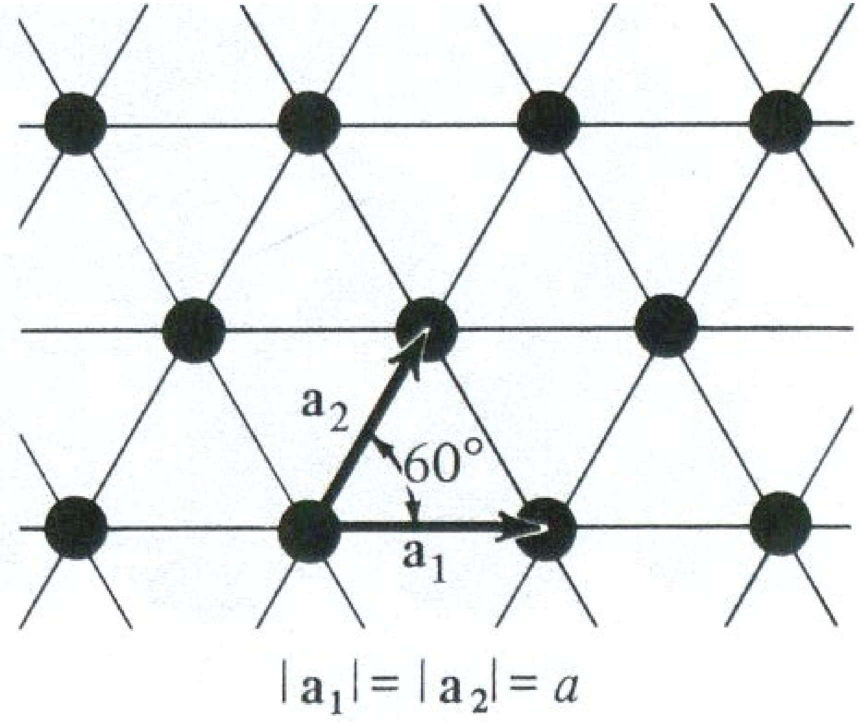
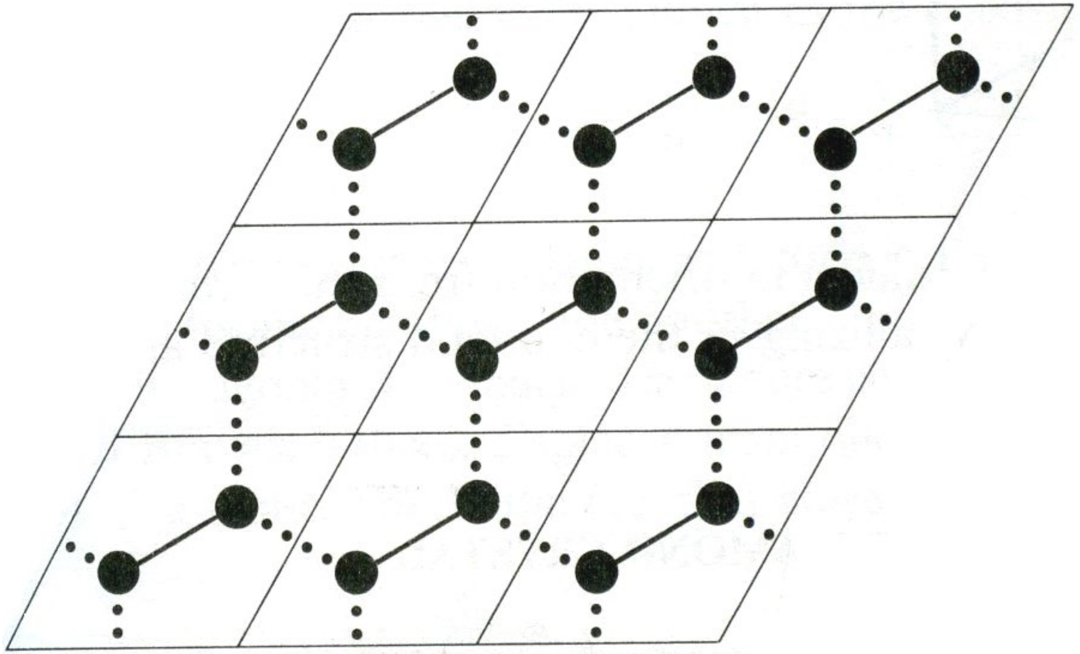
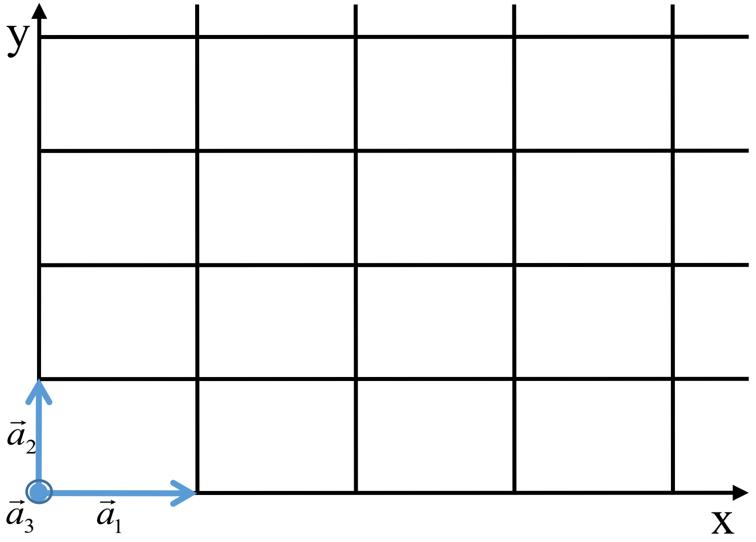
Translation eigenstate

