

# Lecture notes on topological insulators

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## I. REVIEW OF BLOCH THEORY

### A. Translation symmetry

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

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

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,

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

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

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

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

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

$$H\psi = \varepsilon\psi, \quad (1.4)$$

$$T_{\mathbf{R}}\psi = c_{\mathbf{R}}\psi, \quad (1.5)$$

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

$$T_{\mathbf{R}}T_{\mathbf{R}'} = T_{\mathbf{R}'}T_{\mathbf{R}} = T_{\mathbf{R}+\mathbf{R}'}. \quad (1.6)$$

This leads to

$$c_{\mathbf{R}}c_{\mathbf{R}'} = c_{\mathbf{R}'}c_{\mathbf{R}} = c_{\mathbf{R}+\mathbf{R}'}. \quad (1.7)$$

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

$$H\psi_{\varepsilon\mathbf{k}} = \varepsilon\psi_{\varepsilon\mathbf{k}}, \quad (1.8)$$

$$T_{\mathbf{R}}\psi_{\varepsilon\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\varepsilon\mathbf{k}}. \quad (1.9)$$

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

If one writes the Bloch state in the following form,

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

then Eq. (1.9) gives

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

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.

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

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

in which

$$\tilde{H}_{\mathbf{k}}(\mathbf{r}) \equiv e^{-i\mathbf{k}\cdot\mathbf{r}}H(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \quad (1.13)$$

$$= \frac{1}{2m}(\mathbf{p} + \hbar\mathbf{k})^2 + V_L(\mathbf{r}). \quad (1.14)$$

Since  $u_{\varepsilon\mathbf{k}}$  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  $\mathbf{k}$ , and write

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

The quantum numbers  $n$  and  $\mathbf{k}$  are called the **band index** and the **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)),

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

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

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

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 phase), one can no longer set  $\phi(\mathbf{k}) = 0$  for *all*  $\mathbf{k}$ . This is called the **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.

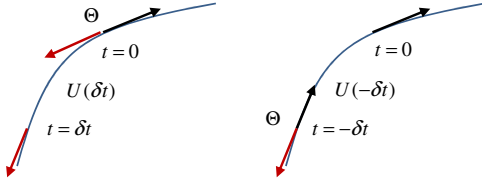


FIG. 1 Time reversal  $\Theta$  followed by  $U(\delta t)$  (left) and  $U(-\delta t)$  followed by time reversal  $\Theta$  (right) result in the same state.

## B. Time reversal symmetry

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

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

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)

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

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  $-H\Theta = \Theta H$ . That is, if a state has energy  $\varepsilon$ , 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,  $\Theta$  must be an **anti-unitary operator**, which can be written as

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

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

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

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

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

*Pf:*

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle UK\beta|UK\alpha\rangle \quad (1.23)$$

$$= \langle K\beta|K\alpha\rangle^* \quad (1.24)$$

$$= \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle. \quad QED \quad (1.25)$$

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

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

*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  $|\tilde{\gamma}\rangle = O^\dagger|\tilde{\beta}\rangle$ , or

$$\Theta|\gamma\rangle = O^\dagger\Theta|\beta\rangle, \quad (1.27)$$

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

$$\langle\tilde{\beta}|O|\tilde{\alpha}\rangle = \langle\tilde{\gamma}|\tilde{\alpha}\rangle \quad (1.28)$$

$$= \langle\alpha|\gamma\rangle \quad (1.29)$$

$$= \langle\alpha|\Theta^{-1}O^\dagger\Theta|\beta\rangle. \quad QED \quad (1.30)$$

If an operator  $O$  transforms under time reversal as,

$$\Theta^{-1}O^\dagger\Theta = \pm O, \quad (1.31)$$

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

$$\langle\psi|\Theta^{-1}\mathbf{r}\Theta|\psi\rangle = \langle\psi|\mathbf{r}|\psi\rangle, \quad (1.32)$$

$$\langle\psi|\Theta^{-1}\mathbf{p}\Theta|\psi\rangle = -\langle\psi|\mathbf{p}|\psi\rangle, \quad (1.33)$$

