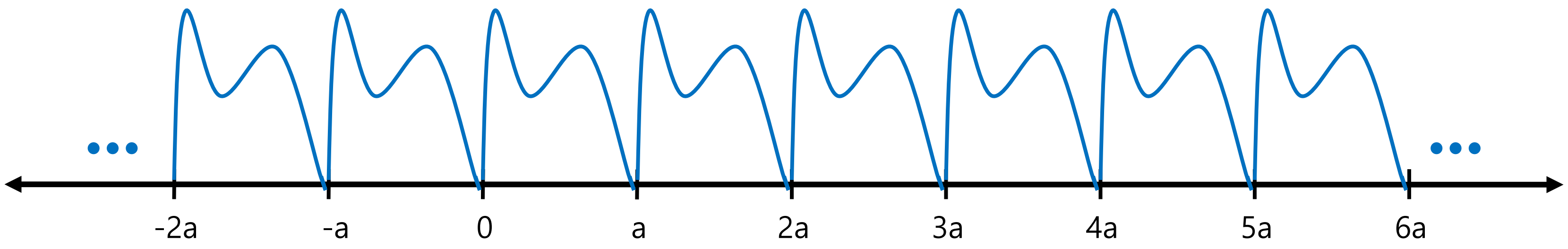
Fourier Transformation



$\rho(x) = \rho(x+a)$: A function with the periodicity of a

Fourier expansion : mathematics : Why &How this expansion is useful ?

$$\rho(x) = \sum_{n=-\infty}^{\infty} A_n e^{i\frac{2\pi n}{a}x} = \sum_{n=0}^{\infty}\left[\alpha_n \cos(\frac{2\pi}{a}nx) + \beta_n \sin(\frac{2\pi}{a}nx)\right]$$

Fourier Transformation

$$\rho(x) = \sum_{n=-\infty}^{\infty} A_n e^{i\frac{2\pi n}{a}x} = \sum_{n=0}^{\infty}\left[\alpha_n \cos(\frac{2\pi}{a}nx) + \beta_n \sin(\frac{2\pi}{a}nx)\right]$$

$$\rho(x) = \sum_{n=\infty}^{\infty} A_n e^{iG^n x}$$

Fourier component

Basis function

$$G^n = \frac{2\pi}{a}n$$, n integer

The orthogonality between the two basis functions

$$\int_0^a (e^{iG^m x})^* e^{iG^n x} dx = \int_{-\frac{a}{2}}^{\frac{a}{2}} e^{-iG^m x} e^{iG^n x} dx = \int_{-0.3a}^{0.7a} (e^{iG^m x})^* e^{iG^n x} dx$$

$$= \int_0^a e^{i\frac{2\pi}{a}(n-m)x} dx = a\,\delta_{n,m}$$

Fourier Transformation

1. Using the Dirac notation $e^{i\frac{2\pi}{a}nx} \Rightarrow |n\rangle$, and $(e^{i\frac{2\pi}{a}nx})^* \Rightarrow \langle n|$

2. The inner product $\langle f|g\rangle = \int_0^a f^*(x)g(x)dx$

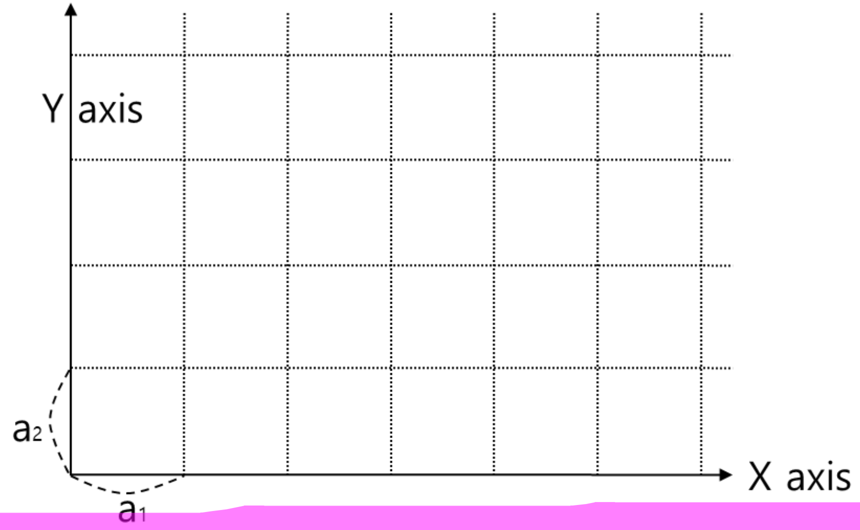
3. Orthogonality of the basis $\langle n|m\rangle = a\delta_{n,m}$

4. A periodic function $\rho(x)$ $|\rho\rangle = \sum_{n=-\infty}^{\infty} A_n |n\rangle$ $\rho(x) = \sum_{n=-\infty}^{\infty} A_n e^{i\frac{2\pi n}{a}x}$

5. Multiply $\langle m|$ on both sides, we have

$$\langle m|g\rangle = \sum_{n=-\infty}^{\infty} A_n \langle m|n\rangle = A_m a, \qquad A_m = \frac{1}{a}\langle m|g\rangle = \frac{1}{a}\int_0^a e^{-i\frac{2\pi}{a}mx} g(x)dx$$

Fourier transformation in 3D



$$\int_0^{a_1}\int_0^{a_2}\int_0^{a_3}$$

$$\rho(x,y,z)=\rho(x+a_1,y,z)=\rho(x,y+a_2,z)=\rho(x,y,z+a_3)$$

The periodicities are a_1, a_2, a_3, in x, y, z directions, respectively.