I. The concept of translation eigenstate can be straightly applied to the lattices of non-orthorhombic cell.





Discrete translation in three dimension

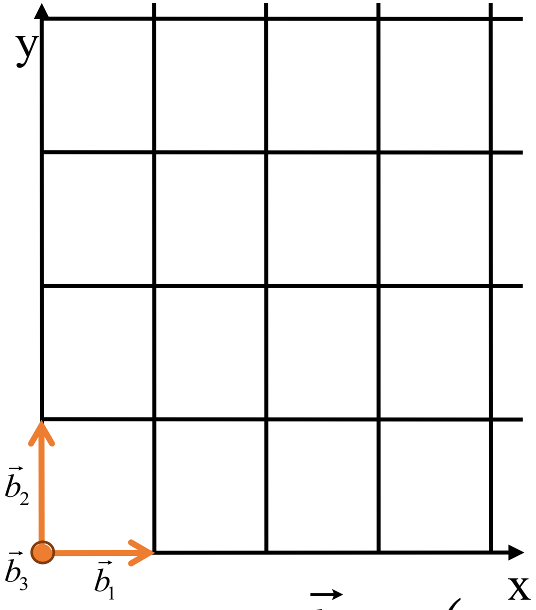


Primitive Lattice Vector

$$\vec{a}_1 = a_1\hat{x}$$

