Lecture notes on topological insulators

Ming-Che Chang

Department of Physics, National Taiwan Normal University, Taipei, Taiwan

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Contents

I. REVIEW OF BLOCH THEORY

A. Translation symmetry

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

$$H = \frac{p^2}{2m} + V_L(\mathbf{r}), \text{ with } V_L(\mathbf{r}+\mathbf{R}) = V_L(\mathbf{r}), \tag{1.1}$$

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

$$T_\mathbf{R}\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{R}). \tag{1.2}$$

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

$$T_\mathbf{R}H(\mathbf{r})\psi(\mathbf{r}) = H(\mathbf{r})T_\mathbf{R}\psi(\mathbf{r}). \tag{1.3}$$

That is, $[T_\mathbf{R}, H] = 0$.

Because $T_\mathbf{R}$ commutes with $H(\mathbf{r})$, one can find their simultaneous eigenstates,

$$\begin{aligned} H\psi &= \varepsilon\psi, & (1.4)\\ T_\mathbf{R}\psi &= c_\mathbf{R}\psi, & (1.5)\end{aligned}$$

where ε and $c_\mathbf{R}$ are eigenvalues of H and $T_\mathbf{R}$, and $|c_\mathbf{R}| = 1$. Furthermore, successive translations satisfy

$$T_\mathbf{R}T_{\mathbf{R}'} = T_{\mathbf{R}'}T_\mathbf{R} = T_{\mathbf{R}+\mathbf{R}'}. \tag{1.6}$$

This leads to

$$c_\mathbf{R}c_{\mathbf{R}'} = c_{\mathbf{R}'}c_\mathbf{R} = c_{\mathbf{R}+\mathbf{R}'}. \tag{1.7}$$

To satisfy these equations, $c_\mathbf{R}$ needs to be an exponential, $c_\mathbf{R} = e^{i\mathbf{k}\cdot\mathbf{R}}$. Therefore,

$$\begin{aligned} H\psi_{\varepsilon\mathbf{k}} &= \varepsilon\psi_{\varepsilon\mathbf{k}}, & (1.8)\\ T_\mathbf{R}\psi_{\varepsilon\mathbf{k}} &= e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\varepsilon\mathbf{k}}. & (1.9)\end{aligned}$$

The simultaneous eigenstate of H and $T_\mathbf{R}$ is called **Bloch state**.

If one writes the Bloch state in the following form,

$$\psi_{\varepsilon\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\varepsilon\mathbf{k}}(\mathbf{r}), \tag{1.10}$$

then Eq. (1.9) gives

$$u_{\varepsilon\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\varepsilon\mathbf{k}}(\mathbf{r}). \tag{1.11}$$

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

The Schrödinger equation for $u_{\varepsilon\mathbf{k}}$ is,

$$\tilde{H}_\mathbf{k}(\mathbf{r})u_{\varepsilon\mathbf{k}} = \varepsilon u_{\varepsilon\mathbf{k}}, \tag{1.12}$$

in which

$$\begin{aligned} \tilde{H}_\mathbf{k}(\mathbf{r}) &\equiv e^{-i\mathbf{k}\cdot\mathbf{r}}H(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} & (1.13)\\ &= \frac{1}{2m}(\mathbf{p}+\hbar\mathbf{k})^2 + V_L(\mathbf{r}). & (1.14)\end{aligned}$$

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

$$\tilde{H}_\mathbf{k}(\mathbf{r})u_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}}u_{n\mathbf{k}}. \tag{1.15}$$

The quantum numbers n and $\mathbf{k}$ are called **band index** and **Bloch momentum**, and $\varepsilon_{n\mathbf{k}}$ are the energy dispersions of Bloch bands.

The Bloch state $\psi_{n\mathbf{k}}$ translates under $\mathbf{R}$ as (see Eq. (1.9)),

$$\psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r}). \tag{1.16}$$

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

$$\psi_{n\mathbf{k}+\mathbf{G}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}+\mathbf{G}}(\mathbf{r}). \tag{1.17}$$

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 $\phi(\mathbf{k})$. For convenience, one can choose the **periodic gauge** with $\phi(\mathbf{k}) = 0$, $\psi_{n\mathbf{k}+\mathbf{G}} = \psi_{n\mathbf{k}}$. Note that for a quantum phase with non-trivial topology (such as the quantum Hall state), one can no longer set $\phi(\mathbf{k}) = 0$ for *all* $\mathbf{k}$. This is called **topological obstruction** (see Chap. **??**). In any case, $\psi_{n\mathbf{k}}$ (or $u_{n\mathbf{k}}$) in the first Brillouin zone should contain enough information of the electronic state.

