TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Solid State Theory (SS2020)

Lecture 9: Bloch theorem

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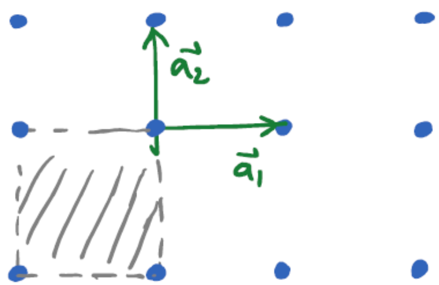
§ 3.1 Bloch theorem

- Electrons in a periodic potential:

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

Presence due to the crystal structure:



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

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

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

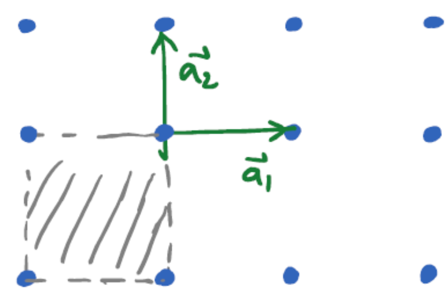
§ 3.1 Bloch theorem

- Electrons in a periodic potential:

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

Info. about $V(\vec{r})$: sufficient within a unit cell!

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



Fourier transform:

$$V(\vec{r}) = \sum_m V_m e^{i\vec{G}_m \cdot \vec{r}}$$

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

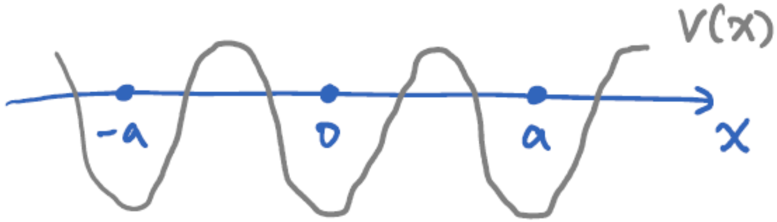
§ 3.1 Bloch theorem

- Before considering the particular form of $V(\vec{r})$ and diagonalizing H, it is always fruitful to derive general results from the symmetry of H, without going into the microscopic details.

  - Consider a single electron in a 1D periodic potential:

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

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



§ 3.1 Bloch theorem

- Before considering the particular form of $V(\vec{r})$ and diagonalizing H, it is always fruitful to derive general results from the symmetry of H, without going into the microscopic details.

  - Consider a single electron in a 1D periodic potential:

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

No potential: $V(x)=0$

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

§ 3.1 Bloch theorem

- Before considering the particular form of $V(\vec{r})$ and diagonalizing H, it is always fruitful to derive general results from the symmetry of H, without going into the microscopic details.

  - Consider a single electron in a 1D periodic potential:

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

With potential:

Eigenstates can be expanded using plane waves !

complete basis

§ 3.1 Bloch theorem

- 1D periodic potential:

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

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

$$= \frac{\hbar^2 k^2}{2m}\phi_k(x) + V(x)\,\phi_k(x)$$

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

§ 3.1 Bloch theorem

- 1D periodic potential:

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

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

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

$$H\,\phi_k(x) = \frac{\hbar^2 k^2}{2m}\phi_k(x) + \sum_{m\in\mathbb{Z}} V_m \, e^{im\frac{2\pi}{a}x}\phi_k(x)$$

$$\phi_{k+m\frac{2\pi}{a}}x$$

$$= \left(\frac{\hbar^2 k^2}{2m} + V_0\right)\phi_k(x) + V_1\,\phi_{k+\frac{2\pi}{a}}(x)$$

$$+ V_2\,\phi_{k+\frac{4\pi}{a}}(x) + \cdots$$

§ 3.1 Bloch theorem

$$H\,\phi_k(x) = \frac{\hbar^2 k^2}{2m}\phi_k(x) + \sum_{m\in\mathbb{Z}} V_m\, \underbrace{e^{im\frac{2\pi}{a}x}\phi_k(x)}_{\to\ \phi_{k+m\frac{2\pi}{a}}x}$$

$$= \left(\frac{\hbar^2 k^2}{2m} + V_0\right)\phi_k(x) + V_1\,\phi_{k+\frac{2\pi}{a}}(x)$$

$$+ V_2\,\phi_{k+\frac{4\pi}{a}}(x) + \cdots$$

Hilbert space can be divided into subspaces :

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

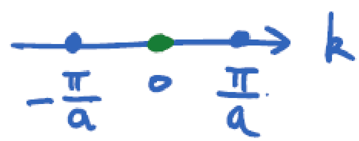
$k \in$ FBZ !