$$\vec{a}_2 = a_2\hat{y}$$

$$\vec{a}_3 = a_3\hat{z}$$



Reciprocal Lattice: Primitive Vector

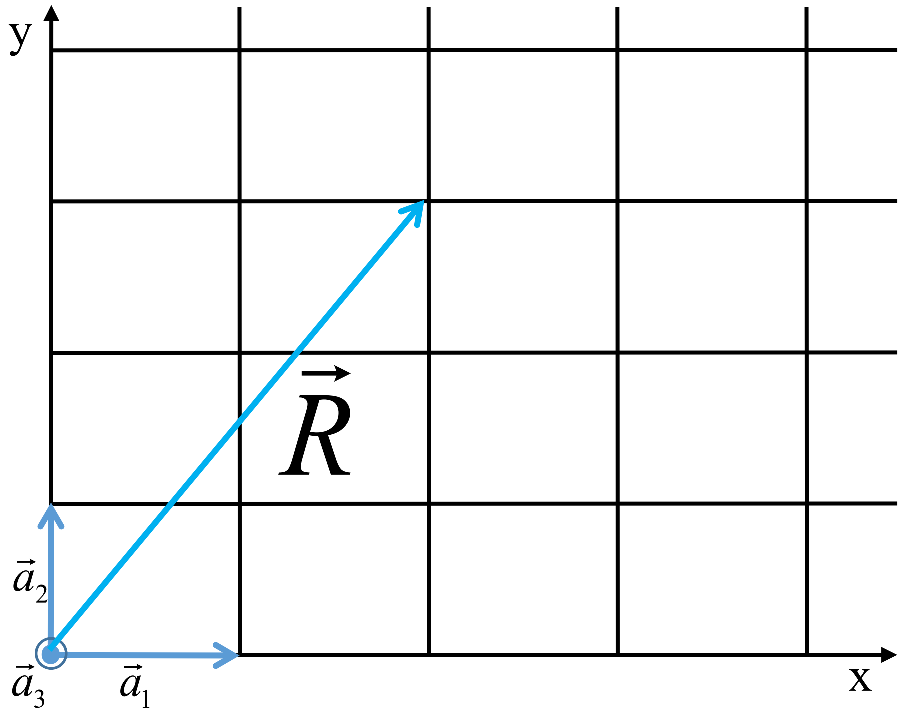
$$\vec{b}_1 = \left(2\pi/a_1\right)\hat{x}$$

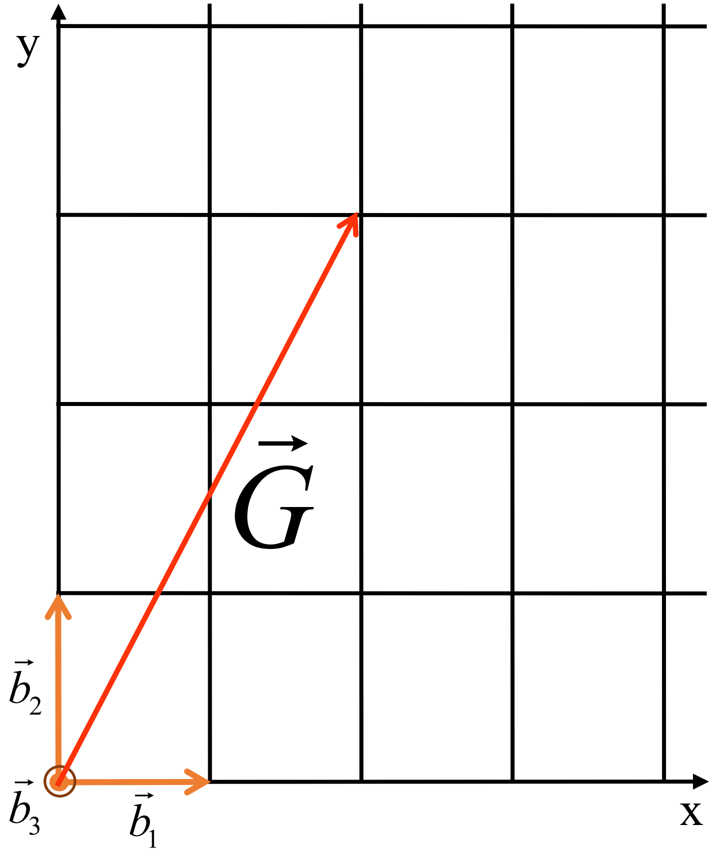
$$\vec{b}_2 = \left(2\pi/a_2\right)\hat{y}$$