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

$$\Theta^{-1}\mathbf{r}\Theta = \mathbf{r}, \quad (1.34)$$

$$\Theta^{-1}\mathbf{p}\Theta = -\mathbf{p}. \quad (1.35)$$

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

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

Furthermore, given the Schrödinger equation,

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

its complex-conjugate counterpart is,

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

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,

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

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

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

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

For a Bloch state, one has

$$\psi_{n\mathbf{k}}(\mathbf{r}) \rightarrow \Theta\psi_{n\mathbf{k}}(\mathbf{r}) = \psi_{n\mathbf{k}}^*(\mathbf{r}). \quad (1.41)$$

Under a translation,

$$T_{\mathbf{R}}\psi_{n\mathbf{k}}^*(\mathbf{r}) = \psi_{n\mathbf{k}}^*(\mathbf{r} + \mathbf{R}) \quad (1.42)$$

$$= e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}^*(\mathbf{r}). \quad (1.43)$$

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),

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

## 2. Spin-1/2 state

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

$$\Theta^{-1}\mathbf{s}\Theta = -\mathbf{s}. \quad (1.45)$$

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

$$s_x\Theta = -\Theta s_x, \quad (1.46)$$

$$s_y\Theta = -\Theta s_y, \quad (1.47)$$

$$s_z\Theta = -\Theta s_z. \quad (1.48)$$

Using the standard representation for Pauli matrices, where only  $\sigma_y$  has complex matrix elements, we have

$$\sigma_x U = -U\sigma_x, \quad (1.49)$$

$$\sigma_y U = +U\sigma_y, \quad (1.50)$$

$$\sigma_z U = -U\sigma_z. \quad (1.51)$$

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

$$\Theta = -i\sigma_y K = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K. \quad (1.52)$$

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

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

$$\Theta = e^{-iJ_y\pi/\hbar}K, \quad (1.53)$$

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

$$\Theta = e^{-is_y\pi/\hbar}K = -i\sigma_y K. \quad (1.54)$$

A Bloch state with spin-1/2 transforms as

$$\begin{pmatrix} \varphi_{\mathbf{k}1} \\ \varphi_{\mathbf{k}2} \end{pmatrix} \xrightarrow{TR} \Theta \begin{pmatrix} \varphi_{\mathbf{k}1} \\ \varphi_{\mathbf{k}2} \end{pmatrix} = \begin{pmatrix} -\varphi_{\mathbf{k}2}^* \\ +\varphi_{\mathbf{k}1}^* \end{pmatrix}. \quad (1.55)$$

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

$$\Theta^2 = -1. \quad (1.56)$$

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.

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

$$H\Theta\psi = \Theta H\psi = \varepsilon\Theta\psi. \quad (1.57)$$

That is,  $\Theta\psi$  is also an eigenstate with energy  $\varepsilon$ .

Furthermore, using the identity  $\langle\beta|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\beta}\rangle$ , one has

$$\langle\psi|\Theta\psi\rangle = \langle\Theta(\Theta\psi)|\Theta(\psi)\rangle \quad (1.58)$$

$$= -\langle\psi|\Theta\psi\rangle, \quad (1.59)$$

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. (1.55)) 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* symmetries, there is a two-fold degeneracy at each  $\mathbf{k}$ -point,

$$\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n\mathbf{k}-s}. \quad (1.60)$$

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 space inversion symmetry, so that  $\varepsilon_{n-\mathbf{k}s} \neq \varepsilon_{n\mathbf{k}s}$ , then the two-fold degeneracy at a  $\mathbf{k}$ -point is not guaranteed, except at the

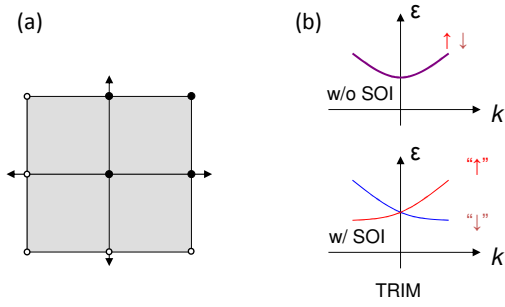


FIG. 2 (a) The TRIM are shown as black and white dots in the first Brillouin zone. Only four of them (black dots) are independent. (b) The Bloch energy levels of a system with time-reversal symmetry but without space-inversion symmetry.

