I. REVIEW OF BLOCH THEORY

A. Bloch state

For a perfect crystal with discrete translation symmetry, the Hamiltonian is

\[ H = \frac{p^2}{2m} + V_L(r), \tag{1.1} \]

in which \( V_L(r) \) is the potential of the atomic lattice, and \( R \) is a lattice translation vector. Define a lattice translation operator \( T_R \) that acts on electronic states as follows,

\[ T_R \psi(r) = \psi(r + R). \tag{1.2} \]

It can be shown that, because \( H \) has the translation symmetry,

\[ T_R H(r) \psi(r) = H(r) T_R \psi(r). \tag{1.3} \]

That is, \([T_R, H] = 0\).

Because \( T_R \) commutes with \( H(r) \), one can find their simultaneous eigenstates,

\[ H \psi = \varepsilon \psi, \tag{1.4} \]

\[ T_R \psi = \epsilon_R \psi, \tag{1.5} \]

where \( \varepsilon \) and \( \epsilon_R \) are eigenvalues of \( H \) and \( T_R \), and \(|\epsilon_R| = 1\). Furthermore, successive translations satisfy

\[ T_R T_{R'} = T_{R+R'} T_R = T_R T_{R+R'}. \tag{1.6} \]

This leads to

\[ \epsilon_R \epsilon_{R'} = \epsilon_{R+R'} = \epsilon_R \epsilon_{R+R'}. \tag{1.7} \]

To satisfy these equations, \( \epsilon_R \) needs to be an exponential, \( \epsilon_R = e^{ik \cdot R} \). Therefore,

\[ H \psi_{ck} = \varepsilon \psi_{ck}, \tag{1.8} \]

\[ T_R \psi_{ck} = e^{i k \cdot R} \psi_{ck}. \tag{1.9} \]

The simultaneous eigenstate of \( H \) and \( T_R \) is called the Bloch state.

If one writes the Bloch state in the following form,

\[ \psi_{ck}(r) = e^{i k \cdot r} u_{ck}(r), \tag{1.10} \]

then Eq. (1.9) gives

\[ u_{ck}(r + R) = u_{ck}(r). \tag{1.11} \]

That is, a Bloch state is a plane wave times a cell-periodic function \( u_{ck}(r) \). The latter contains, in one unit cell, all information of the Bloch state.

The Schrödinger equation for \( u_{ck} \) is,

\[ \tilde{H}_k(r) u_{ck} = \varepsilon u_{ck}, \tag{1.12} \]

in which

\[ \tilde{H}_k(r) \equiv e^{-i k \cdot r} H(r) e^{i k \cdot r} \]

\[ = \frac{1}{2m} (p + i \hbar \nabla)^2 + V_L(r). \tag{1.13} \]

Since \( u_{ck} \) can be restricted to one unit cell (with periodic boundary condition), we expect it to have discrete energy eigenvalues \( \varepsilon_n \) (\( n \in \mathbb{Z}^+ \)) for each \( k \), and write

\[ \tilde{H}_k(r) u_{nk} = \varepsilon_{nk} u_{nk}. \tag{1.15} \]

The quantum numbers \( n \) and \( k \) are called the band index and the Bloch momentum, and \( \varepsilon_{nk} \) are the energy dispersions of Bloch bands.

The Bloch state \( \psi_{nk} \) translates under \( R \) as (see Eq. (1.9)),

\[ \psi_{nk}(r + R) = e^{i k \cdot R} \psi_{nk}(r). \tag{1.16} \]

If one shifts the momentum \( k \) by a reciprocal lattice vector \( G \), then since \( e^{i G \cdot R} = 1 \) (for any \( R \)),

\[ \psi_{nk+G}(r + R) = e^{i k \cdot R} \psi_{nk+G}(r). \tag{1.17} \]