$$\vec{b}_3 = \left(2\pi/a_3\right)\hat{z}$$

Discrete translation in three dimension

3D lattice





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

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

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

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

Born-von-Karman boundary condition

1. For a very large number N_1, N_2, N_3

$$\hat{T}[N_1\vec{a}_1]\psi_{k_1}(x,y,z) = \psi_{k_1}(x+N_1a_1,y,z) = e^{iN_1k_1a_1}\psi_{k_1}(x,y,z)\ ,\ \ k_1 = \frac{2\pi}{a_1}\frac{l}{N_1}$$

$$\hat{T}[N_2\vec{a}_2]\psi_{k_2}(x,y,z) = \psi_{k_2}(x,y+N_2a_2,z) = e^{iN_2k_2a_2}\psi_{k_2}(x,y,z)\ ,\ \ k_2 = \frac{2\pi}{a_2}\frac{m}{N_2}$$

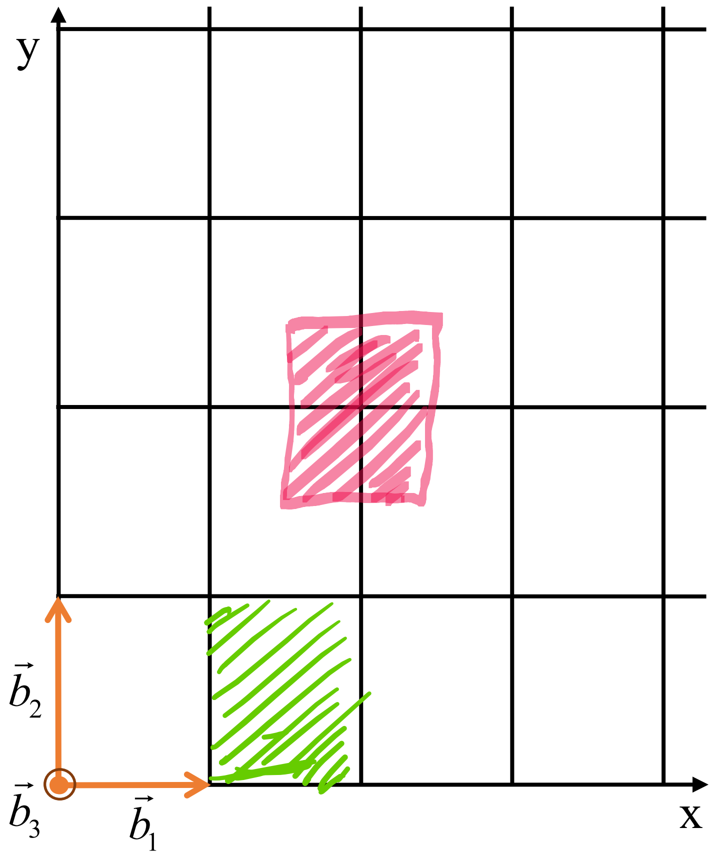
$$\hat{T}[N_3\vec{a}_3]\psi_{k_3}(x,y,z) = \psi_{k_3}(x,y,z+N_3a_3) = e^{iN_3k_3a_3}\psi_{k_3}(x,y,z)\ ,\ \ k_2 = \frac{2\pi}{a_3}\frac{n}{N_3}$$

2. For an arbitrary discrete translations

$$\vec{k} = (k_1,k_2,k_3) = \frac{l}{N_1}\vec{b}_1 + \frac{m}{N_2}\vec{b}_2 + \frac{n}{N_3}\vec{b}_3$$

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.