★

$$\rho(x,y,z)=\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\sum_{n_3=-\infty}^{\infty}A_{n_1,n_2,n_3}e^{i\frac{2\pi}{a_1}n_1x}e^{i\frac{2\pi}{a_2}n_2y}e^{i\frac{2\pi}{a_3}n_3z}$$

$$A_{n_1,n_2,n_3}=\frac{1}{a_1a_2a_3}\int dx\int dy\int dz\,\rho(\vec{r})e^{-i\frac{2\pi n_1}{a_1}x}e^{-i\frac{2\pi n_2}{a_2}y}e^{-i\frac{2\pi n_3}{a_3}z}$$

Fourier Transformation

$$\vec{b_1} = \frac{2\pi}{a_1}\hat{x}\ ,\quad \vec{b_2} = \frac{2\pi}{a_2}\hat{y}\ ,\quad \vec{b_3} = \frac{2\pi}{a_3}\hat{z}$$

$$\rho(x,y,z) = \sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\sum_{n_3=-\infty}^{\infty} A_{n_1n_2n_3}\, e^{i\frac{2\pi}{a_1}n_1x}\, e^{i\frac{2\pi}{a_2}n_2y}\, e^{i\frac{2\pi}{a_3}n_3z}$$

$$\frac{2\pi}{a_1}n_1x + \frac{2\pi}{a_2}n_2y + \frac{2\pi}{a_3}n_3z = (n_1\vec{b_1} + n_2\vec{b_2} + n_3\vec{b_3})\cdot\vec{r}$$

$$\vec{G}(n_1, n_2, n_3) = n_1\vec{b_1} + n_2\vec{b_2} + n_3\vec{b_3}$$

$$= \vec{G}(n_1, n_2, n_3)\cdot\vec{r}$$

Note the lattice vector and reciprocal

$$\vec{a}_1 = a_1\hat{x} \;, \vec{a}_2 = a_2\hat{y} \;, \vec{a}_3 = a_3\hat{y}$$

$$\vec{b}_1 = \frac{2\pi}{a_1}\hat{x} \;, \quad \vec{b}_2 = \frac{2\pi}{a_2}\hat{y} \;, \quad \vec{b}_3 = \frac{2\pi}{a_3}\hat{z}$$

G-vector (Reciprocal Lattice Vector)

Let's give number to each member of this G-vectors (n_1, n_2, n_3)

(0, 0, 0) ⇒ " 1 "
(1, 0, 0) ⇒ " 2 "
(0, 1, 0) ⇒ " 4 "
(0, 0, 1) ⇒ " 6 "
(1, 1, 0) ⇒ " 8 "
(1, 0, 1) ⇒ "10 "
(0, 1, 1) ⇒ "11 "

(-1, 0, 0) ⇒ " 3 "
(0, -1, 0) ⇒ " 5 "
(0, 0, -1) ⇒ " 7 "
(1, -1, 0) ⇒ " 9 "

⋮

(n_1, n_2, n_3) ⇒ "X"

$$\overrightarrow{G_1} = \vec{0}$$

$$\overrightarrow{G_1} = \overrightarrow{b_1} \qquad \overrightarrow{G_2} = \overrightarrow{b_2} \qquad \overrightarrow{G_3} = \overrightarrow{b_3}$$

$$\overrightarrow{G_4} = -\overrightarrow{b_1} \qquad \overrightarrow{G_5} = -\overrightarrow{b_2} \qquad \overrightarrow{G_6} = -\overrightarrow{b_3}$$

$$\overrightarrow{G_7} = \overrightarrow{b_1} + \overrightarrow{b_2} \qquad \overrightarrow{G_8} = \overrightarrow{b_2} + \overrightarrow{b_3}$$

$$\vdots$$

$$\overrightarrow{G_N} = l\overrightarrow{b_1} + m\overrightarrow{b_2} + n\overrightarrow{b_3}$$

$$\rho(x,y,z) = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_3=-\infty}^{\infty} A_{n_1 n_2 n_3} e^{i\frac{2\pi}{a_1}n_1 x} e^{i\frac{2\pi}{a_2}n_2 y} e^{i\frac{2\pi}{a_3}n_3 z}$$

$$= \sum_{l} A_l e^{i\vec{G}_l \bullet \vec{r}}$$

Fourier expansion : mathematics : Why &How this expansion is useful ?

Dirac' notation and orthogonality

$$\rho(x,y,z) = \rho(\vec{r}) = \sum_{N=1}^{\infty} A_N \, e^{i\,\vec{G}_N \cdot \vec{r}}$$

Fourier transformation of 3D periodic function

$$\left|N\right\rangle \Rightarrow \frac{1}{\sqrt{\Omega}} e^{i\vec{G}_N \cdot \vec{r}} \text{ , and } \left\langle M\right| \Rightarrow \frac{1}{\sqrt{\Omega}} \left(e^{i\vec{G}_M \cdot \vec{r}}\right)^* = \frac{1}{\sqrt{\Omega}} e^{-i\vec{G}_M \cdot \vec{r}}$$

$$\left\langle N\middle|M\right\rangle = \frac{1}{\Omega}\iiint d^3\vec{r}\ e^{i(\vec{G}_M - \vec{G}_N)\cdot\vec{r}} d^3\vec{r} = \frac{1}{\Omega}\int_0^{a_1} dx \int_0^{a_2} dy \int_0^{a_3} dz\ \left(e^{i\vec{G}_N \cdot \vec{r}}\right)^* e^{i\vec{G}_M \cdot \vec{r}} = \delta_{N,M}$$

Fourier component of 3D periodic function.

$$\rho(\vec{r}) = \sum_{N=1}^{\infty} A_N e^{i\vec{G_N}\cdot\vec{r}}$$

$$A_N = \frac{1}{\Omega}\iiint \rho(\vec{r})e^{-i\vec{G_N}\cdot\vec{r}}\, d^3\vec{r}$$