Since the two Bloch states \( \psi_{nk} \) and \( \psi_{nk+G} \) satisfy the same Schrödinger equation (with \( \varepsilon_{nk} = \varepsilon_{nk+G} \)) and the same boundary condition (Eqs. (1.16) and (1.17)), they can differ (for non-degenerate states) at most by a phase factor \( \phi(k) \). For convenience, one can choose the periodic gauge with \( \phi(k) = 0 \), \( \psi_{nk+G} = \psi_{nk} \). Note that for a quantum phase with non-trivial topology (such as the quantum Hall phase), one can no longer set \( \phi(k) = 0 \) for all \( k \). This is called the topological obstruction (see Chap. ??). In any case, \( \psi_{nk} \) (or \( \psi_{nk} \)) in the first Brillouin zone should contain enough information of the electronic state.
B. Time reversal symmetry

**Time reversal operator** $\Theta$ maps a state to its time-reversed state,

$$|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle = \Theta|\alpha\rangle.$$  \hfill (1.18)

Naturally, if a dynamical system has time-reversal symmetry (TRS), then for a state $|\alpha\rangle$ evolving with $U(t) = e^{-iHt/\hbar}$, one expects

$$U(t)\Theta|\alpha\rangle = \Theta U(-t)|\alpha\rangle.$$  \hfill (1.19)

For an infinitesimal evolution $U(\delta t) \simeq 1 - iH\delta t/\hbar$, Eq. (1.18) leads to $-iH\Theta = \Theta iH$. If $\Theta$ is a unitary operator, then we have $-H\Theta = \Theta H$. This causes the eigenenergies to be not bounded from below (see Sasaki, 1985, p.272), which is unreasonable.

According to Wigner’s study, an operator that preserves inner product $|\langle \beta | \alpha \rangle |$ can only be either unitary or anti-unitary. Therefore, $\Theta$ must be an **anti-unitary operator**. We thus write it as

$$\Theta = U_T K,$$  \hfill (1.20)

where $U_T$ is an unitary operator, and $K$ is a **complex conjugate operator**, $Ki = -iK$. As a result, if $H$ has TRS, then

$$H\Theta = \Theta H.$$  \hfill (1.21)

A remark: even though $[H, \Theta] = 0$, there is no conserved quantity associated with TRS since $U(t)\Theta \neq \Theta U(t)$.

For states under TR, one has

$$\langle \tilde{\beta} | \tilde{\alpha} \rangle = \langle \alpha | \beta \rangle, \quad \text{or} \quad \langle \beta | \alpha \rangle^*.$$  \hfill (1.22)

**Pf:** Assume $\{|n\rangle\}$ is a complete set of basis of the system, and choose a basis such that $K|n\rangle = |n\rangle$. The completeness relation is $1 = \sum_n |n\rangle \langle n|$. Then,

$$|\tilde{\alpha}\rangle = U_T K|\alpha\rangle = \sum_n U_T^n |n\rangle \langle n| \alpha \rangle^*,$$  \hfill (1.23)

$$\langle \tilde{\tilde{\beta}} | \tilde{\alpha} \rangle = \sum_m \langle m| \beta \rangle \langle m| U_T^n \rangle, \quad \text{for } n,m = 1,2,\ldots$$  \hfill (1.24)

\[ \vdots \]

$$\langle \tilde{\beta} | \tilde{\alpha} \rangle = \sum_{m,n} \langle m U_T^n | n \rangle \langle n | \alpha \rangle \langle m | \beta \rangle = \langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^*.$$  \hfill (1.25)

For the matrix elements of an operator $O$, one has

$$\langle \tilde{\beta} | O | \tilde{\alpha} \rangle = \langle \tilde{\tilde{\beta}} | \Theta O^\dagger \Theta^{-1} | \tilde{\alpha} \rangle.$$  \hfill (1.26)

**Pf:** We would try **not** to use the dual operation of $\Theta$ explicitly. That is, $\Theta$ is only allowed to act on ket states. First define $|\gamma\rangle = O^\dagger |\beta\rangle$, then $\langle \gamma | = \langle \beta | O$.

$$\langle \beta | O | \alpha \rangle = \langle \gamma | \alpha \rangle = \langle \tilde{\tilde{\beta}} | O^\dagger | \tilde{\alpha} \rangle, \quad \langle \beta | O | \alpha \rangle = \langle \tilde{\tilde{\beta}} | O^\dagger | \tilde{\alpha} \rangle.$$  \hfill (1.27)