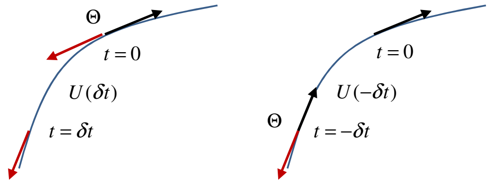

FIG. 1 Time reversal Θ of $|\alpha\rangle$ followed by $U(\delta t)$ (left), and $U(-\delta t)$ of $|\alpha\rangle$ followed by time reversal Θ (right). Both result in the same state.

B. Time reversal symmetry

Time reversal operator Θ maps a state to its time-reversed state (or, motion-reversed state),

$$|\alpha\rangle \to |\tilde{\alpha}\rangle = \Theta|\alpha\rangle. \tag{1.18}$$

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 (see Fig. 1)

$$U(t)\Theta|\alpha\rangle = \Theta U(-t)|\alpha\rangle. \tag{1.19}$$

For an infinitesimal evolution $U(\delta t) \simeq 1 - iH\delta t/\hbar$, Eq. (1.18) leads to $-iH\Theta = \Theta iH$. If Θ is a unitary operator, then we have $-H\Theta = \Theta H$. That is, if a state has energy ε, then its time-reversed state has energy $-\varepsilon$. This causes the eigen-energies to be bottomless, which is unreasonable (see Sakurai, 1985, p.272).

Time-reversal transformation, like translation or rotation, preserves the squared modulus $\langle\alpha|\alpha\rangle$ of a quantum state $|\alpha\rangle$ if the system under consideration has that symmetry. According to Wigner's study, an operator of transformation that preserves $|\langle\beta|\alpha\rangle|$ can only be either unitary or anti-unitary. Therefore, Θ must be an **anti-unitary operator**, which can be written as

$$\Theta = UK, \tag{1.20}$$

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

$$H\Theta = \Theta H. \tag{1.21}$$

Note: 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

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

Pf:

$$\begin{aligned} \langle\tilde{\beta}|\tilde{\alpha}\rangle &= \langle UK\beta|UK\alpha\rangle && (1.23)\\ &= \langle U\alpha|U\beta\rangle && (1.24)\\ &= \langle\alpha|\beta\rangle. \quad QED && (1.25)\end{aligned}$$

For the matrix elements of an operator O, one has

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

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

$$\Theta|\gamma\rangle = O^\dagger\Theta|\beta\rangle, \tag{1.27}$$

then $\langle\tilde{\gamma}| = \langle\tilde{\beta}|O$, and

$$\begin{aligned} \langle\tilde{\beta}|O|\tilde{\alpha}\rangle &= \langle\tilde{\gamma}|\tilde{\alpha}\rangle && (1.28)\\ &= \langle\alpha|\gamma\rangle && (1.29)\\ &= \langle\alpha|\Theta^{-1}O^\dagger\Theta|\beta\rangle. \quad QED && (1.30)\end{aligned}$$

If an operator O transforms under time reversal as,

$$\Theta^{-1}O^\dagger\Theta = \pm O, \tag{1.31}$$

then $\langle\Theta\alpha|O|\Theta\alpha\rangle = \pm\langle\alpha|O|\alpha\rangle$.

1. Spinless state

Given a time-reversed state $|\tilde{\psi}\rangle = \Theta|\psi\rangle$, one expects

$$\begin{aligned} \langle\psi|\Theta^{-1}\mathbf{r}\Theta|\psi\rangle &= \langle\psi|\mathbf{r}|\psi\rangle, && (1.32)\\ \langle\psi|\Theta^{-1}\mathbf{p}\Theta|\psi\rangle &= -\langle\psi|\mathbf{p}|\psi\rangle, && (1.33)\end{aligned}$$

Since this is valid for every time-reversed state, we demand

$$\begin{aligned} \Theta^{-1}\mathbf{r}\Theta &= \mathbf{r}, && (1.34)\\ \Theta^{-1}\mathbf{p}\Theta &= -\mathbf{p}. && (1.35)\end{aligned}$$

This also implies that the angular momentum operator $\mathbf{L} = \mathbf{r}\times\mathbf{p}$ changes sign under TR.

A spin-less state is described by a scalar function, and this two relations can be satisfied with $\Theta = K$ (i.e. $U = 1$). Hence

$$\psi(\mathbf{r},t) \xrightarrow{TR} \Theta\psi(\mathbf{r},t) = \psi^*(\mathbf{r},t). \tag{1.36}$$

Given the Schrödinger equation,

$$H\psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t), \tag{1.37}$$

its complex-conjugate counterpart is,

$$H\psi^*(\mathbf{r},t) = i\hbar\frac{\partial}{\partial(-t)}\psi^*(\mathbf{r},t). \tag{1.38}$$

That is $\psi^*(\mathbf{r},t)$ evolves to $-t$ the same way as $\psi(\mathbf{r},t)$ evolves to t. Hence, $\psi^*(\mathbf{r},t)$ is indeed a time-reversed state.