Translation eigenstate

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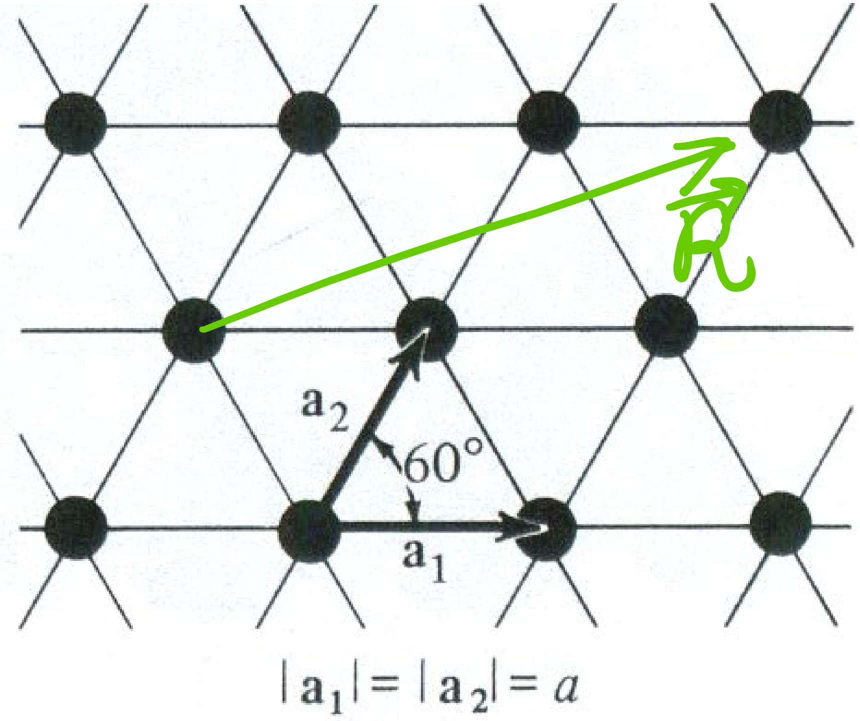
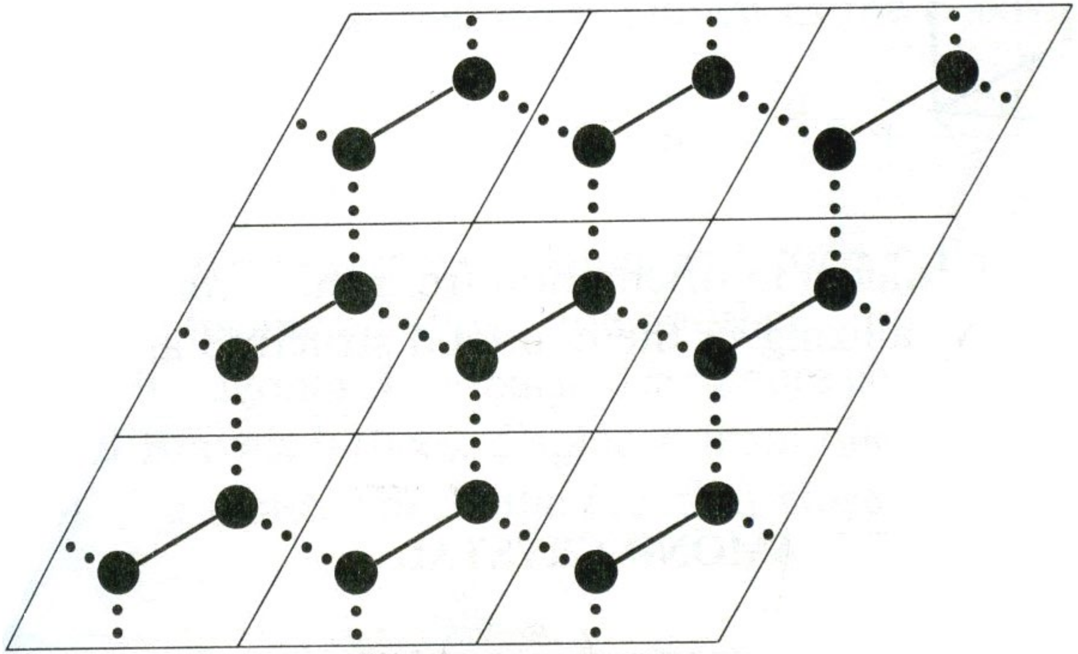




