I. Review of Bloch theory

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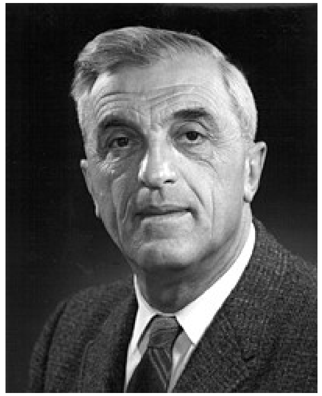


I. REVIEW OF BLOCH THEORY

A. Translation symmetry

Lattice Hamiltonian

$$H = \frac{p^2}{2m} + V_L(\mathbf{r}), \text{ with } V_L(\mathbf{r}+\mathbf{R}) = V_L(\mathbf{r})$$

Lattice translation operator

$$T_{\mathbf{R}}\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{R})$$

$$T_{\mathbf{R}}H(\mathbf{r})\psi(\mathbf{r}) = H(\mathbf{r})T_{\mathbf{R}}\psi(\mathbf{r})$$

➡ Simultaneous eigenstates (Bloch states)

$$\begin{cases} H\psi = \varepsilon\psi, \\ T_{\mathbf{R}}\psi = c_{\mathbf{R}}\psi, \end{cases}$$

$|c_R|=1$

$$T_{\mathbf{R}}T_{\mathbf{R}'} = T_{\mathbf{R}'}T_{\mathbf{R}} = T_{\mathbf{R}+\mathbf{R}'}$$

➡ $$c_{\mathbf{R}}c_{\mathbf{R}'} = c_{\mathbf{R}'}c_{\mathbf{R}} = c_{\mathbf{R}+\mathbf{R}'}$$

➡ $$c_{\mathbf{R}} = e^{i\mathbf{k}\cdot\mathbf{R}}$$

$$\begin{aligned} H\psi_{\varepsilon\mathbf{k}} &= \varepsilon\psi_{\varepsilon\mathbf{k}}, \\ T_{\mathbf{R}}\psi_{\varepsilon\mathbf{k}} &= e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\varepsilon\mathbf{k}}. \end{aligned}$$

write $$\psi_{\varepsilon\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\varepsilon\mathbf{k}}(\mathbf{r})$$

then $$u_{\varepsilon\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\varepsilon\mathbf{k}}(\mathbf{r})$$ Cell-periodic function

- The Bloch wave differs from the plane wave of free electrons only by a periodic modulation.
- $u_{\varepsilon k}(\boldsymbol{r})$ contains, in one unit cell, all info of $\psi_{\varepsilon\mathbf{k}}(\mathbf{r})$

Schrodinger eq. for $u_{\varepsilon \boldsymbol{k}}(\boldsymbol{r})$

$$\tilde{H}_{\mathbf{k}}(\mathbf{r})u_{\varepsilon\mathbf{k}} = \varepsilon u_{\varepsilon\mathbf{k}}$$

$$\begin{aligned}\tilde{H}_{\mathbf{k}}(\mathbf{r}) &\equiv e^{-i\mathbf{k}\cdot\mathbf{r}}H(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \\ &= \frac{1}{2m}(\mathbf{p}+\hbar\mathbf{k})^2 + V_L(\mathbf{r})\end{aligned}$$

Solve diff eq with with PBC

$$u_{\varepsilon\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\varepsilon\mathbf{k}}(\mathbf{r})$$

➡ Discrete energy levels

$$\tilde{H}_{\mathbf{k}}(\mathbf{r})u_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}}u_{n\mathbf{k}}$$

Band index *n*,
Bloch momentum ***k***

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

$$e^{i\mathbf{G}\cdot\mathbf{R}} = 1$$

➡ $$\psi_{n\mathbf{k}+\mathbf{G}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}+\mathbf{G}}(\mathbf{r})$$

Since the two Bloch states $\psi_{n\mathbf{k}}$ and $\psi_{n\mathbf{k}+\mathbf{G}}$ satisfy the same Schrödinger equation (with $\varepsilon_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}+\mathbf{G}}$) and the same boundary condition (Eqs. (1.16)and (1.17)), they can differ (for non-degenerate states) at most by a phase factor $\phi(\mathbf{k})$.