§ 3.1 Bloch theorem

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!



§ 3.1 Bloch theorem

- 1D periodic potential:
  - General wave-function ansatz within the subspace S_k:

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

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

§ 3.1 Bloch theorem

- 1D periodic potential:
  - General wave-function ansatz within the subspace S_k:

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

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

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

periodic function:

$$u_k(x+a) = u_k(x)$$

§ 3.1 Bloch theorem

- 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.

$u_k(x)$ $\quad\quad$ e^{ikx}

$$\boxed{\psi_k(x) = u_k(x) e^{ikx} \text{ with } u_k(x+a) = u_k(x)}$$

§ 3.1 Bloch theorem

- Other symmetries, if exist, could also be very useful.

  - Example: reflection symmetry in 1D

$$V(\hat{x}) = V(-\hat{x})$$

$$\Rightarrow \quad \underline{PV(\hat{x})P^\dagger} = V(-\hat{x}) = V(\hat{x})$$

action on operators

$$\Rightarrow \quad PHP^\dagger = H$$

action on states:
$$Pf(x) = f(-x)$$

f: functions

Consequence: If $\phi_k(x)$ is an eigenstate, $P\phi_k(x)$ is also an eigenstate.

§ 3.1 Bloch theorem

- Reflection symmetry in 1D:

  - If $\psi_k(x)$ is an eigenstate, $P\psi_k(x)$ is also an eigenstate (with the same energy).

$$H[P\psi_k(x)] = PHP^\dagger P\psi_k(x) = PH\psi_k(x) = \varepsilon_k[P\psi_k(x)]$$

use $P^\dagger P = I$

  - $P\psi_k(x)$ lives in the subspace S_{-k}, so it's sufficient to consider half of the FBZ.

$$P\psi_k(x) = P[u_k(x)e^{ikx}] = u_k(-x)e^{-ikx} \qquad \text{with } k \in \mathrm{FBZ}$$

§ 3.1 Bloch theorem

- Bloch theorem:

Straightforward generalization to arbitrary dimensions:

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

> Hint: use $V(\vec{r}) = \sum_m V_m e^{i\vec{G}_m\cdot\vec{r}}$

§ 3.1 Bloch theorem

- Bloch theorem:

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}$$

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

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

§ 3.1 Bloch theorem

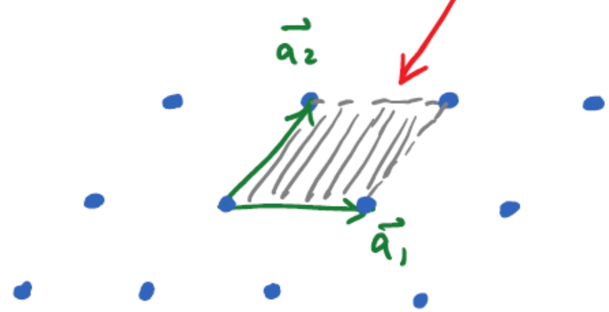
- Bloch theorem:

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

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

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

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



§ 3.1 Bloch theorem

- Bloch theorem is a consequence of the discrete translation symmetry:

Action on states: $T_{\vec{R}} f(\vec{r}) = f\left(\vec{r} + \vec{R}\right)$ f: functions

translation operator

Action on operators: $T_{\vec{R}} V\left(\hat{\vec{r}}\right) T_{\vec{R}}^{\dagger} = \hat{V}\left(\hat{\vec{r}} + \vec{R}\right)$

$= \hat{V}(\vec{r})$ if $\vec{R}$ is a lattice vector

$$\Rightarrow \quad T_{\vec{R}} H T_{\vec{R}}^{\dagger} = H$$

§ 3.1 Bloch theorem

- Bloch theorem is a consequence of the discrete translation symmetry:

  - Hamiltonian commutes with $T_{\vec{R}}$, so we should be able to find common eigenstates of H and $T_{\vec{R}}$:

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

$$\Rightarrow \quad T_{\vec{R}}\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}\left(\vec{r}+\vec{R}\right)e^{i\vec{k}\cdot(\vec{r}+\vec{R})}$$

$$= u_{\vec{k}}\ (\vec{r})e^{i\vec{k}\cdot\vec{r}}e^{i\vec{k}\cdot\vec{R}}$$

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

$\psi_{\vec{k}}(\vec{r})$ is an eigenstate of $T_{\vec{R}}$ with eigenvalue $e^{i\vec{k}\cdot\vec{R}}$.