$\mathbf{k}$ -point that differs from  $-\mathbf{k}$  by a reciprocal lattice vector  $\mathbf{G}$ ,

$$\mathbf{k} = -\mathbf{k} + \mathbf{G}. \quad (1.61)$$

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

$$\varepsilon_{n\mathbf{k}s} = \varepsilon_{n-\mathbf{k}-s} = \varepsilon_{n,-\mathbf{k}+\mathbf{G},-s} = \varepsilon_{n\mathbf{k}-s}. \quad (1.62)$$

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.

### C. Rotation symmetry

A crystal can be invariant under a rotation with respect to a lattice point. Because of the rotation, a position vector  $\mathbf{r}$  changes to  $\mathbf{r}'$ ,

$$\mathbf{r} \rightarrow \mathbf{r}' = \mathbf{R}\mathbf{r}, \quad (1.63)$$

where  $\mathbf{R}$  is the rotation matrix. A quantum state  $\psi$  changes as,

$$\psi(\mathbf{r}) \rightarrow \psi'(\mathbf{r}) = \psi(\mathbf{R}^{-1}\mathbf{r}) = D_R\psi(\mathbf{r}), \quad (1.64)$$

$$\text{or } |\psi'\rangle = D_R|\psi\rangle. \quad (1.65)$$

where  $D_R$  is a rotation operator. We have used a *passive rotation*  $\mathbf{R}^{-1}\mathbf{r}$  to simulate an active rotation of  $\psi$ .

After rotation, an operator  $O$  changes to  $O'$ , and we demand that

$$\langle \psi' | O | \psi' \rangle = \langle \psi | O' | \psi \rangle. \quad (1.66)$$

Thus,

$$O \rightarrow O' = D_R^\dagger O D_R. \quad (1.67)$$

For example, a Hamiltonian transforms as,

$$H' = D_R^\dagger H D_R. \quad (1.68)$$

The Hamiltonian is invariant under rotation,  $H' = H$ , if  $H$  commutes with  $D_R$ .

The Schrödinger equation for cell-periodic state is,

$$\tilde{H}_{\mathbf{k}}(\mathbf{r}, \mathbf{p})u_{\mathbf{k}}(\mathbf{r}) = \varepsilon_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{r}), \quad (1.69)$$

where

$$\tilde{H}_{\mathbf{k}} = \frac{p^2}{2m} + \frac{\mathbf{p} \cdot \mathbf{k}}{m} + \frac{k^2}{2m} + V_L(\mathbf{r}). \quad (1.70)$$

After rotation (Kittel, 1963),

$$\tilde{H}_{\mathbf{k}}(\mathbf{R}^{-1}\mathbf{r}, \mathbf{R}^{-1}\mathbf{p})u_{\mathbf{k}}(\mathbf{R}^{-1}\mathbf{r}) = \varepsilon_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{R}^{-1}\mathbf{r}). \quad (1.71)$$

Since  $p^2$  and  $k^2$  are invariant under rotation, and

$$\mathbf{k} \cdot \mathbf{R}^{-1}\mathbf{p} = \mathbf{R}\mathbf{k} \cdot \mathbf{p}, \quad (1.72)$$

we have

$$\tilde{H}_{\mathbf{R}\mathbf{k}}(\mathbf{r}, \mathbf{p})D_R u_{\mathbf{k}}(\mathbf{r}) = \varepsilon_{\mathbf{k}}D_R u_{\mathbf{k}}(\mathbf{r}). \quad (1.73)$$

If a Hamiltonian is invariant under  $D_R$ ,

$$D_R^\dagger \tilde{H}_{\mathbf{R}\mathbf{k}} D_R = \tilde{H}_{\mathbf{k}}, \quad (1.74)$$

then its Bloch energy is invariant under the rotation.

In general, symmetry operations on a crystal consist of translation, rotation, mirror reflection, space inversion, or their combinations. These operations form a **space group**. Rotation, mirror reflection, and space inversion leaves a point fixed. These operations form a **point group**.

### Exercise

1. Suppose  $Q = UK$  is an anti-unitary operator, prove that  $Q^2$  can only be  $+1$  or  $-1$ .

Hint: Since performing time reversal 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,

$$\Theta O \Theta^{-1} = O^\dagger, \quad (1.75)$$

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  $\psi$  being scattered to its time-reversal state is zero.

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