Lecture notes on topological insulators

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I. 2D TOPOLOGICAL INSULATOR

A. General theory

Analogous to the connection between 1D charge pump and 2D quantum Hall effect (see ??), there is also a close connection between 1D spin pump and 2D topological insulator (TI). The key ingredient that leads to the $Z_2$ connection between 1D spin pump and 2D topological insulator is the TRS of the 1D lattice at $t = 0, T/2$. We can identify the parameter $t$ with the Bloch momentum $k_y$ of a 2D lattice system (see Fig. 1), then $k_y = 0, \pi$ play similar roles to $t = 0, T/2$. Mathematically, one expects a similar $Z_2$ number from the following expression,

$$(-1)^\nu = \prod_n \frac{w_n(\Lambda_1)}{w_n(\Lambda_2)} \frac{w_n(\Lambda_2)}{w_n(\Lambda_3)} \frac{w_n(\Lambda_3)}{w_n(\Lambda_4)} \frac{w_n(\Lambda_4)}{w_n(\Lambda_1)} = \pm 1,$$

(1.1)

where $\Lambda_i$ are the TRIM shown in Fig. 1.

Introducing the sewing matrix for $N$ filled Kramer pairs,

$$w(k) = \begin{pmatrix} 0 & e^{i\chi\nu} & 0 & 0 & 0 \\ -e^{-i\chi\nu} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\chi\nu} & 0 \\ 0 & 0 & -e^{i\chi\nu} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$  

(1.2)

Then one can show that its determinant at a TRIM is,

$$\det w(\Lambda_i) = \prod_{n=1}^{N} w_n^2(\Lambda_i),$$

(1.3)

where $w_n(k) = e^{i\chi\nu k}$.

For an antisymmetric $2N \times 2N$ matrix $M$, one can define its pfaffian (H.E. Haber’s note),

$$\text{pf } M = \sum_P (-1)^P M_{i_1 j_1} M_{i_2 j_2} \cdots M_{i_{2N} j_{2N}},$$  

(1.4)

where $P$ is a permutation from $(1, 2, \ldots, 2N)$ to $(i_1, i_2, \cdots, i_{2N})$, such that

$$i_1 < j_1, i_2 < j_2, \cdots, j_{2N} < j_{2N}, \text{ and } i_1 < i_2 < \cdots < i_{2N}.$$  

$(-1)^P$ is the sign of permutation $p$. For example,

$$\text{pf } \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix} = a.$$  

(1.5)

For the determinant in Eq. (1.3), we have

$$\text{pf } w(\Lambda_i) \prod_{n=1}^{N} w_n(\Lambda_i).$$  

(1.6)

Pfaffian $\text{pf } M$ can be considered as the square root of determinant $\det M$, because of the general relation,

$$\det M = (\text{pf } M)^2.$$  

(1.7)

If we define the a cumulative index for filled bands at each TRIM as,

$$\delta_i = \prod_n \frac{w_n(\Lambda_i)}{\sqrt{\det w(\Lambda_i)}},$$  

(1.8)

then Eq. (1.1) can be re-written as

$$(-1)^\nu = \prod_{i=1}^{4} \frac{\text{pf } w(\Lambda_i)}{\sqrt{\det w(\Lambda_i)}} = \prod_{i=1}^{4} \delta_i.$$  

(1.9)
1. Edge state in 2D topological insulator

If the 1D spin pump or the 2D lattice in Fig. 1 has an edge at certain cutoff $x$, then $k$ (or $k_x$) is no longer a good quantum number. For the evolution of the edge states in a spin pump, by analogy, a 2D TI would have similar edge states inside the energy gap, crossing each other at TRIM (Fig. 2(b)).

In comparison, even though the edge states in a trivial insulator also need to cross each other at TRIM (Fig. 2(c)), the ways they link together are different. This is due to the fact that when $\delta_1 \delta_2$ and $\delta_3 \delta_4$ have opposite signs, $\nu = 1$, and we have a TI accompanied by a switch of Kramer-pair partner. When $\delta_1 \delta_2$ and $\delta_3 \delta_4$ have same sign, $\nu = 0$, and we have a trivial insulator with no switch of Kramer-pair partner.