Unit-cell volume

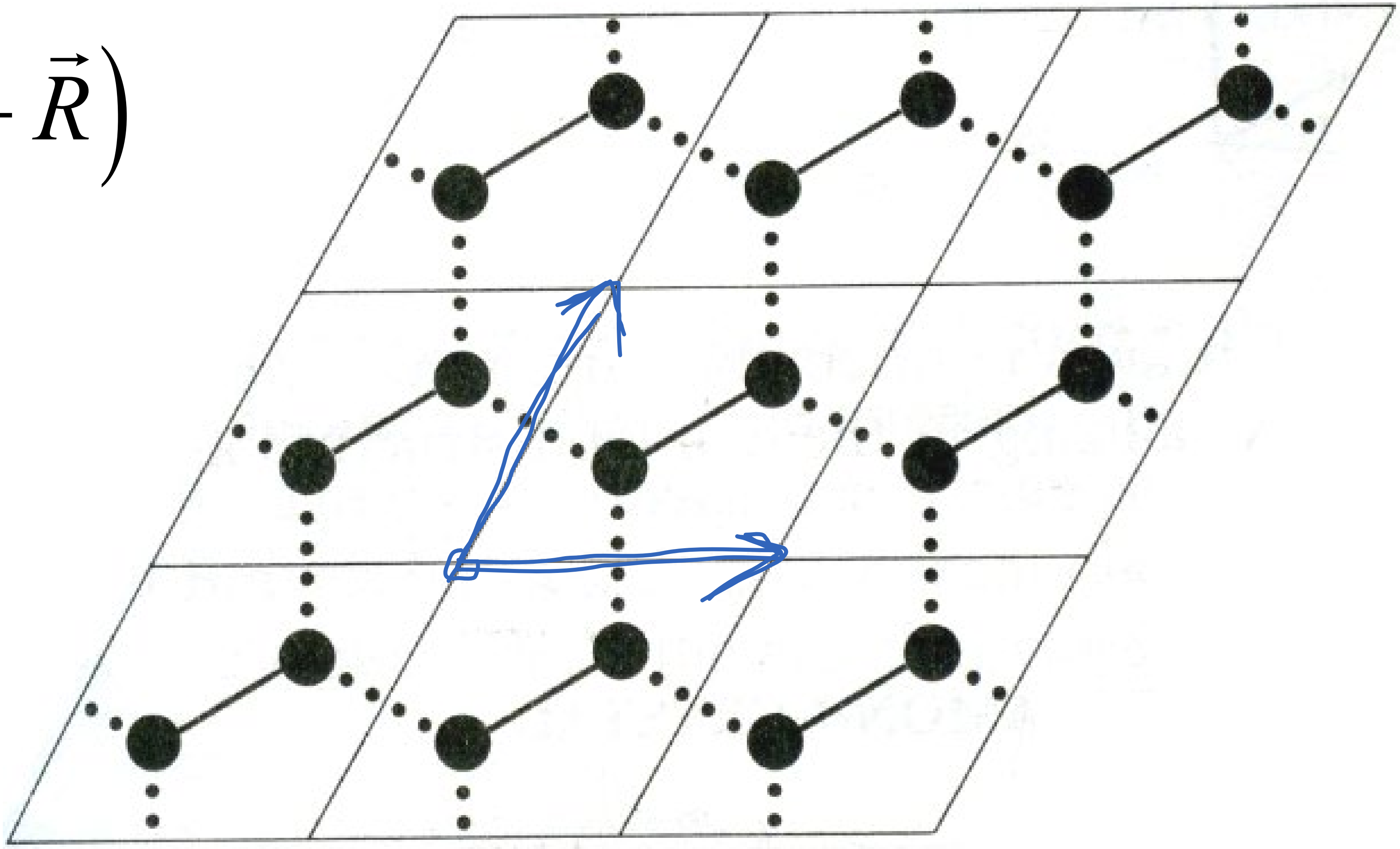
Unit-cell

$$|\rho\rangle = \sum_{N=1}^{\infty} A_N |N\rangle$$

$$A_M = \langle M|\rho\rangle = \sum_{N=1}^{\infty} A_N \langle M|N\rangle$$

Periodic but in non-orthorhombic crystal.

$$\rho\left(\vec{r}'\right)=\rho\left(\vec{r}'+\vec{R}\right)$$



We have three vectors

$$\rho(\vec{r}') = \rho(\vec{r}' + \vec{R})$$

1. Lattice vectors

$$\vec{R} = n\vec{a}_1 + l\vec{a}_2 + m\vec{a}_3$$

2. Reciprocal Lattice vectors

$$\vec{G} = n\vec{b}_1 + l\vec{b}_2 + m\vec{b}_3$$

Fourier transformation,,

Fourier **wave vector** = Reciprocal Lattice vector

3. Bloch vectors

$$\vec{k} = \alpha\vec{b}_1 + \beta\vec{b}_2 + \gamma\vec{b}_3$$

For a lattice defined by $\vec{a}_1, \vec{a}_2, \vec{a}_3$

1. Unit cell volume

$$V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

2. The primitive lattice vectors for the reciprocal lattice

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

3. Show that

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{i,j}$$

$$\vec{a}_1 \cdot \vec{b}_1 = ???$$

$$\vec{a}_1 \cdot \vec{b}_2 = ???$$

$$\vec{a}_1 \cdot \vec{b}_1 = 2\pi \qquad \vec{a}_1 \cdot \vec{b}_3 = 0$$

$$\vec{a}_1 \cdot \vec{b}_2 = 0 \qquad \vec{a}_2 \cdot \vec{b}_2 = 2\pi$$

$$\vdots$$

$$\boxed{\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}}$$

Direct Lattice	Reciprocal Lattice
$\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$	$\{\vec{b}_1, \vec{b}_2, \vec{b}_3\}$
$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$	$\vec{G} = l_1\vec{b}_1 + l_2\vec{b}_2 + l_3\vec{b}_3$