1. Time reversal transformation of a spinless state

First, expand the state as

$$|\psi\rangle = \int d^3r |r\rangle (r|\psi\rangle).$$  \hfill (1.33)

It follows that,

$$\Theta|\psi\rangle = \int d^3r (\Theta|r\rangle)(r|\psi\rangle^*) = \int d^3r |r\rangle (r|\psi\rangle^*).$$  \hfill (1.34)

Therefore,

$$\psi(r) \xrightarrow{TR} \Theta \psi(r) = \psi^*(r).$$  \hfill (1.35)

For a Bloch state, one has

$$\psi_{nk}(r) \xrightarrow{\Theta} \Theta \psi_{nk}(r) = \psi_{nk}^*(r).$$  \hfill (1.36)

Under a translation,

$$T_R \psi_{nk}^*(r) = \psi_{nk}^*(r + R) = e^{-iK^T R} \psi_{nk}^*(r).$$  \hfill (1.37)

If the state is not degenerate, then according to Eq. (1.9), $\psi_{nk}^*(r)$ with the eigenvalue $e^{-iK^T R}$ could be identified as $\psi_{n-k}(r)$. That is (see Sec. 16.3 of Dresselhaus et al., 2008),

$$\psi_{nk}^*(r) = \psi_{n-k}(r).$$  \hfill (1.38)

2. Time reversal transformation of a spin-1/2 state

Consider two spinor states $|\tilde{n}, \pm\rangle$ that are respectively up and down along the direction $\hat{n}$ in Fig. 1. They can be reached from rotating the state $|+\rangle$ that is spin-up along the $z$-direction (see Sakurai, 1985, chap 3),

$$|\tilde{n}, +\rangle = e^{-iS_z \phi/h} e^{-iS_\theta \theta/h} |+, \rangle, \quad \text{and} \quad |\tilde{n}, -\rangle = e^{-iS_z \phi/h} e^{-iS_\theta (\theta+x)h} |+, \rangle.$$  \hfill (1.39, 1.40)

Under time reversal,

$$\Theta |\tilde{n}, +\rangle = |\tilde{n}, -\rangle.$$  \hfill (1.41, 1.42)
which can be re-written as
\[
\Theta e^{-iS_\epsilon/\hbar} \Theta^{-1} \Theta e^{-iS_\epsilon/\hbar} \Theta^{-1} |+\rangle = e^{-iS_\epsilon/\hbar} e^{-iS_\epsilon/\hbar} e^{-iS_\epsilon/\hbar} |+\rangle,
\]
(1.44)
Since \(\Theta S \Theta^{-1} = -S\), one has
\[
\Theta e^{-iS_\epsilon/\hbar} \Theta^{-1} = e^{-iS_\epsilon/\hbar}, \quad (\alpha = x, y, z).
\]
(1.45)
Note that the \(K\) operator in \(\Theta\) changes the sign of \(i\), which compensates the change of sign of \(S\). Comparing the two sides of Eq. (1.44), and noting that \(K|+\rangle = |+\rangle\), one would get
\[
\Theta = e^{-i\sigma y \epsilon/\hbar} K = \left( \begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \right) K.
\]
(1.46)
As a result, a Bloch state with spin-1/2 transforms as
\[
\begin{pmatrix} \psi_{k\uparrow} \\ \psi_{k\downarrow} \end{pmatrix} \xrightarrow{\text{TR}} \Theta \begin{pmatrix} \psi_{k\uparrow} \\ \psi_{k\downarrow} \end{pmatrix} = \begin{pmatrix} -\psi_{k\downarrow} \\ \psi_{k\uparrow} \end{pmatrix}.
\]
(1.48)
Applying the time-reversal transformation twice gives \(\Theta^2 = -1\).

It is not difficult to see that the derivation of \(\Theta\) remains valid even for states with higher spins. One only needs to replace the operator \(S\) with the operator \(J\) of higher spins.

