Day-4

I. Momentum operator and translation operator

II. Angular momentum operator and rotation operator

Momentum = translation generator

1. Defining property of the momentum operator

$$\left\langle \mathbf{x} \middle| \hat{T}[\mathbf{d}] \middle| \psi \right\rangle = \psi(\mathbf{x}+\mathbf{d}), \text{ where } \left\langle \mathbf{x} \middle| \psi \right\rangle = \psi(\mathbf{x})$$

$$\hat{T}[\mathbf{d}] = e^{i\frac{1}{\hbar}\mathbf{d}\cdot\hat{\mathbf{p}}} \doteq e^{i\frac{1}{\hbar}\mathbf{d}\cdot(-i\hbar\nabla)} = e^{\mathbf{d}\cdot\nabla}$$

2. For example, in one-dimension

$$e^{i\frac{1}{\hbar}d\cdot\hat{p}}\psi(x) = e^{d\frac{\partial}{\partial x}}\psi(x) = \sum_{n=0}^{\infty}\frac{1}{n!}d^n\frac{\partial^n}{\partial x^n}\psi(x) = \psi(x+d)$$

Momentum = translation generator

1. Eigenstates of momentum operator = eigenstates of translation operator

$$\hat{\mathbf{p}}\,\psi_{\mathbf{k}}(\mathbf{r}) = \hbar\mathbf{k}\,\psi_{\mathbf{k}}(\mathbf{r})$$

$$e^{i\frac{1}{\hbar}\mathbf{d}\cdot\hat{\mathbf{p}}}\psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r}+\mathbf{d}) = e^{i\mathbf{k}\cdot\mathbf{d}}\psi_{\mathbf{k}}(\mathbf{r})$$

2. The momentum eigenstates are the eigenstates of translation operators with $\vec{d}$ being finite or infinitesimal.

Angular momentum = Rotation generator

1. Defining property of the momentum operator

$$\left\langle \mathbf{x} \middle| \hat{R}_z[\varphi] \middle| \psi \right\rangle = \psi(r,\theta,\phi+\varphi), \text{ where } \left\langle \mathbf{x} \middle| \psi \right\rangle = \psi(r,\theta,\phi)$$

$$\hat{R}_z[\varphi] = e^{i\frac{1}{\hbar}\hat{L}_z\varphi} \doteq e^{i\frac{1}{\hbar}\varphi(-i\hbar\frac{\partial}{\partial\varphi})} = e^{\varphi\frac{\partial}{\partial\varphi}}$$

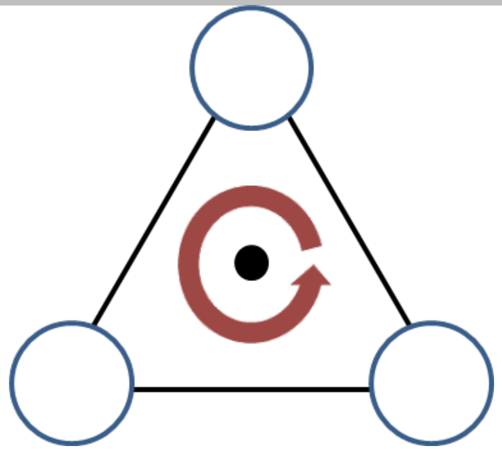
2. For example, for a given axis of rotation

$$e^{i\frac{1}{\hbar}\hat{L}_z\varphi}\psi(r,\theta,\phi) = \sum_{n=0}^{\infty}\frac{1}{n!}\varphi^n\frac{\partial^n}{\partial\varphi^n}\psi(r,\theta,\phi) = \psi(r,\theta,\phi+\varphi)$$

3. The Angular momentum eigenstates are the eigenstate of rotation operator with finite or infinitesimal rotation.

Discrete rotation

1. The system might not be fully isotropic, but symmetric for finite rotation. Then, we may need to consider the rotation operator with finite rotation.