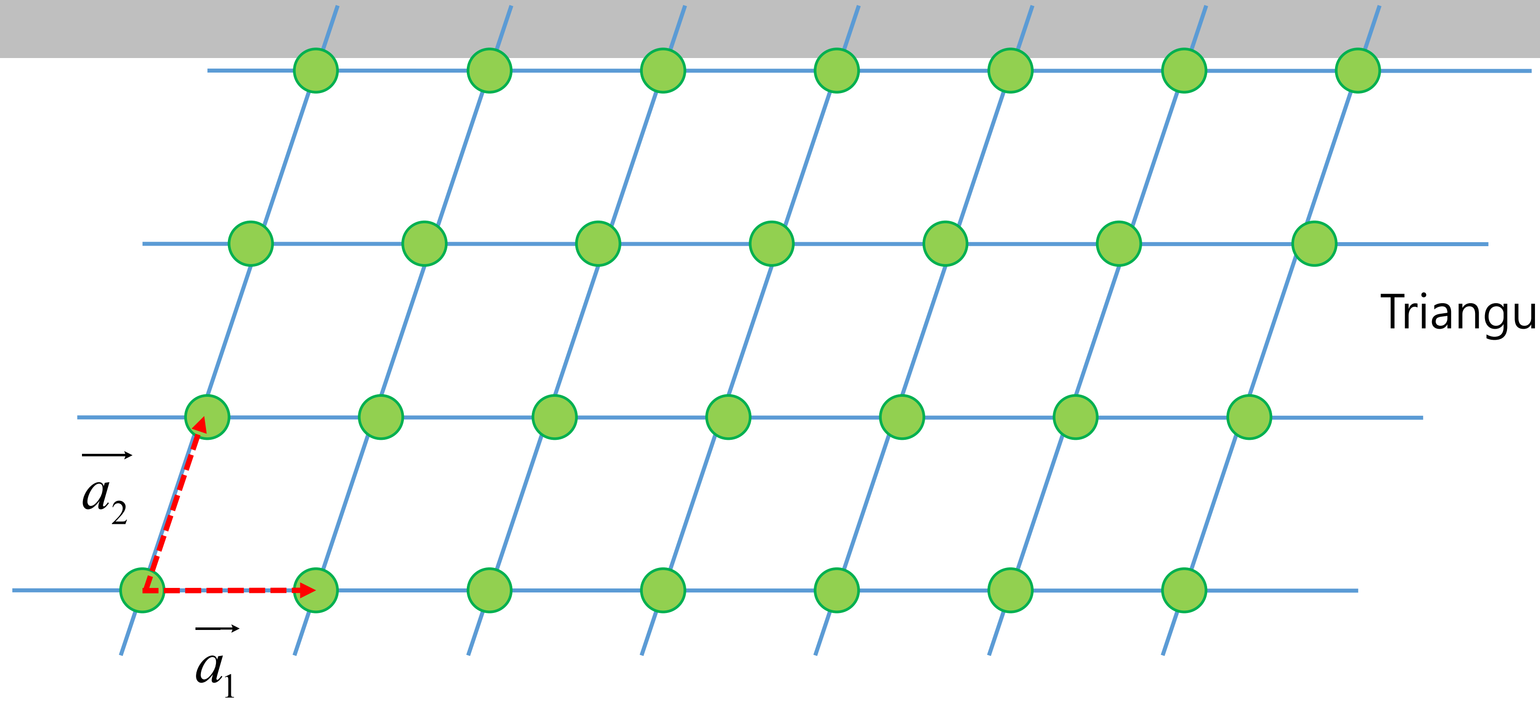
$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

$$\vec{R} \cdot \vec{G} = 2\pi\,(n_1 l_1 + n_2 l_2 + n_3 l_3)$$

$$= 2\pi \times (\text{ integer})$$

(a lattice vector) • (a Reciprocal lattice vector) = integer multiple of 2π

Again, the Fourier Transform of 3D



Triangular lattice

Again, the Fourier Transform of 3D

$$\rho(\vec{r}) = \sum_N A_N e^{i\overrightarrow{G_N}\cdot\vec{r}}$$

$$\rho(\vec{r}+\vec{R}) = \sum_N A_N e^{i\overrightarrow{G_N}\cdot(\vec{r}+\vec{R})} = \sum_N A_N e^{i\overrightarrow{G_N}\cdot\vec{r}} e^{i\overrightarrow{G_N}\cdot\vec{R}}$$

