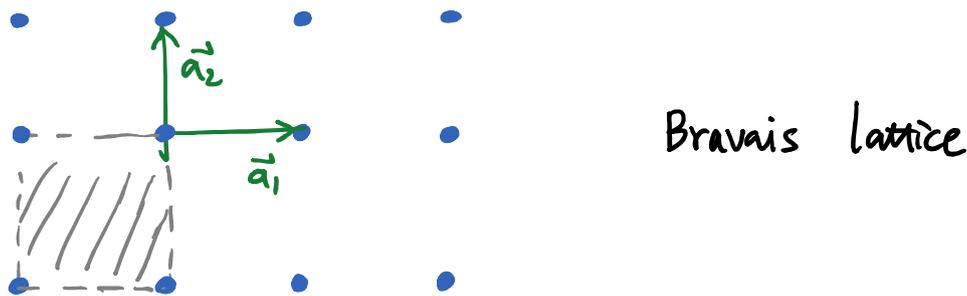


§3. Band electrons

* Electrons in a periodic potential

Single-electron problem:

$$H = -\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 + \underbrace{V(\vec{r})}_{\text{periodic potential}}$$



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

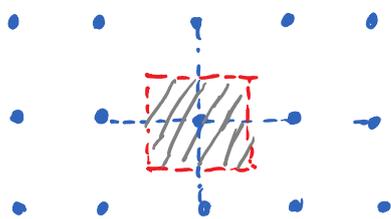
$$n_1, n_2, n_3 \in \mathbb{Z} \quad (\text{integers})$$

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

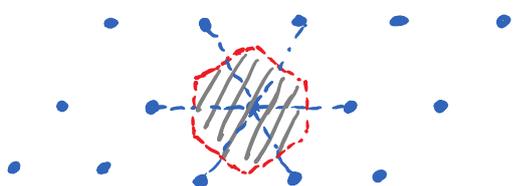
Periodic potential means $V(\vec{r}) = V(\vec{r} + \vec{R}_n)$.

⇒ Info. about $V(\vec{r})$ within a "unit cell" is sufficient!
(see, e.g. shaded region)

Wigner-Seitz cell: one choice of unit cell



Draw perpendicular lines
(planes in 3d) through
the center of all lines
connecting neighboring sites
of the Bravais Lattice.



Wigner-Seitz cell: shaded region

We certainly want to diagonalize H .

Before that, some general results can be derived
from the (discrete) translation symmetry, without
going into the microscopic details of $V(\vec{r})$.

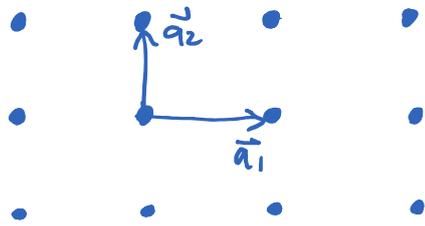
Fourier transformation:

$$V(\vec{r}) = \sum_m V_m e^{i\vec{G}_m \cdot \vec{r}} \quad \left. \begin{array}{l} \\ \\ \\ \end{array} \right\} \Rightarrow e^{i\vec{G}_m \cdot \vec{R}_n} = 1$$

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

\vec{G}_m : allowed Fourier components

- Reciprocal Lattice



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

$$n \in \mathbb{Z}$$

We need to determine all allowed \vec{G}_m satisfying

$$e^{i\vec{G}_m \cdot \vec{R}_n} = 1$$

$$\Rightarrow \vec{G}_m \cdot \vec{R}_n = 0, \pm 2\pi, 4\pi, \dots$$

Example: square lattice

$$\begin{cases} \vec{a}_1 = a \hat{x} \\ \vec{a}_2 = a \hat{y} \end{cases}$$

$$\vec{G} = G_x \hat{x} + G_y \hat{y}$$

$$\Rightarrow \begin{cases} e^{i\vec{G} \cdot \vec{a}_1} = e^{iG_x a} = 1 \\ e^{i\vec{G} \cdot \vec{a}_2} = e^{iG_y a} = 1 \end{cases}$$

$$G_x = 0, \pm \frac{2\pi}{a}, \pm \frac{4\pi}{a}, \dots \quad (\text{same for } G_y)$$

Solution for \vec{G}_m :

$$\vec{G}_m = m_1 \frac{2\pi}{a} \hat{x} + m_2 \frac{2\pi}{a} \hat{y}, \quad m_1, m_2 \in \mathbb{Z}$$

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④

General solution in 3D:

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

$$e^{i \vec{G}_m \cdot \vec{R}_n} = 1$$

$$\vec{G}_m = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \quad i, j = 1, 2, 3$$

\Rightarrow

$$\vec{b}_i = 2\pi \frac{\vec{a}_j \times \vec{a}_k}{\vec{a}_i \cdot (\vec{a}_j \times \vec{a}_k)}$$