Periodic gauge (choose $\phi(k)=0$)

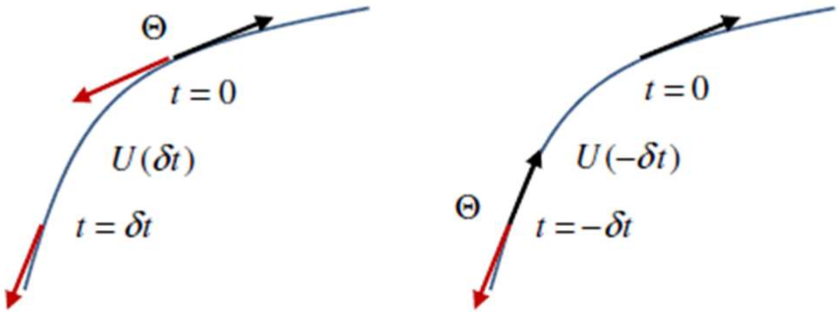
$$\psi_{n\mathbf{k}+\mathbf{G}} = \psi_{n\mathbf{k}}$$

Not applicable to topological state, e.g., quantum Hall state (this is called topological obstruction)

Ref: Sakurai, Modern quantum mechanics

B. Time reversal symmetry

$$|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle = \Theta|\alpha\rangle$$



$$U(t)\Theta|\alpha\rangle = \Theta U(-t)|\alpha\rangle.$$

$$U(\delta t) \simeq 1 - iH\delta t/\hbar$$

➡ $$-iH\Theta = \Theta iH$$

Wigner's theorem

An operator of transformation that preserves <α|α> can only be either unitary or anti-unitary:

$$\langle U\psi_1|U\psi_2\rangle = \langle\psi_1|\psi_2\rangle$$

or $$\langle U^A\psi_1|U^A\psi_2\rangle = \langle\psi_2|\psi_1\rangle$$

If Θ is unitary, then –HΘ=ΘH

→ energy is bottomless

So Θ has to be anti-unitary,

➡ $\Theta = UK \quad Ki = -iK$

➡ $H\Theta = \Theta H$ but $U(t)\Theta \neq \Theta U(t)$

No conserved quantity from Θ

For states under TR, one has

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\alpha|\beta\rangle, \quad \text{or} \quad \langle\beta|\alpha\rangle^*.$$

Pf:

$$\begin{aligned}\langle\tilde{\beta}|\tilde{\alpha}\rangle &= \langle UK\beta|UK\alpha\rangle \\ &= \langle K\beta|K\alpha\rangle \\ &= \langle\alpha|\beta\rangle. \qquad QED\end{aligned}$$

For the matrix elements of an operator O, one has

$$\langle\tilde{\beta}|O|\tilde{\alpha}\rangle = \langle\alpha|\Theta^{-1}O^{\dagger}\Theta|\beta\rangle.$$

(for a proof, see my latex note)

1. Spinless state Θ=K

$$\psi(\mathbf{r},t) \xrightarrow{TR} \Theta\psi(\mathbf{r},t) = \psi^*(\mathbf{r},t)$$

- In a magnetic field

$$H = \frac{(\mathbf{p}-q\mathbf{A})^2}{2m} + V_L(\mathbf{r})$$

$$K^{-1}HK = \frac{(\mathbf{p}+q\mathbf{A})^2}{2m} + V_L(\mathbf{r}) \neq H$$

Magnetic field breaks TRS

- Bloch state under TR

$$\psi_{n\mathbf{k}}(\mathbf{r}) \xrightarrow{TR} \Theta\psi_{n\mathbf{k}}(\mathbf{r}) = \psi^*_{n\mathbf{k}}(\mathbf{r})$$