$$\hat{R}\left(\frac{2\pi}{3}\right)|\psi\rangle = \lambda|\psi\rangle$$

$$\left[\hat{R}\left(\frac{2\pi}{3}\right)\right]^3|\psi\rangle = \hat{R}\left(\frac{2\pi}{3}\right)\hat{R}\left(\frac{2\pi}{3}\right)\hat{R}\left(\frac{2\pi}{3}\right)|\psi\rangle = \lambda^3|\psi\rangle$$

$$\lambda^3 = 1, \lambda = \exp\left(i\frac{2\pi l}{3}\right), l = 0,1,2$$

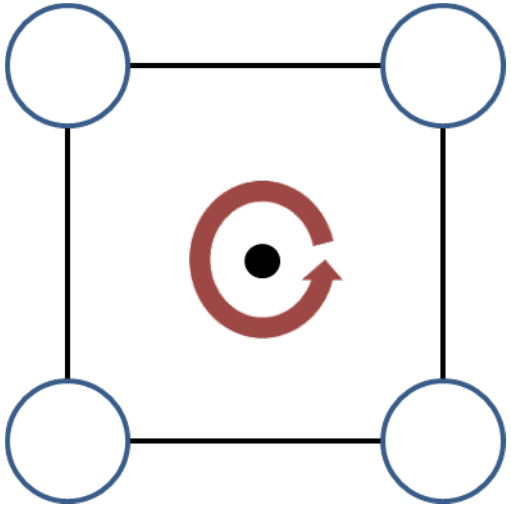
2. Three distinct eigenstates for $\hat{R}[\frac{2\pi}{3}]$

$$\hat{R}\left(\frac{2\pi}{3}\right)\psi_l(\theta) = \psi_l\left(\theta + \frac{2\pi}{3}\right) = e^{i\frac{2\pi}{3}l}\ \psi_l(\theta),$$

$$l = 0,1,2(any \text{ consecutive three integer})$$

Discrete rotation

4. Four distinct eigenstates for $\hat{R}[\frac{2\pi}{4}]$



$$\hat{R}\left(\frac{2\pi}{4}\right)|\psi\rangle = \lambda|\psi\rangle$$

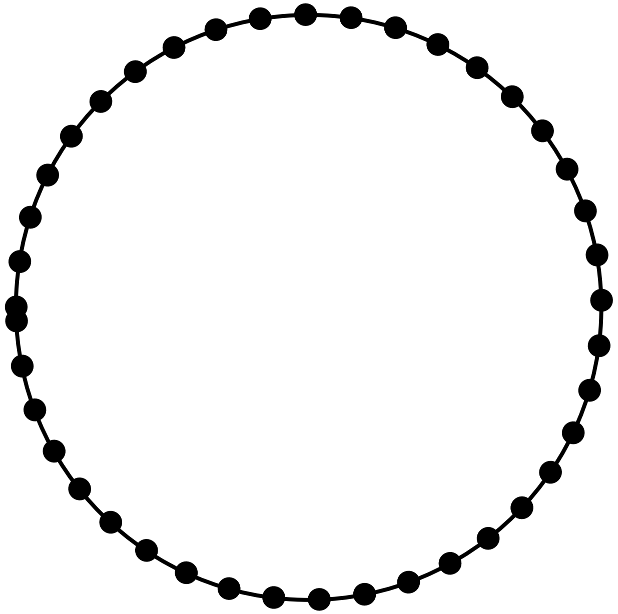
$$\left[\hat{R}\left(\frac{2\pi}{4}\right)\right]^4 |\psi\rangle = \lambda^4|\psi\rangle$$

$$\lambda^4 = 1, \lambda = \exp\left(i\frac{2\pi l}{4}\right)(l = 0,1,2,3)$$

eigen state of $\hat{R}\left(\frac{2\pi}{4}\right)$ $|\psi_l\rangle$

$$\hat{R}\left(\frac{2\pi}{4}\right)\psi_l(\theta) = \psi_l\left(\theta + \frac{2\pi}{4}\right) = e^{i\frac{2\pi}{4}l}\ \psi_l(\theta)$$

Discrete rotation operator of $\hat{R}[\frac{2\pi}{N}]$



$$\hat{R}\left(\frac{2\pi}{N}\right)|\psi\rangle = \lambda|\psi\rangle$$

$$\left[\hat{R}\left(\frac{2\pi}{N}\right)\right]^N = \hat{R}\left(\frac{2\pi}{N}\right)\cdots\hat{R}\left(\frac{2\pi}{N}\right)|\psi\rangle = \lambda^N|\psi\rangle$$