If one plots a horizontal line (chemical potential) inside the energy gap, then it would cut the edge states in (b) odd number of times, but cut those in (c) even number of times. The former cannot be avoided by shifting or distorting the energy levels of edge states, while the latter can be avoided. Thus, the edge states in TI are robust, while those in trivial insulator are not.

2. Lattice with inversion symmetry

Even though $\nu$ is known to have two possible values, 0 and 1, it is not a trivial task to get explicit values of $\chi_{n\Lambda_i}$ at the first place. Fortunately, if the lattice has space inversion symmetry (SIS), then $\psi_{n\Lambda_i} / \sqrt{w_n(\Lambda_i)}$ is simply equal to the parity $\zeta$ of the Bloch state $\psi_{n\Lambda_i \pm}$ (a Kramer pair with index $\alpha = \pm$). This fact is proved below, following Nomura, 2013.

First, under space inversion,

$$\psi_{n\kappa}(r) \rightarrow \Pi \psi_{n\kappa}(r) = \psi_{n\kappa}(-r) = \psi_{n-k}(r), \quad (1.10)$$

where $\Pi$ is the SI operator. The same is true for the cell-periodic state,

$$u_{n\kappa}(r) \rightarrow \Pi u_{n\kappa}(r) = u_{n-k}(r). \quad (1.11)$$

If the lattice has SIS, then $\psi_{n\kappa}$ (but not $u_{n\kappa}$) are parity eigenstates at $k = \Lambda_i$,

$$\Pi \psi_{n\Lambda_i \alpha}(r) = \zeta_{\Lambda_i} \psi_{n\Lambda_i \alpha}(r). \quad (1.12)$$

The parity eigenvalue $\zeta_{n\Lambda_i} = \pm 1$ is the same for the two Bloch states (with $\alpha = \pm$) in a Kramer pair.

Note that there is a slight difference between Bloch state $\psi_{n\kappa}$ and cell-periodic state $u_{n\kappa}$,

$$\psi_{n\kappa + G} = \psi_{n\kappa}, \quad (1.13)$$

but

$$u_{n\kappa + G} = e^{-iG \kappa} u_{n\kappa}. \quad (1.14)$$

Therefore, only the Bloch state can have $\psi_{n \pm \frac{1}{2} \alpha} = \psi_{n \pm \alpha}$.

Second, define a different type of sewing matrix as follows, for a particular Kramer pair with index $n$ (suppressed),

$$v_{\alpha\beta}(k) = \langle u_{\kappa} | \Pi | \Theta | u_{\beta} \rangle. \quad (1.15)$$

(1) The matrix $v_{\alpha\beta}$ is anti-symmetric.

$Pf$: Using the relation $\langle \psi_1 | \Theta | \psi_2 \rangle = -\langle \Theta^2 \psi_1 | \Theta | \psi_2 \rangle = -\langle \psi_2 | \Theta | \psi_1 \rangle$, and $\Pi^2 = \Pi$, one has

$$v_{\alpha\beta} = \langle u_{\kappa} | \Pi \Theta | u_{\beta} \rangle = \langle u_{\kappa} | \Theta (\Pi | u_{\beta} \rangle = -\langle u_{\beta} | \Pi \Theta | u_{\kappa} \rangle = -v_{\beta\alpha}. \quad (1.16)$$

(2) The matrix $v_{\alpha\beta}$ is unitary.