2D: $\vec{G}_m = m_1 \vec{b}_1 + m_2 \vec{b}_2$ and $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2$
(x-y plane)

take $\vec{a}_3 = a \hat{z}$ and use the above formula

\Rightarrow \vec{b}_1, \vec{b}_2 in x,y plane

$$\vec{b}_3 = \frac{2\pi}{a} \hat{z}$$

1D: $\vec{G}_m = m_1 \vec{b}_1 = m_1 b \hat{x}$ and $\vec{R}_n = n_1 \vec{a}_1 = n_1 a \hat{x}$

$$\Rightarrow b = \frac{2\pi}{a}$$

$$\vec{G}_m = m_1 \frac{2\pi}{a} \hat{x}, \quad m_1 \in \mathbb{Z}$$

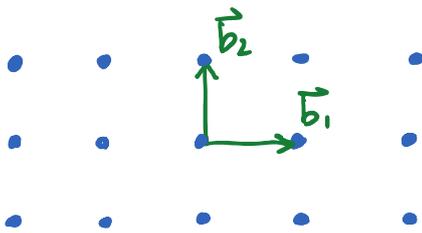
\vec{G}_m is called reciprocal lattice vectors,

which forms a reciprocal lattice.

Example: Reciprocal lattice of the square lattice

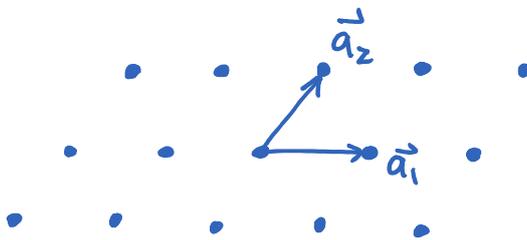
$$\vec{G}_m = m_1 \vec{b}_1 + m_2 \vec{b}_2 \quad \vec{R}_n : \begin{cases} \vec{a}_1 = a \hat{x} \\ \vec{a}_2 = a \hat{y} \end{cases}$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \Rightarrow \begin{cases} \vec{b}_1 = \frac{2\pi}{a} \hat{x} \\ \vec{b}_2 = \frac{2\pi}{a} \hat{y} \end{cases}$$



reciprocal lattice: square

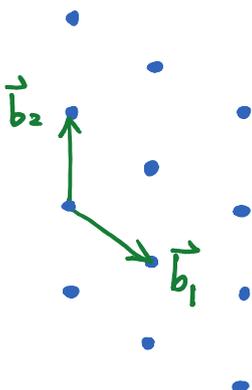
Example: Reciprocal lattice of the triangular lattice



$$\vec{R}_n : \begin{cases} \vec{a}_1 = a \hat{x} \\ \vec{a}_2 = \frac{a}{2} \hat{x} + \frac{\sqrt{3}a}{2} \hat{y} \end{cases}$$

$$\vec{G}_m = m_1 \vec{b}_1 + m_2 \vec{b}_2$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \Rightarrow \begin{cases} \vec{b}_1 = \frac{2\pi}{a} \hat{x} - \frac{2\pi}{\sqrt{3}a} \hat{y} \\ \vec{b}_2 = \frac{4\pi}{\sqrt{3}a} \hat{y} \end{cases}$$



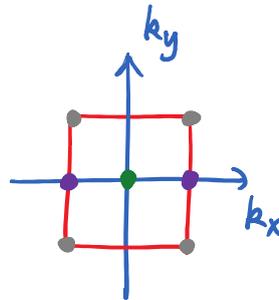
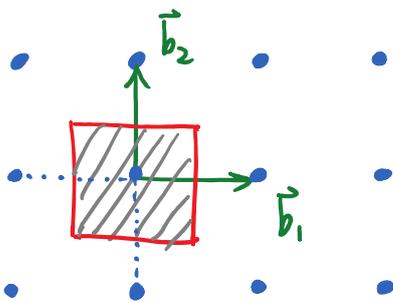
reciprocal lattice: triangular

- First Brillouin zone (FBZ)

The Wigner-Seitz primitive cell of the reciprocal lattice is called the FBZ.

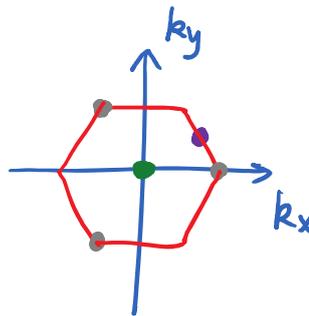
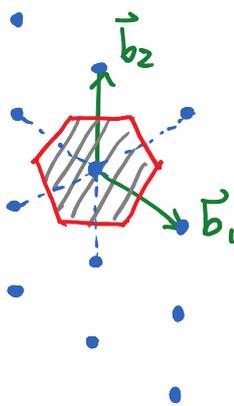
Other points are related to a point within the FBZ by shifting a proper \vec{G}_m .