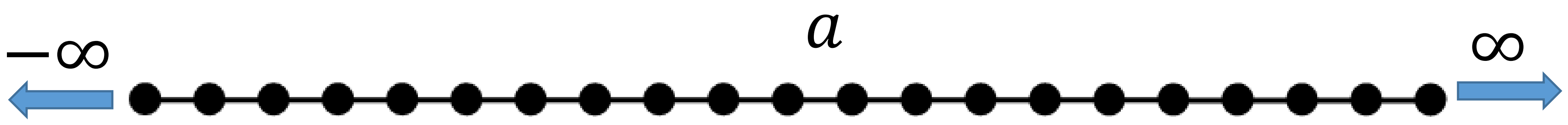
$$\lambda^N = 1, \lambda = \exp\left(i\frac{2\pi l}{N}\right)(l = 0,\cdots, N-1)$$

The eigenstate of $\hat{R}\left(\frac{2\pi}{N}\right)$, $|\psi_l\rangle$

$$\hat{R}\left(\frac{2\pi}{N}\right)\psi_l(\theta) = \psi_l\left(\theta + \frac{2\pi}{N}\right) = e^{i\frac{2\pi}{N}l}\ \psi_l(\theta)$$

Discrete translation

1. The system might not be fully homogeneous, but symmetric with respect to finite translations.

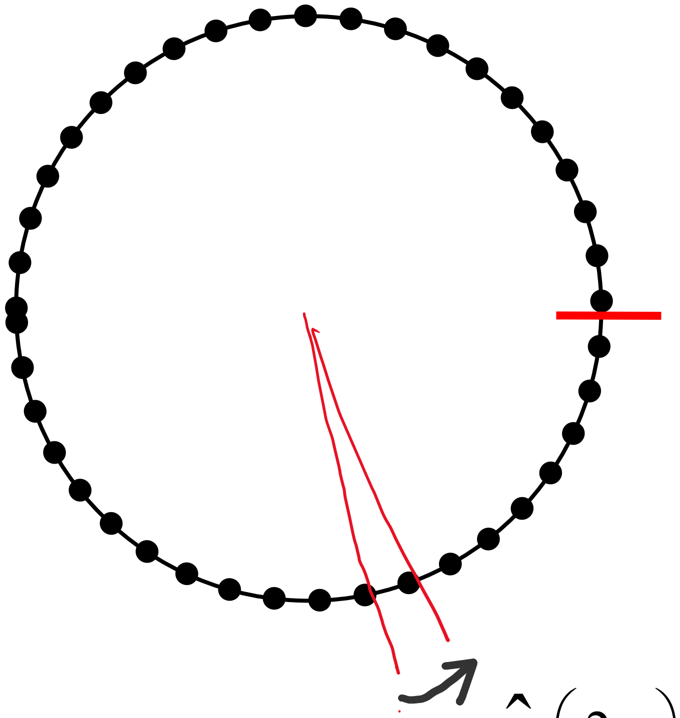


2. Now, let us think of the eigenstates of translation operator

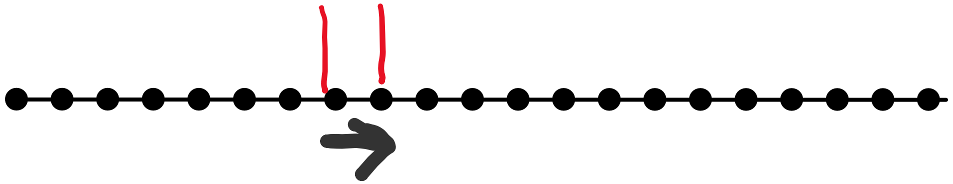
$$\hat{T}[a]\psi_{\lambda}(x) = \psi_{\lambda}(x+a) = \lambda\psi_{\lambda}(x)$$