$Pf$: Using the relation $\langle \psi_1 | \psi_2 \rangle^* = \langle \psi_2 | \psi_1 \rangle$, one has

$$(vv^\dagger)_{\alpha\gamma} = \sum_{\beta} v_{\alpha\beta} v_{\beta\gamma} = \sum_{\beta} \langle u_{\kappa} | \Pi \Theta | u_{\beta} \rangle \langle u_{\gamma} | \Pi \Theta | u_{\beta} \rangle^* = \langle u_{\kappa} | u_{\gamma} \rangle = \delta_{\alpha\gamma}. \quad (1.20)$$

Similarly, one can also show that $\langle v^\dagger v \rangle_{\alpha\gamma} = \delta_{\alpha\gamma}$. Therefore, it is unitary.

The matrix $w_{\alpha\beta}$ is also unitary, and is antisymmetric at $\Lambda_i$. Therefore, sewing matrices $w_{\alpha\beta}(\Lambda_i)$ and $v_{\alpha\beta}(\Lambda_i)$ differ by a multiplicative constant (the parity!)

$$w_{\alpha\beta}(\Lambda_i) = \langle u_{-\Lambda_i \alpha} | \Theta | u_{\Lambda_i \beta} \rangle = \langle \psi_{-\Lambda_i \alpha} | \Theta | \psi_{\Lambda_i \beta} \rangle = \langle \psi_{\Lambda_i \alpha} | \Pi^2 \Theta | \psi_{\Lambda_i \beta} \rangle = \zeta_{\Lambda_i} \langle u_{\Lambda_i \alpha} | \Pi \Theta | u_{\Lambda_i \beta} \rangle = \zeta_{\Lambda_i} v_{\alpha\beta}(\Lambda_i). \quad (1.24)$$

Under a gauge transformation,

$$u_{k+} \rightarrow u_{k+}^L = e^{i\phi_k} u_{k+}, \quad (1.30)$$

$$u_{k-} \rightarrow u_{k-}^L = u_{k-}, \quad (1.31)$$

the off-diagonal matrix element of $v(k)$ transforms as,

$$v(k) \rightarrow v'(k) = e^{-i\phi_k} v(k). \quad (1.32)$$

FIG. 2 Comparison of the edge states in (a) 1D spin pump, (b) 2D topological insulator, and (c) 2D trivial insulator. (a) is a schematic plot of the edge state in Fig. ??.. (b) and (c) show the energy levels in edge BZ.
Therefore, one can adjust its phase such that \( v(\Lambda_i) = 1 \).

Thus,

\[
  w_n(\Lambda_i) = \zeta_n(\Lambda_i)v_n(\Lambda_i) = \zeta_n(\Lambda_i). \tag{1.33}
\]

As a result,

\[
  \frac{w_n(\Lambda_i)}{\sqrt{w_n^2(\Lambda_i)}} = \zeta_n(\Lambda_i). \tag{1.34}
\]

It follows that,

\[
  \delta_i = \prod_{n \in \text{filled}} \zeta_n(\Lambda_i), \tag{1.35}
\]

which is the cumulative parity of filled Bloch states (pick only one \( \zeta_n(\Lambda_i) \) for each Kramer pair) at a TRIM, and

\[
  (-1)^\nu = \prod_{i=1}^{4} \delta_i. \tag{1.36}
\]

3. \( Z_2 \) integer \( \nu \) as a topological invariant

To understand the \( Z_2 \) topology, we follow Moore and Balents’ argument for 2D TI (Moore and Balents, 2007). Because of time-reversal symmetry, the degenerate Bloch states for \( k \) and \(-k\) in a Brillouin zone are time-reversal conjugate (see Fig. 3(a)). As their Berry curvatures cancel with each other, the first Chern number for a filled band vanishes. Since the domain of independent Bloch states cover only half of the BZ (called effective Brillouin zone, or EBZ), one may wonder if the integral of the Berry curvature over the EBZ could be quantized.

Unfortunately, since the EBZ does not form a closed surface (see Fig. 3(b)), no quantization is guaranteed. To fix this, one can put two caps with TR conjugation to close the EBZ. This closed surface should have an integer \( C_1 \), but its value depends on the caps of choice. However, Moore and Balents proved that, because of the TR conjugation, \( C_1 \) mod 2 is independent of the caps of choice. Therefore, \( C_1 \) mod 2 should be an intrinsic property of the EBZ itself. We thus have two topological classes: 0 being the usual insulator, and 1 being the topological insulator.