Discrete translation

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

$$\hat{T}[\vec{a}_1]\psi_{\vec{k}}(\mathbf{r}) = \psi_{\vec{k}}(\mathbf{r}+\vec{a}_1) = e^{i\vec{k}\cdot\vec{a}_1}\psi_{\vec{k}}(\mathbf{r})$$

$$\hat{T}[\vec{a}_2]\psi_{\vec{k}}(\mathbf{r}) = \psi_{\vec{k}}(\mathbf{r}+\vec{a}_1) = e^{i\vec{k}\cdot\vec{a}_2}\psi_{\vec{k}}(\mathbf{r})$$

$$\hat{T}[\vec{a}_2]\psi_{\vec{k}}(\mathbf{r}) = \psi_{\vec{k}}(\mathbf{r}+\vec{a}_3) = e^{i\vec{k}\cdot\vec{a}_3}\psi_{\vec{k}}(\mathbf{r})$$

$$T[l\vec{a}_1 + m\vec{a}_2 + n\vec{a}_3]\psi_{\vec{k}}(\mathbf{r}) = \hat{T}[l\vec{a}_3]\hat{T}[m\vec{a}_2]\hat{T}[n\vec{a}_1]\psi_{\vec{k}}(\mathbf{r}) = \exp[i\vec{k}\cdot(l\vec{a}_1 + m\vec{a}_2 + n\vec{a}_3)]\psi_{\vec{k}}(\mathbf{r})$$

2. For an arbitrary discrete translations

Born-von-Karman boundary condition

1. Think of Born-von-Karman boundary condition along $\vec{a}_1$, $\vec{a}_2$,$\vec{a}_3$ direction.

$$\hat{T}[N_1\vec{a}_1]\psi_{\vec{k}}(\mathbf{r}) = \psi_{\vec{k}}(\mathbf{r} + N_1\vec{a}_1) = e^{iN_1\vec{k}\cdot\vec{a}_1}\psi_{\vec{k}}(\mathbf{r})$$

$$\hat{T}[N_2\vec{a}_2]\psi_{\vec{k}}(\mathbf{r}) = \psi_{\vec{k}}(\mathbf{r} + N_1\vec{a}_1) = e^{iN_2\vec{k}\cdot\vec{a}_2}\psi_{\vec{k}}(\mathbf{r})$$

$$\hat{T}[N_3\vec{a}_2]\psi_{\vec{k}}(\mathbf{r}) = \psi_{\vec{k}}(\mathbf{r} + N_3\vec{a}_3) = e^{iN_3\vec{k}\cdot\vec{a}_3}\psi_{\vec{k}}(\mathbf{r})$$

2. For an arbitrary discrete translations

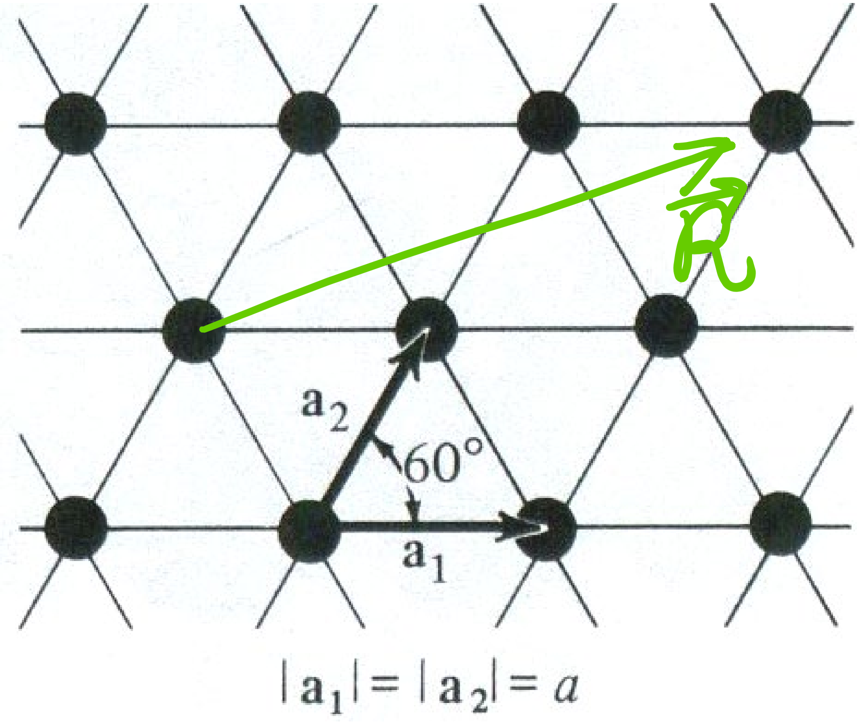
$$\vec{k}\cdot\vec{a}_1 = \frac{2\pi}{N_1}l \;,\quad \vec{k}\cdot\vec{a}_2 = \frac{2\pi}{N_2}m \;,\quad \vec{k}\cdot\vec{a}_3 = \frac{2\pi}{N_3}n$$