$$\vec{R} \cdot \vec{G} = 2\pi N$$

Fourier Transform in 3D or 2D

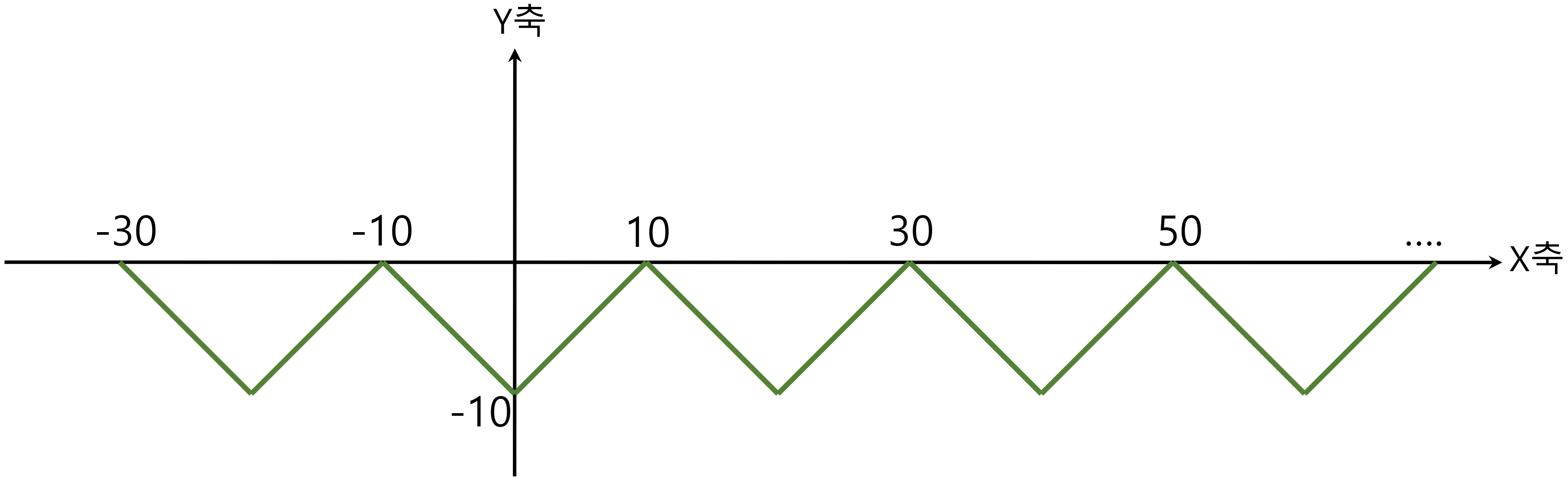
$$\rho(\vec{r}) = \rho(\vec{r} + \vec{R}) :$$

$$\rho(\vec{r}) = \sum_{j=1}^{\infty} e^{i\vec{G_j}\cdot\vec{r}} A(\vec{G_j}) \ , \quad A(\vec{G_j}) = \frac{1}{V}\int \rho(\vec{r}) e^{i\vec{G_j}\cdot\vec{r}}\, d^3\vec{r}$$

Caution: G-vector should be ordered in their magnitude ? …WHY ?

$$\rho(\vec{r}) \approx \sum_{j=1}^{N} e^{i\vec{G_j}\cdot\vec{r}} A(\vec{G_j})$$

Let's consider the quality of Fourier Series



$$\rho(x) = \begin{cases} -x-10 & (-10 \le x \le 0) \\ x-10 & (0 \le x \le 10) \end{cases}$$

$$\rho(x) = \rho(x+20)$$

Say, the lower component is more important. Particularly, what does it mean by the zeroth component of Fourier coeff.

Primitive lattice vector $a = 20$

Primitive reciprocal lattice vector $b = \frac{2\pi}{a}$

reciprocal lattice vector $G^n = nb$

G-vector should be order in their magnitude!

$$G_1 = 0\ ,\ G_2 = b\ ,\ G_3 = -b\ ,\ G_4 = 2b\ ,\ G_5 = -2b$$

$$f(x) \approx \sum_{j=1}^{N} e^{i\overrightarrow{G_j}\vec{x}} A(\overrightarrow{G_x})$$

$$A(G_1)=\frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} f(x)\,dx=-5$$

$$A(G_2)=\frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} e^{iG_2x} f(x)\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(G_2x)(x-\frac{a}{2})\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(\frac{2\pi}{a}x)(x-\frac{a}{2})\,dx=-\frac{a}{\pi^2}=-\frac{20}{\pi^2}$$

$$A(G_3)=\frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} e^{iG_3x} f(x)\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(G_3x)(x-\frac{a}{2})\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(\frac{2\pi}{a}x)(x-\frac{a}{2})\,dx=-\frac{20}{\pi^2}$$

$$A(G_4)=\frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} e^{iG_4x} f(x)\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(G_4x)(x-\frac{a}{2})\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(\frac{4\pi}{a}x)(x-\frac{a}{2})\,dx=0$$