For the Hamiltonian in Eq. (1.1), $K^{-1}HK = H$ (note that $K^{-1} = K$). However, for a crystal in a magnetic field,

$$H = \frac{(\mathbf{p}-q\mathbf{A})^2}{2m} + V_L(\mathbf{r}), \tag{1.39}$$

where $q=-e$ is the charge of an electron and $\mathbf{A}$ is the vector potential, we have

$$K^{-1}HK = \frac{(\mathbf{p}+q\mathbf{A})^2}{2m} + V_L(\mathbf{r}) \neq H. \tag{1.40}$$

That is, the magnetic field breaks the TRS, as expected.

For a Bloch state, one has

$$\psi_{n\mathbf{k}}(\mathbf{r}) \xrightarrow{TR} \Theta\psi_{n\mathbf{k}}(\mathbf{r}) = \psi^*_{n\mathbf{k}}(\mathbf{r}). \tag{1.41}$$

Under a translation,

$$\begin{aligned} T_{\mathbf{R}}\psi^*_{n\mathbf{k}}(\mathbf{r}) &= \psi^*_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) && (1.42)\\ &= e^{-i\mathbf{k}\cdot\mathbf{R}}\psi^*_{n\mathbf{k}}(\mathbf{r}). && (1.43)\end{aligned}$$

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

$$\psi^*_{n\mathbf{k}}(\mathbf{r}) = \psi_{n-\mathbf{k}}(\mathbf{r}). \tag{1.44}$$

2. Spin-1/2 state

For a quantum state with spin, in addition to Eqs. (1.34), (1.35), we also require the spin operator under TR to satisfy

$$\Theta^{-1}\mathbf{s}\Theta = -\mathbf{s}. \tag{1.45}$$

A spin-1/2 state is a two-component **spinor**, and the spin operators $\mathbf{s}=\frac{\hbar}{2}\boldsymbol{\sigma}$, where $\boldsymbol{\sigma}$ are the **Pauli matrices**,

$$\sigma_x = \begin{pmatrix} 0 & 1\\ 1 & 0\end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i\\ i & 0\end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix}. \tag{1.46}$$

Obviously, $\Theta=K$ cannot satisfy Eq. (1.45), and a unitary rotation U (not operating on $\mathbf{r}$ and $\mathbf{p}$) in $\Theta=UK$ is required.

From Eq. (1.45), one has

$$\begin{aligned} s_x\Theta &= -\Theta s_x, && (1.47)\\ s_y\Theta &= -\Theta s_y, && (1.48)\\ s_z\Theta &= -\Theta s_z. && (1.49)\end{aligned}$$

Using the standard representation for Pauli matrices in Eq. (1.46), where only σ_y has *complex* matrix elements, we have

$$\begin{aligned} \sigma_x U &= -U\sigma_x, && (1.50)\\ \sigma_y U &= +U\sigma_y, && (1.51)\\ \sigma_z U &= -U\sigma_z. && (1.52)\end{aligned}$$

U is a 2×2 matrix (for spin-1/2 states), which can be expanded by Pauli matrices. Since U anti-commutes with $\sigma_{x,z}$, but commutes with σ_y, the equations above can be satisfied with $U=\sigma_y$, or $U=e^{i\delta}\sigma_y$, where δ is an arbitrary phase. A popular choice of $e^{i\delta}$ is $-i$. Thus,

$$\Theta = -i\sigma_y K = \begin{pmatrix} 0 & -1\\ 1 & 0\end{pmatrix} K. \tag{1.53}$$

Other choices of $e^{i\delta}$ are allowed, such as $+i$ or 1.

In general, for a state with spin quantum number j, which can be an integer or a half-integer,

$$\Theta = e^{-iJ_y\pi/\hbar}K, \tag{1.54}$$

in which J_y is a spin operator (Sakurai, 1985). For spin 1/2,

$$\Theta = e^{-is_y\pi/\hbar}K = -i\sigma_y K. \tag{1.55}$$

A Bloch state with spin-1/2 transforms as

$$\begin{pmatrix} \varphi_{\mathbf{k}\uparrow}\\ \varphi_{\mathbf{k}\downarrow}\end{pmatrix} \xrightarrow{TR} \Theta\begin{pmatrix} \varphi_{\mathbf{k}\uparrow}\\ \varphi_{\mathbf{k}\downarrow}\end{pmatrix} = \begin{pmatrix} -\varphi^*_{\mathbf{k}\downarrow}\\ +\varphi^*_{\mathbf{k}\uparrow}\end{pmatrix}. \tag{1.56}$$

Applying the time-reversal transformation twice gives $\Theta^2=-1$.