Square:



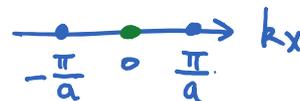
- P: $(0, 0)$
- M: $(\frac{\pi}{a}, \frac{\pi}{a})$
- X: $(\frac{\pi}{a}, 0)$

Triangular:



- P: $(0, 0)$
- K: $(\frac{4\pi}{3a}, 0)$
- M: $(\frac{\pi}{a}, \frac{\pi}{\sqrt{3}a})$

1D:



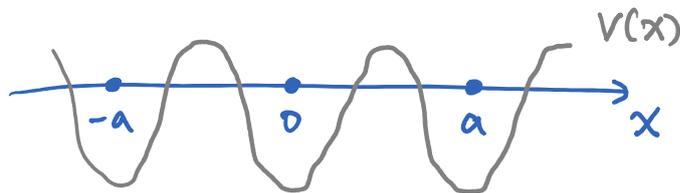
$$\text{FBZ: } k_x \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$$

- Floquet / Bloch theorem

Consider a single electron in a 1D periodic potential:

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

$$V(x) = V(x+na), \quad n \in \mathbb{Z}$$



$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E \psi(x)$$

No potential: $V(x) = 0$

Plane waves $\phi_k(x) = \frac{1}{\sqrt{L}} e^{ikx}$

With potential:

Eigenstates can be expanded using plane waves!
complete basis

Periodicity of $V(x)$ should be used for further simplifying the problem.

Give it a try and act H on a plane wave:

$$\begin{aligned} H \phi_k(x) &= \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \cdot \frac{1}{\sqrt{L}} e^{ikx} \\ &= \frac{\hbar^2 k^2}{2m} \phi_k(x) + V(x) \phi_k(x) \end{aligned}$$

Obviously, $\phi_k(x)$ is not an eigenstate, unless $\underline{V(x) = V}$.
trivial

Use the Fourier expansion of $V(x)$:

$$V(x) = \sum_{m \in \mathbb{Z}} V_m e^{iG_m x}$$

\downarrow
 $G_m = m \frac{2\pi}{a}, m \in \mathbb{Z}$

Required by $V(x) = V(x+na), n \in \mathbb{Z}$!

$$\begin{aligned} H \phi_k(x) &= \frac{\hbar^2 k^2}{2m} \phi_k(x) + \sum_{m \in \mathbb{Z}} V_m e^{im \frac{2\pi}{a} x} \phi_k(x) \\ &= \left(\frac{\hbar^2 k^2}{2m} + V_0 \right) \phi_k(x) + V_1 \phi_{k + \frac{2\pi}{a}}(x) \\ &\quad + V_2 \phi_{k + \frac{4\pi}{a}}(x) + \dots \end{aligned}$$

Hilbert space can be divided into subspaces:

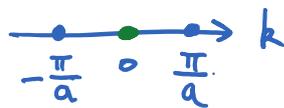
$$S_k = \left\{ \phi_k, \phi_{k \pm \frac{2\pi}{a}}, \phi_{k \pm \frac{4\pi}{a}}, \dots \right\}$$

$\rightarrow k \in \text{FBZ} !$

Thus, we just have to pick up a k -point in the FBZ and diagonalize H within the subspace S_k .

much smaller than the full Hilbert space

This is why we introduced the FBZ!



Remaining problem:

Consider a general ansatz within S_k

$$\psi_k(x) = \sum_{m \in \mathbb{Z}} f_{k,m} \phi_{k+m\frac{2\pi}{a}}(x)$$

superposition coefficient

and determine $f_{k,m}$ so that ψ_k is an eigenstate of H .

The particular form of $f_{k,m}$ depends on microscopic details, i.e. the form of $V(x)$.

The general eigenstates can be rewritten as

$$\psi_k(x) = \sum_{m \in \mathbb{Z}} f_{k,m} \underbrace{\phi_{k+m \frac{2\pi}{a}}(x)}_{= \frac{1}{\sqrt{L}} e^{i(k+m \frac{2\pi}{a})x}}$$

$$= \underbrace{u_k(x)} e^{ikx}$$

$$u_k(x) = \frac{1}{\sqrt{L}} \sum_{m \in \mathbb{Z}} f_{k,m} e^{im \frac{2\pi}{a} x}$$

Note that $u_k(x)$ is periodic in real space:

$$u_k(x+na) = u_k(x), \quad n \in \mathbb{Z}$$

So we only need $u_k(x)$ within a unit cell!
 $x \in [0, a]$

Floquet theorem:

The single-particle eigenstates of an electron

in a 1D periodic potential are product of

a periodic function and a plane-wave factor.

$$u_k(x)$$

$$e^{ikx}$$

30.04.19

①

Straightforward generalization to arbitrary dimensions:

$$\left[-\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 + \underbrace{V(\vec{r})} \right] \psi(\vec{r}) = E \psi(\vec{r})$$

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

Bloch theorem:

$$\psi_{\vec{k}}(\vec{r}) = \underbrace{u_{\vec{k}}(\vec{r})}_{\text{periodic}} e^{i\vec{k} \cdot \vec{r}}$$

$$\vec{k} \in \text{FBZ}$$

$$u_{\vec{k}}(\vec{r} + \vec{R}_n) = u_{\vec{k}}(\vec{r})$$

It's sufficient to determine $u_{\vec{k}}(\vec{r})$ within a unit cell.