Discrete translation, Born-von-Karman

1. Apply the Born-von-Karman boundary condition.



$$\hat{R}\left(\frac{2\pi}{N}\right)$$



$$\hat{T}[a]$$

Discrete translation, Born-von-Karman

$$\hat{T}[a]\psi(x) = \lambda\psi(x)$$

$$\left\{\hat{T}[a]\right\}^N \psi(x) = \psi(x+Na) = \lambda^N\psi(x)$$

$$\lambda^N = 1, \lambda_l = \exp\left(i\frac{2\pi l}{N}\right) \quad \left(l = 0, \cdots, N-1\right)$$

$$\lambda_l = \exp\left(i\frac{2\pi}{a}\frac{l}{N}a\right), \quad k_l = \frac{2\pi}{a}\frac{l}{N}, \ \lambda_l = \exp\left(ik_l a\right)$$

$$N \to \infty, 0 \le k < \frac{2\pi}{a}$$

Discrete translation

1. The eigenstate of discrete translation $R = Na$

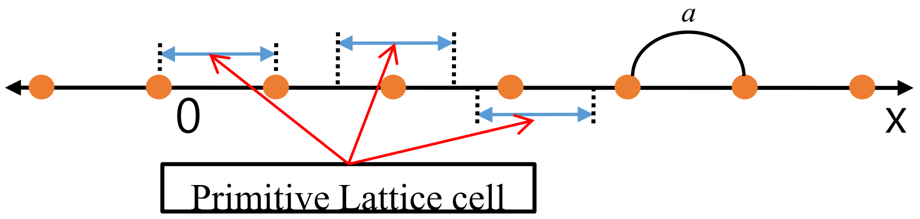
$$\hat{T}[a]\psi_k(x) = \psi_k(x+a) = e^{ika}\psi_k(x)$$

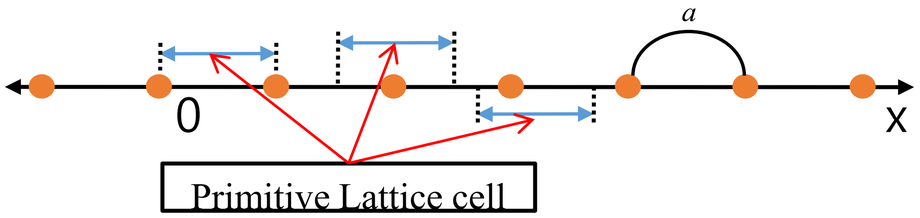
$$\hat{T}[R]\psi_k(x) = \psi_k(x+Na) = (e^{ika})^N\psi_k(x) \text{ , with } R = Na.$$

$$\hat{T}[R]\psi_k(x) = e^{ikR}\psi_k(x)$$

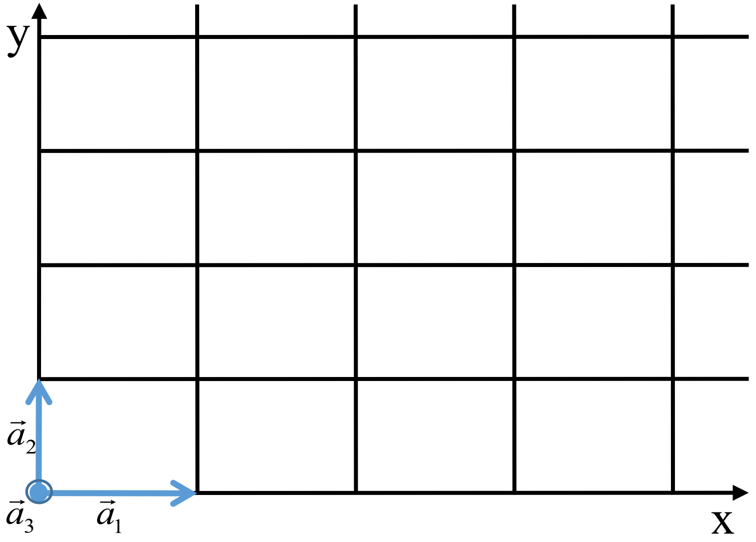
2. *k* can be found in the unit cell of reciprocal lattice, or the first Brillouin zone.

$$k \in \begin{cases} \left\{k \middle| 0 \le k < \frac{2\pi}{a}\right\} \\ or \\ \left\{k \middle| -\frac{\pi}{a} \le k < \frac{\pi}{a}\right\} \\ or \\ \cdots \end{cases}$$