$$\vec{k} = \frac{l}{N_1}\vec{b}_1 + \frac{m}{N_2}\vec{b}_2 + \frac{n}{N_3}\vec{b}_3$$

Summary

The eigenstates for the lattice translation, the discrete translation

$\hat{T}[\vec{R}]\psi(\vec{r}) = \psi(\vec{r}+\vec{R})$ defintion of $\hat{T}[\vec{R}]$



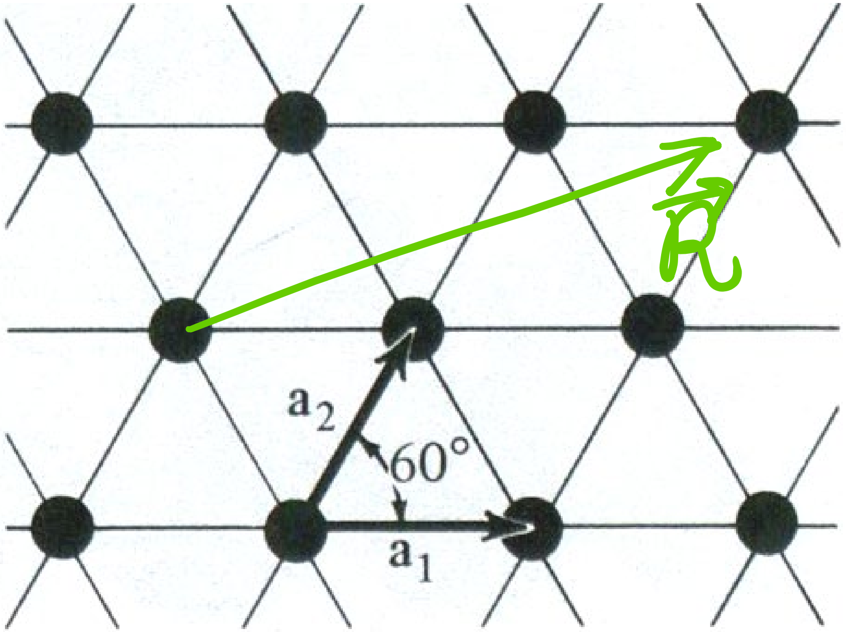
The eigenstate of $\hat{T}[\vec{R}]$

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

All distinct $\vec{k}$ can be found in the unit-cell of reciprocal la

Summary

Show that the eigenfunction for a discrete lattice translation, $\hat{T}[\vec{R}]$, can be written as $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r})$, where $u(\vec{r})$ is periodic over the translation.



$$\text{Set} \quad \psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r})$$

$$\text{Want to have} \quad \psi_{\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\psi_{\vec{k}}(\vec{r})$$

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

$$\text{We must have} \quad u(\vec{r}+\vec{R}) = u(\vec{r})$$