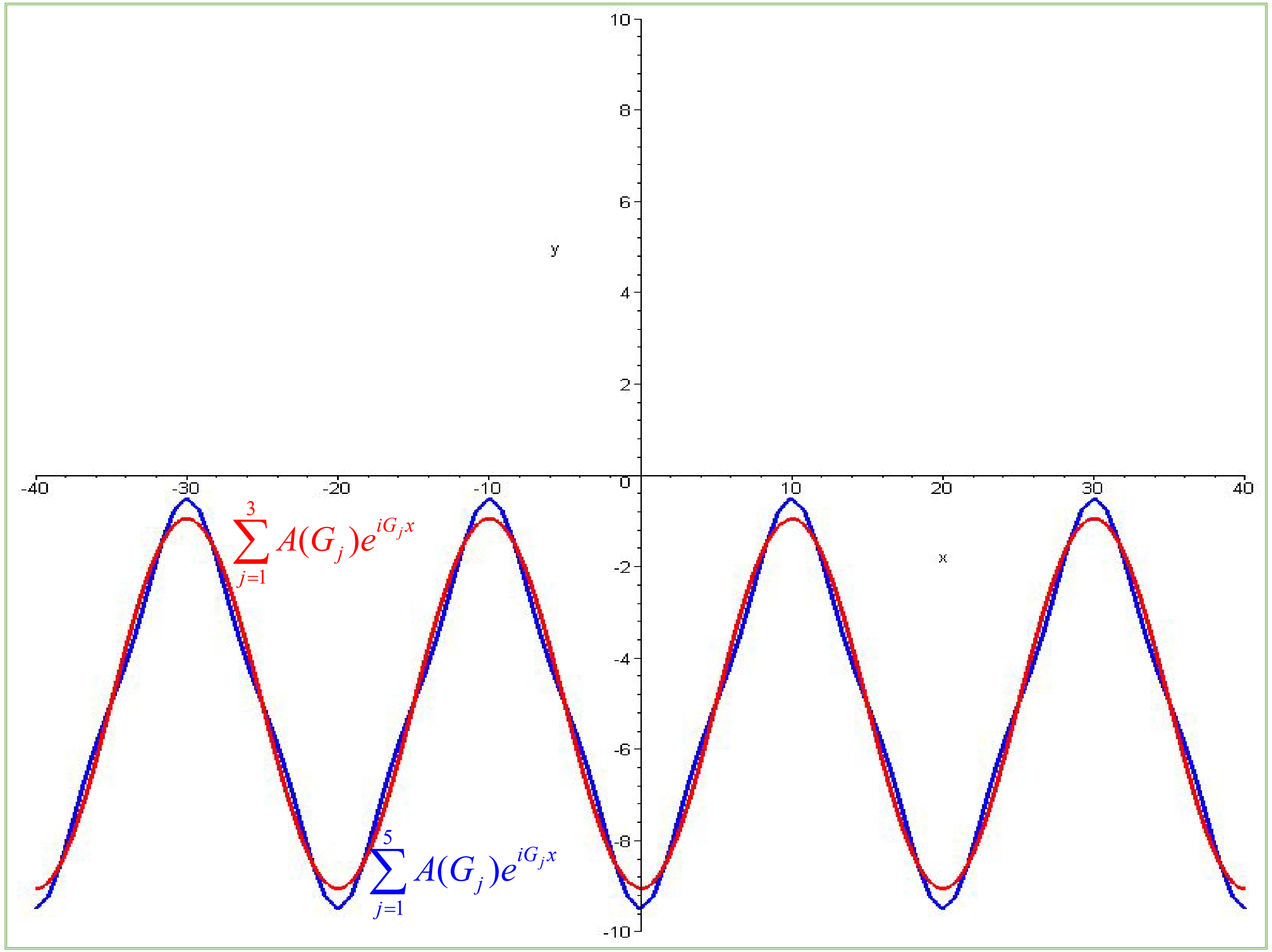
$$A(G_5)=\frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} e^{iG_5x} f(x)\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(G_5x)(x-\frac{a}{2})\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(\frac{4\pi}{a}x)(x-\frac{a}{2})\,dx=0$$

$$A(G_6)=\frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} e^{iG_6x} f(x)\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(G_6x)(x-\frac{a}{2})\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(\frac{6\pi}{a}x)(x-\frac{a}{2})\,dx=-\frac{a}{9\pi^2}=-\frac{20}{9\pi^2}$$

$$A(G_7)=\frac{1}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} e^{iG_7x} f(x)\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(G_7x)(x-\frac{a}{2})\,dx=2\frac{1}{a}\int_0^{\frac{a}{2}}\cos(\frac{6\pi}{a}x)(x-\frac{a}{2})\,dx=-\frac{20}{9\pi^2}$$

$$\vdots$$

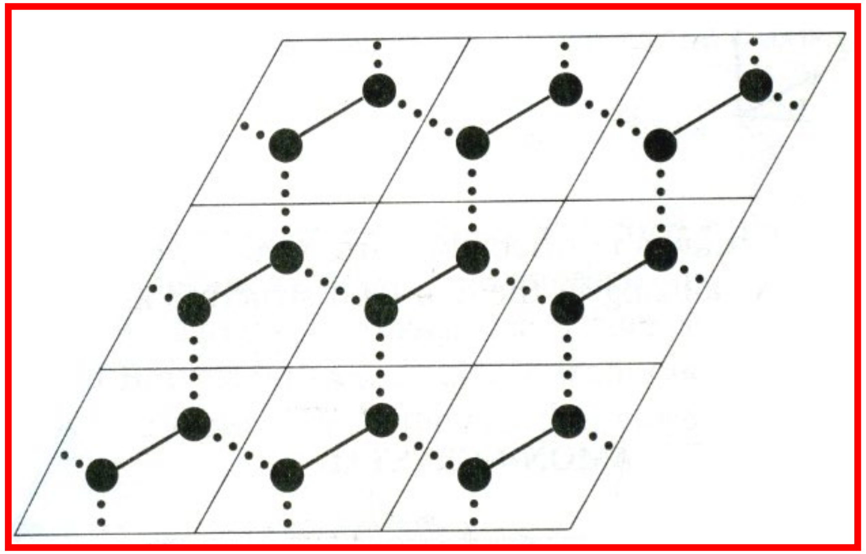
$$\begin{cases} \sum_{j=1}^{3} A(G_j)e^{iG_j x} = -5 - 2\times\frac{20}{\pi^2}\cos(\frac{2\pi}{a}x) = -5 - \frac{40}{\pi^2}\cos(\frac{\pi}{10}x) \\ \sum_{j=1}^{5} A(G_j)e^{iG_j x} = -5 - \frac{40}{\pi^2}\cos(\frac{\pi}{10}x) - \frac{40}{9\pi^2}\cos(\frac{3\pi}{10}x) \end{cases}$$