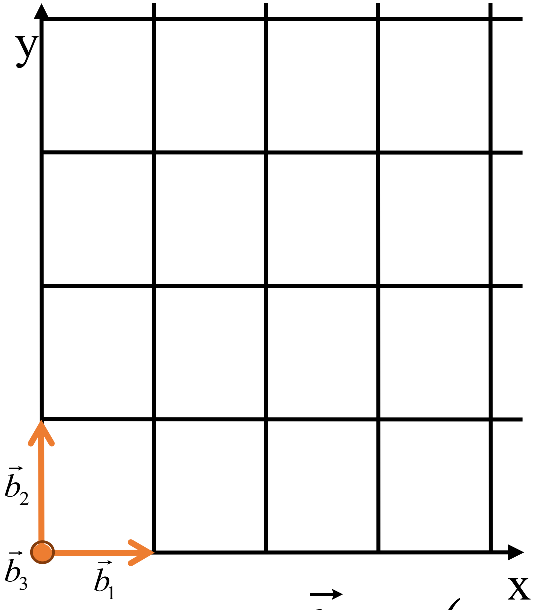


Discrete translation in three dimension



Primitive Lattice Vector

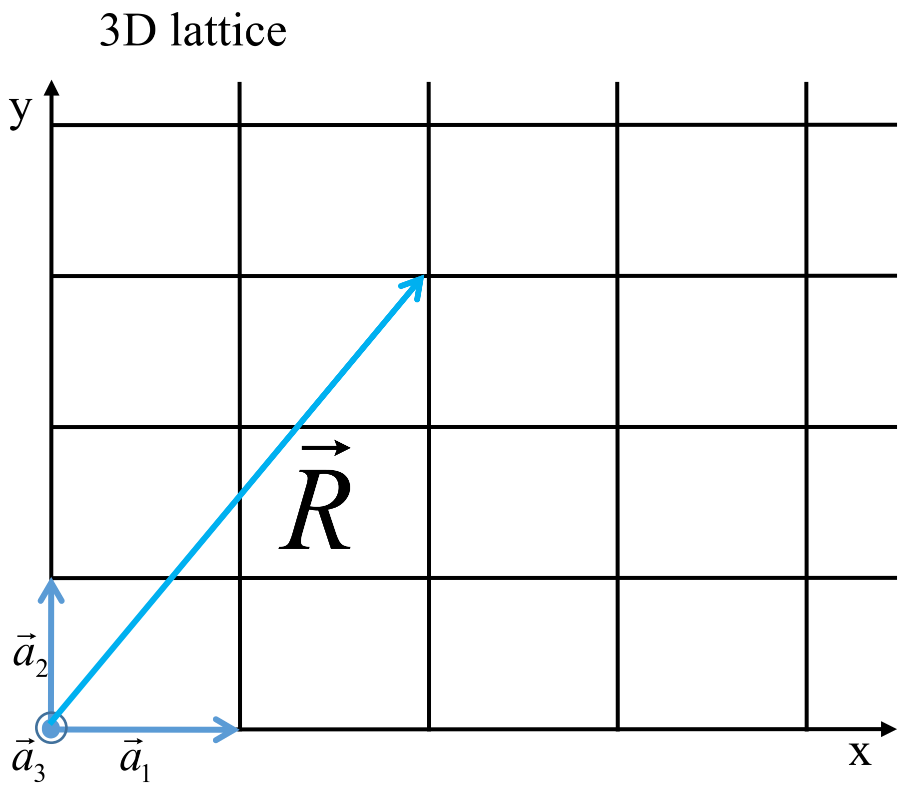
$$\vec{a}_1 = a_1\hat{x}$$
$$\vec{a}_2 = a_2\hat{y}$$
$$\vec{a}_3 = a_3\hat{z}$$

