdot\vec{r}}}_{n(\vec{r})}\, e^{i\vec{G}\cdot\vec{T}}$$

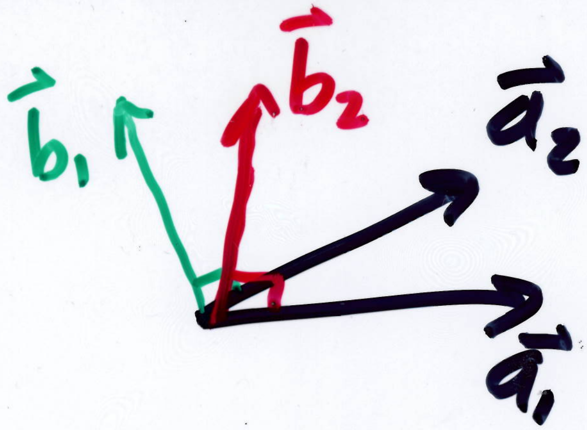
$$\Rightarrow e^{i\vec{G}\cdot\vec{T}} = 1 \Rightarrow \vec{G}\cdot\vec{T} = 2\pi(\text{integer})$$

$$\vec{T} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$\vec{G} = \nu_1\vec{b}_1 + \nu_2\vec{b}_2 + \nu_3\vec{b}_3$$

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

e.g. $\vec{b}_1$ is perpendicular to $\vec{a}_2$ and $\vec{a}_3$.



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

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

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cyclic permutation of $\{1, 2, 3\}$

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

volume of primitive cell "p-cell"

$$n(\vec{r}) = \sum_{\vec{p}} \tilde{n}_{\vec{p}}\, e^{i\vec{G}\cdot\vec{r}}$$

$$\tilde{n}_{\vec{p}} = \frac{1}{V} \iiint_{cell} e^{-i\vec{G}\cdot\vec{r}}\, n(\vec{r})\, dV$$

volume of p-cell