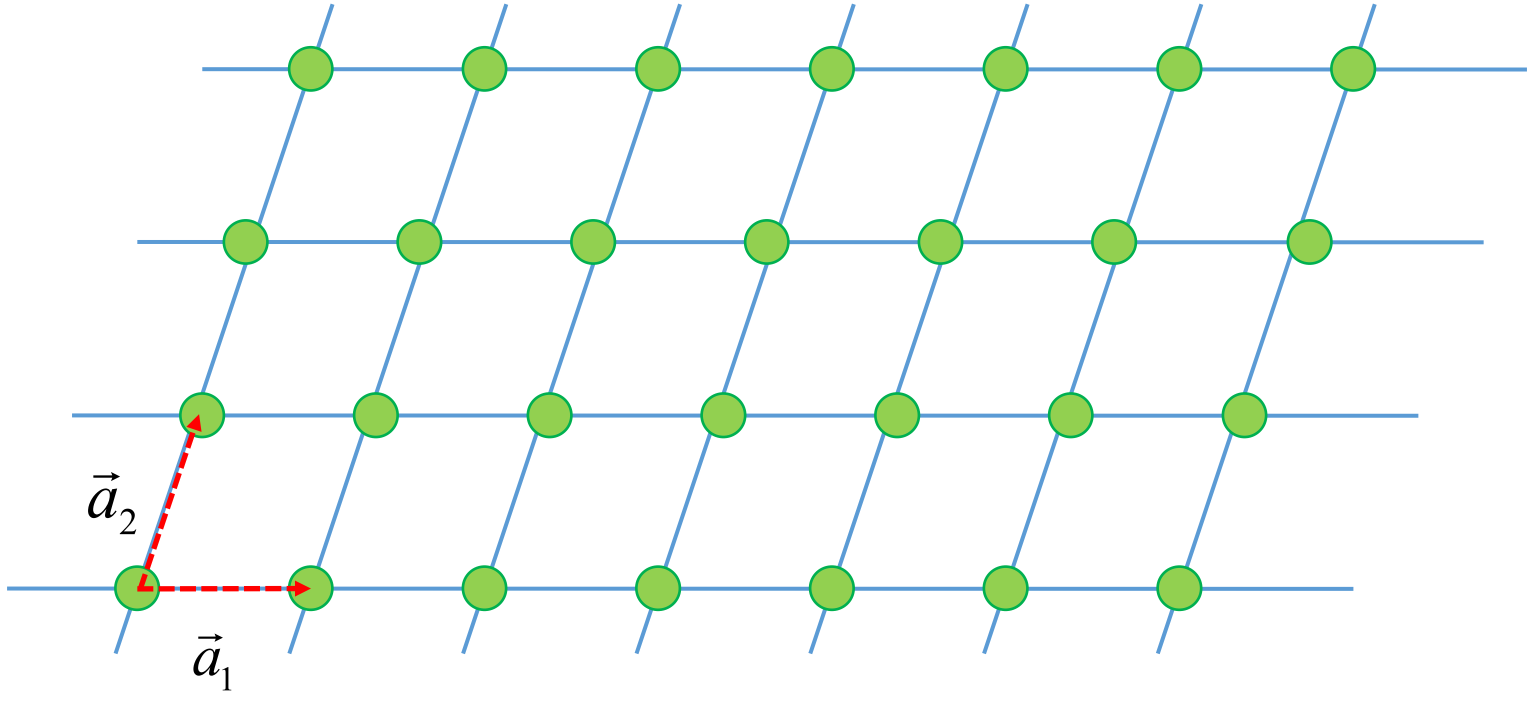
Example-1, the set of G-vectors

1. Consider the graphene structure, as a triangular lattice with $d_{CC} = 1.42\text{Å}$ and $a = \sqrt{3}d$.

2. Generate the set of the reciprocal vectors and give the labels in the increasing orders of its magnitude.



Part of solution for Example-1



Triangular lattice

$$\vec{a}_1 = (a,0,0)\ ,\ \vec{a}_2 = a(1/2,\sqrt{3}/2,0)\ ,\ \vec{a}_3 = (0,0,c)$$

$$\vec{b}_1 = \frac{2\pi}{V}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a}(1,-\frac{1}{\sqrt{3}},0)$$

$$\vec{b}_2 = \frac{2\pi}{V}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{a}(0,\frac{2}{\sqrt{3}},0)$$

$$\vec{G} = n\vec{b}_1 + l\vec{b}_2 + m\vec{b}_3$$

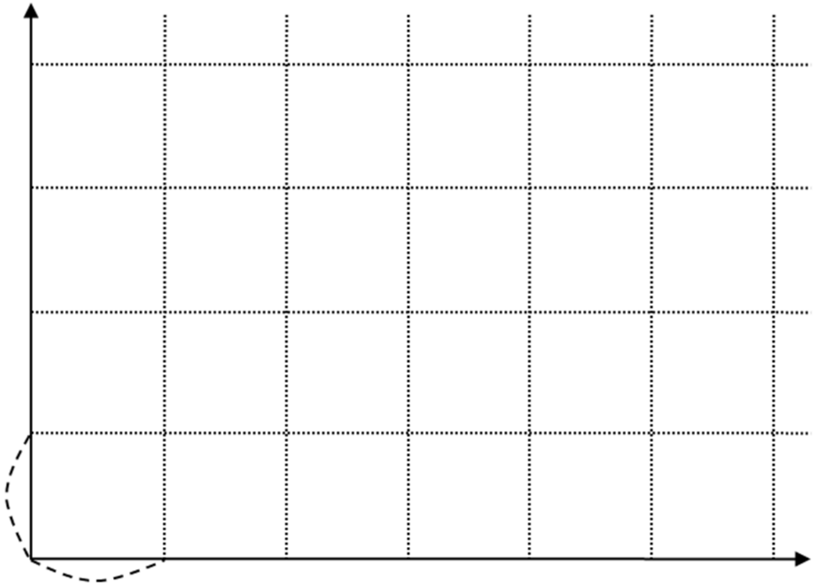
Example-2,

1. Think of a simple cubic lattice with the lattice constant of $3a$.

$$\vec{a}_1 = (a, 0, 0),\ \vec{a}_2 = (0, a, 0),\ \vec{a}_3 = (0, 0, a)$$

2. An atom is placed at the lattice point, as a source of the potential

$$v_{atom}(r) = \begin{cases} \dfrac{e^2}{a_c^{\ 3}}(r^2 - 2a_c^{\ 2}) & \text{for } r < a_c \\ -\dfrac{e^2}{r} & \text{for } r > a_c \end{cases}$$