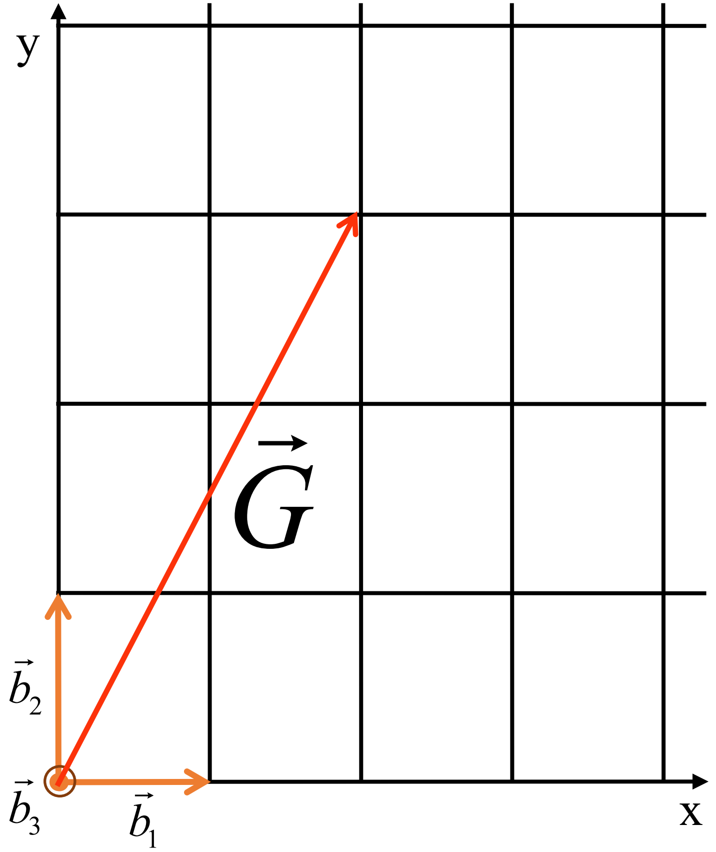


Reciprocal Lattice: Primitive Vector

$$\vec{b}_1 = (2\pi/a_1)\hat{x}$$
$$\vec{b}_2 = (2\pi/a_2)\hat{y}$$
$$\vec{b}_3 = (2\pi/a_3)\hat{z}$$

Discrete translation in three dimension





Lattice Vector

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

Reciprocal Lattice Vector

$$\vec{G} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$$

Discrete translation

1. Very straightforward extension of the theory for one dimension.

$$\hat{T}[\vec{a}_1]\psi_{k_1}(x,y,z) = \psi_{k_1}(x+a_1,y,z) = e^{ik_1a_1}\psi_{k_1}(x,y,z)$$

$$\hat{T}[\vec{a}_2]\psi_{k_2}(x,y,z) = \psi_{k_2}(x,y+a_2,z) = e^{ik_2a_2}\psi_{k_2}(x,y,z)$$

$$\hat{T}[\vec{a}_3]\psi_{k_3}(x,y,z) = \psi_{k_3}(x,y,z+a_3) = e^{ik_3a_3}\psi_{k_3}(x,y,z)$$

$$T[\vec{a}_1+\vec{a}_2+\vec{a}_3]\psi_{k_1,k_2,k_3}(x,y,z) = \hat{T}[\vec{a}_3]\hat{T}[\vec{a}_2]\hat{T}[\vec{a}_1]\psi_{k_1,k_2,k_3}(x,y,z) = \exp[i(k_1a_1+k_2a_2+k_3a_3)]\psi_{k_1,k_2,k_3}(x,y,z)$$

2. For an arbitrary discrete translations

$$T[l\vec{a}_1+m\vec{a}_2+n\vec{a}_3]\psi_{k_1,k_2,k_3}(x,y,z) = (\hat{T}[\vec{a}_3])^l(\hat{T}[\vec{a}_2])^m(\hat{T}[\vec{a}_1])^n\psi_{k_1,k_2,k_3}(x,y,z) = \exp[i(lk_1a_1+mk_2a_2+nk_3a_3)]\psi_{k_1,k_2,k_3}(x,y,z)$$

$$\text{with } \vec{R} = l\vec{a}_1+m\vec{a}_2+n\vec{a}_3 \quad \text{and } \vec{k} = (k_x,k_y,k_z)$$

$$T[\vec{R}]\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\psi_{\vec{k}}(\vec{r})$$

Discrete translation

1. All the distinct eigenvalue (the $\vec{k}$) can be sufficiently found in the unit cell of the reciprocal lattice or in the first Brillouin zone.