2. Spin-1/2 state

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Theta = -i\sigma_y K = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K$$

or $= e^{-is_y\pi/\hbar} K$

Rotates spin-up to spin-down

In general, for half-integer spin,

$$\Theta = e^{-iJ_y\pi/\hbar} K$$

$$\Rightarrow \quad \Theta^2 = -1$$

for integer spin, $\Theta^2 = +1$

- Spinor Bloch state under TR

$$\begin{pmatrix} \varphi_{\mathbf{k}\uparrow} \\ \varphi_{\mathbf{k}\downarrow} \end{pmatrix} \xrightarrow{TR} \Theta \begin{pmatrix} \varphi_{\mathbf{k}\uparrow} \\ \varphi_{\mathbf{k}\downarrow} \end{pmatrix} = \begin{pmatrix} -\varphi^*_{\mathbf{k}\downarrow} \\ +\varphi^*_{\mathbf{k}\uparrow} \end{pmatrix}$$

3. Kramer degeneracy

For a system with TRS and *half-integer* spin, if ψ is an energy eigenstate, then $\Theta\psi$ is also an energy eigenstate. Furthermore, these two states are degenerate and orthogonal to each other.

Pf. Since $H\Theta = \Theta H$, so if ψ is an eigenstate with energy ε, $H\psi = \varepsilon\psi$, then

$$H\Theta\psi = \Theta H\psi = \varepsilon\Theta\psi. \tag{1.58}$$

That is, $\Theta\psi$ is also an eigenstate with energy ε. Furthermore, using the identity $\langle\beta|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\beta}\rangle$, one has

$$\langle\psi|\Theta\psi\rangle = \langle\Theta(\Theta\psi)|\Theta\psi\rangle \tag{1.59}$$

$$= -\langle\psi|\Theta\psi\rangle, \tag{1.60}$$

in which $\Theta^2 = -1$ has been used to get the second equation. Therefore, $\langle\psi|\Theta\psi\rangle = 0$. QED.

[Spin-Orbit Coupling (SOC) included]

- With both TRS and SIS

$$\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n\mathbf{k}-s}$$

(global 2-fold degeneracy)

- With TRS, without SIS

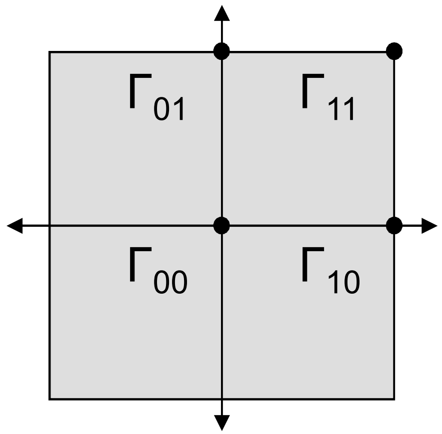
$$\varepsilon_{n-\mathbf{k}s} \neq \varepsilon_{n\mathbf{k}s}$$

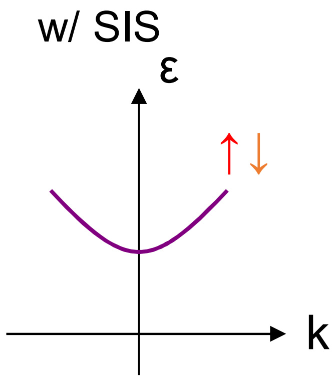
Except at
time-reversal-invariant momentum
(TRIM)

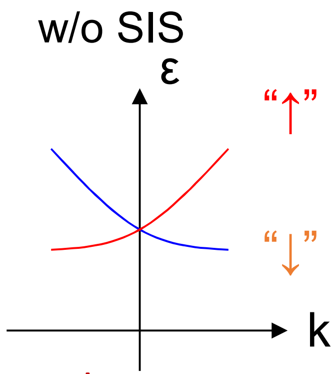
$$\mathbf{k} = -\mathbf{k} + \mathbf{G}$$

At TRIM

$$\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n,-\mathbf{k}+\mathbf{G},-s} = \varepsilon_{n\mathbf{k}-s}$$







Level crossing at TRIM