Example-2,

1. Show that the summed atom potential is a cell-periodic quantity

$$V(\vec{r}) = \sum_{\vec{R}} v_{atom}(\vec{r} - \vec{R})$$

where the lattice translation vector $\vec{R} = n\vec{a}_1 + l\vec{a}_2 + m\vec{a}_3$

Show that

$$V(\vec{r}) = V(\vec{r} + \vec{R})$$

Example-2,

1. Now, let us think of the Fourier transformation of the periodic potential. Calculate the Fourier coefficient corresponding to each G-vecotor.

$$V(\vec{r}) = \sum_{\vec{R}} v_{atom}(\vec{r} - \vec{R}) = \sum_{\vec{G}} V(\vec{G}) e^{i\vec{G}\cdot\vec{r}} \quad ,\ldots, V(\vec{G}) = ???$$

2. Explicitly write the 10 lowest (leading) components of the potential ?

$$V(\vec{G}_1) = \ldots, V(\vec{G}_2) = \ldots, V(\vec{G}_3) = \ldots, V(\vec{G}_{10}) = \ldots$$

Part of the solution for Example-2

1. Fourier transformation of the infinite sum

$$V(\vec{r}) = \sum_{\lambda} v_{atom}(\vec{r} - \vec{R}_{\lambda}) = \sum_{\vec{G}} A(\vec{G}) e^{i\vec{G}\cdot\vec{r}},$$

$$A(\vec{G}) = \frac{1}{V_{cell}} \int_{cell} V(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r} = \frac{1}{V_{cell} N_{cell}} \int_{\infty} V(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r}$$

$$A(\vec{G}) = \frac{1}{V_{cell}} \frac{1}{N_{cell}} \int_{\infty} \sum_{\lambda} v_{atom}(\vec{r} - \vec{R}_{\lambda}) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r}$$

$$= \frac{1}{V_{cell}} \frac{1}{N_{cell}} \int_{\infty} \sum_{\lambda} v_{atom}(\vec{r}) e^{-i\vec{G}\cdot(\vec{r} + \vec{R}_{\lambda})} d^3\vec{r} = \frac{1}{V_{cell}} \frac{1}{N_{cell}} \int_{\infty} \sum_{\lambda} v_{atom}(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r}$$

$$= \frac{1}{V_{cell}} \int_{\infty} v_{atom}(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r}$$

Mathematics !!! For the Example-2

1. Plane waves in terms of spherical Bessel function

$$e^{-i\vec{G}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(Gr) \left[Y_{lm}(\hat{G}) \right]^* Y_{lm}(\hat{r})$$

Mathematics !!! For the Example-2

1. The spherical symmetric atom potential➔ the zeroth spherical Bessel

$$\frac{1}{V_{cell}}\int_{\infty} v_{atom}(r)e^{-i\vec{G}\cdot\vec{r}}d^3\vec{r} = \frac{4\pi}{V_{cell}}\int_{0}^{\infty} v_{atom}(r)r^2 j_0(Gr)dr$$

Example-2, Solution, Part

1. Fourier transformation of the infinite sum

$$U(\vec{r}) = \sum_{\vec{R}} \sum_{\vec{\tau}} v_{atom,\tau}(\vec{r} - \vec{\tau} - \vec{R}) = \sum_{\vec{G}} A(\vec{G}) e^{i\vec{G}\cdot\vec{r}},$$

$$A(\vec{G}) = \frac{1}{V_{cell}} \int \sum_{\vec{R}} \sum_{\vec{\tau}} v_{atom,\tau}(\vec{r} - \vec{\tau} - \vec{R}) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r} = \frac{1}{V_{cell}} \frac{1}{N} \int_{\infty} \sum_{\vec{R}} \sum_{\vec{\tau}} v_{atom,\tau}(\vec{r} - \vec{\tau} - \vec{R}) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r}$$

$$= \frac{1}{V_{cell}} \frac{1}{N} \int_{\infty} \sum_{\vec{R}} \sum_{\vec{\tau}} v_{atom,\tau}(\vec{r}) e^{-i\vec{G}\cdot(\vec{r} + \vec{\tau} + \vec{R}_{\lambda})} d^3\vec{r} = \frac{1}{V_{cell}} \sum_{\vec{\tau}} e^{-i\vec{G}\cdot\vec{\tau}} \int_{\infty} v_{atom,\tau}(r) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r}$$

Mathematics !!! For the Example-2

1. The integral

$$\int_{\infty} v_{atom,\tau}(r) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r} = \int_{\infty} \left(v_{atom,\tau}(r) + \frac{e^2}{r} \right) e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r} - \int_{\infty} \frac{e^2}{r} e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r}$$

$$= 4\pi \int_0^{a_c} \frac{e^2}{a_c{}^3} (r^2 - 2a_c{}^2) r^2 j_0(Gr) dr - \int_{\infty} \frac{e^2}{r} e^{-i\vec{G}\cdot\vec{r}} d^3\vec{r}$$

$$= 4\pi \int_0^{a_c} \frac{e^2}{a_c{}^3} (r^2 - 2a_c{}^2) r^2 \frac{\sin(Gr)}{Gr} dr - \frac{e^2 4\pi}{G^2}$$

$$v_{atom}(r) = \begin{cases} \dfrac{e^2}{a_c{}^3}(r^2 - 2a_c{}^2) & \text{for } r < a_c \\ -\dfrac{e^2}{r} & \text{for } r > a_c \end{cases}$$