3. Kramer degeneracy

In general, if a particle has integer spin, then applying the TR transformation twice gives \(\Theta^2 = 1\). However, if a particle has half-integer spin, then
\[
\Theta^2 = -1.
\]
(1.49)
This fact is crucial to the existence of the Kramer degeneracy: If a system has TRS and its spin is a half-integer, then eigenstates \(\psi\) and \(\Theta\psi\) are degenerate and orthogonal to each other.

**Proof**: Since \(H \Theta = \Theta H\), so if \(\psi\) is an eigenstate with energy \(\epsilon\), \(H \psi = \epsilon \psi\), then
\[
H \Theta \psi = \Theta H \psi = \epsilon \Theta \psi.
\]
(1.50)
That is, \(\Theta \psi\) is also an eigenstate with energy \(\epsilon\). Furthermore, using the identity \(\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle\), one has
\[
\langle \psi | \Theta \psi \rangle = \langle \Theta | \Theta \psi | \Theta \psi \rangle = -\langle \psi | \Theta \psi \rangle,
\]
(1.51)
in which \(\Theta^2 = -1\) has been used to get the second equation. Therefore, \(\langle \psi | \Theta \psi \rangle = 0\).

For example, if a Bloch state \(\psi_{nk}\) has energy \(\epsilon_{nk}\), then its time-reversed state \(\Theta \psi_{nk} = -\psi_{n\rightarrow k}\) has energy \(\epsilon_{n\rightarrow k}\), and with time reversal symmetry \(\epsilon_{nk\uparrow} = \epsilon_{n\rightarrow k\downarrow}\) (Kramer degeneracy). For a solid with space inversion symmetry, one has \(\epsilon_{n\rightarrow k} = \epsilon_{nks}\) (\(s = \uparrow\) or \(\downarrow\)). When the solid has both symmetries, there is a two-fold degeneracy at each \(k\)-point,
\[
\epsilon_{nks} = \epsilon_{n\rightarrow k\downarrow} = \epsilon_{n\rightarrow k\uparrow}.
\]
(1.53)
An energy band thus has a global two-fold degeneracy over the whole Brillouin zone.

On the other hand, if a solid has no space inversion symmetry, so that \(\epsilon_{n\rightarrow k} \neq \epsilon_{nks}\), then the two-fold degeneracy at a \(k\)-point is not guaranteed, except at the \(k\)-point that differs from \(-k\) by a reciprocal lattice vector \(G\).

\[
k = -k + G.
\]
(1.54)
These \(k\)-points are called time-reversal-invariant momenta (TRIM). At a TRIM,
\[
\epsilon_{nks} = \epsilon_{n\rightarrow k\downarrow} = \epsilon_{n\rightarrow k\downarrow} = \epsilon_{n\rightarrow k\uparrow}.
\]
(1.55)
Typical TRIM are located at the corners of a BZ, \(k = G/2\). They play important roles in the theory of topological insulator.

Note: For a crystal without space-inversion symmetry, we often still have \(\epsilon_{nk} = \epsilon_{n\rightarrow k}\). This is due to the fact that, with time-reversal symmetry, \(\epsilon_{nks} = \epsilon_{n\rightarrow k\uparrow}\). In the absence of spin-orbit interaction (SOI), \(\epsilon_{n\rightarrow k\downarrow} = \epsilon_{n\rightarrow k\uparrow}\) and we have a symmetric energy spectrum with global two-fold degeneracy. A SOI breaks the two-fold degeneracy (except at TRIM), but the energy spectrum still looks symmetric because of the Kramer degeneracy.

**Exercise**

1. Show that, if an operator \(O\) transforms under time reversal as,
\[
\Theta O \Theta^{-1} = \pm O^T,
\]
(1.56)
then \(\langle \Theta \psi | O | \Theta \psi \rangle = \pm \langle \psi | O | \psi \rangle\).

2. Show that, if an operator \(O\) (e.g., \(V(r)\)) transforms as,
\[
\Theta O \Theta^{-1} = O^T,
\]
(1.57)
and \(\Theta^2 = -1\), then \(\langle \psi | O | \Theta \psi \rangle = 0\). (Kittel, 1963, p.197).

**References**


Kittel, C., 1963, Quantum theory of solids (Wiley).