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

$$\Theta^2 = -1. \tag{1.57}$$

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 ψ and $\Theta\psi$ 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

$$\begin{aligned} \langle\psi|\Theta\psi\rangle &= \langle\Theta(\Theta\psi)|\Theta\psi\rangle && (1.59)\\ &= -\langle\psi|\Theta\psi\rangle, && (1.60)\end{aligned}$$

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

For example, if a Bloch state $\psi_{n\mathbf{k}\uparrow}$ has energy $\varepsilon_{n\mathbf{k}\uparrow}$, then its time-reversed state $\Theta\psi_{n\mathbf{k}\uparrow} = -\psi_{n-\mathbf{k}\downarrow}$ (see Eq. (1.56)) has energy $\varepsilon_{n-\mathbf{k}\downarrow}$, and with time reversal symmetry, $\varepsilon_{n\mathbf{k}\uparrow}=\varepsilon_{n-\mathbf{k}\downarrow}$ (Kramer degeneracy).

For a solid with space inversion symmetry, one has $\varepsilon_{n-\mathbf{k}s}=\varepsilon_{n\mathbf{k}s}$ ($s=\uparrow$ or $\downarrow$). When the solid has *both* TR and SI symmetries, there is a two-fold degeneracy at each $\mathbf{k}$-point,

$$\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n\mathbf{k}-s}. \tag{1.61}$$

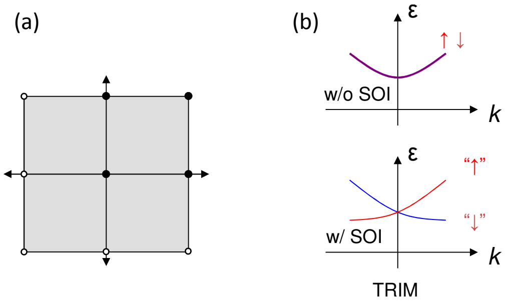

FIG. 2 (a) The TRIM are shown as black and white dots in the first Brillouin zone. Only four of them (black dots) are independent. (b) The Bloch energy levels of a system with time-reversal symmetry but without space-inversion symmetry.

An energy band thus has a *global* two-fold degeneracy over the whole Brillouin zone.

On the other hand, if there is TRS but no SIS, so that $\varepsilon_{n-\mathbf{k}s} \neq \varepsilon_{n\mathbf{k}s}$, then the two-fold degeneracy at a **k**-point is not guaranteed, except at the **k**-point that differs from $-\mathbf{k}$ by a **reciprocal lattice vector G**,

$$\mathbf{k} = -\mathbf{k} + \mathbf{G}. \tag{1.62}$$

These **k**-points are called **time-reversal-invariant momenta** (TRIM), see Fig. 2(a). At a TRIM,

$$\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n,-\mathbf{k}+\mathbf{G},-s} = \varepsilon_{n\mathbf{k}-s}. \tag{1.63}$$

Typical TRIM are located at the corners of a BZ, $\mathbf{k} = \mathbf{G}/2$. They play important roles in the theory of **topological insulator**.

Note: For a crystal *without* space-inversion symmetry, we often still have $\varepsilon_{n\mathbf{k}} = \varepsilon_{n-\mathbf{k}}$ (Fig. 2(b)). This is due to the fact that, with time-reversal symmetry, $\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s}$. In the absence of spin-orbit interaction (SOI), $\varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n-\mathbf{k}s}$ 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. Suppose $Q = UK$ is an anti-unitary operator, prove that Q^2 can only be $+1$ or -1.
Hint: Since performing Q twice would get us back to the original state, differing at most by a phase factor, we can assume $Q^2 = e^{i\delta}$. Check the consistency between mathematical operations to find out $e^{i\delta}$.
2. Show that, if an operator O transforms as,

$$\Theta^{-1} O^\dagger \Theta = O, \tag{1.64}$$

and $\Theta^2 = -1$, then $\langle\psi|O|\Theta\psi\rangle = 0$.

For example, if an electron is scattered by a scalar potential $V(\mathbf{r})$, then to the first-order approximation (**Born approximation**), the scattering amplitude for ψ being scattered to its time-revered state is zero, $\langle\Theta\psi|V|\psi\rangle = 0$.

References

Dresselhaus, M. S., G. Dresselhaus, and A. Jorio, 2008, *Group Theory* (Springer-Verlag Berlin Heidelberg).
Sakurai, J. J., 1985, *Modern quantum mechanics* (Benjamin-Cummings Publishing Company).