Fu and Kane have shown that the \( Z_2 \) integer can also be written as (Fu and Kane, 2006),

\[
  \nu = \frac{1}{2\pi} \left( \int_{EBZ} d^2k \, \Omega_x - \oint_{\partial EBZ} dk \cdot A \right) \mod 2. \tag{1.37}
\]

The second term is the Berry connection integrated around the boundary of the EBZ. This is different from the Chern number in a quantum Hall system, which only has the first term, and is an integral over a closed surface (the whole BZ). The topological number here is for a manifold with edge.

Eq. (1.37) looks like the generalized Gauss-Bonnet formula for a 2D surface \( M \) with edge, in which the Berry curvature is replaced by the Gaussian curvature \( G \), and the Berry connection is replace by the geodesic curvature \( k_g \) of the boundary,

\[
  \chi = \frac{1}{2\pi} \left( \int_M d^2r \, G - \oint_{\partial M} dr \, k_g \right). \tag{1.38}
\]

For example, for a torus, \( \chi = 0 \), for a disk-like surface (which has a boundary), \( \chi = 1 \), and for a sphere, \( \chi = 2 \).

So far we have learned that the \( Z_2 \) topological invariant \( \nu \) can be calculated via,

1. The sign of \( \text{pf} \, w / \sqrt{\text{det} \, w} \) at TRIM (or, the parities of Bloch states at TRIM, if there is inversion symmetry).
2. The Gauss-Bonnet-like integral formula above.
3. The winding number between two patches of gauge choices over the Brillouin zone (Fu and Kane, 2006).
4. The vorticity of the pfaffian of a sewing matrix \( m \) (see Prob. 2).
5. The axion angle of electromagnetic response (see Chap. 9).

Except for the parities in 1., none of these is easy to evaluate. For a crystal without inversion symmetry, one can deform it to one that has SIS and determine its \( \nu \) by parities. This is a valid shortcut if the energy gap remains open during the process of deformation.

B. Bernevig-Hughes-Zhang model

The first experimentally confirmed (2D) TI is made from semiconductor quantum well. Bulk HgTe has inverted band structure (due to spin-orbit coupling) near...
the Fermi energy. Unfortunately, it’s a metal, not an insulator. Nevertheless, one can sandwich it between CdTe (an ordinary insulator), forming a quantum well (QW) and opening an energy gap near the Fermi energy (see Fig. 4). When the HgTe layer is thick, the discrete QW energy levels remain inverted, similar to the bulk CdTe (an ordinary insulator), forming a quantum well (QW) and opening an energy gap near the Fermi energy. However, if the HgTe layer is thinner than a critical width, the vectors \( R \) would switch positions. Therefore, one can check if the topology of the QW states (signified by the emergence of helical edge states) depends on the width of the QW (König et al., 2007).

Typical semiconductor band structure near \( k = 0 \) is shown in Fig. 5. In a QW, the LH bands split off the HH bands, so in the simplified Bernevig-Hughes-Zhang (BHZ) model, only conduction band and one HH valence band are considered (each are two-fold degenerate). In order to investigate the parities of Bloch states at TRIM, we follow the lattice version of the BHZ model proposed by Fu and Kane, 2007 (also, see Nomura, 2016)

For an atom at site \( \mathbf{R} \), four states are considered,

\[
|s \uparrow\rangle, |s \downarrow\rangle, |p_x + ip_y \uparrow\rangle, |p_x - ip_y \downarrow\rangle.
\]  

Without ambiguity, one can write \( |p_x + ip_y \uparrow\rangle \) and \( |p_x - ip_y \downarrow\rangle \) simply as \( |p \uparrow\rangle \) and \( |p \downarrow\rangle \). They are the states with quantum numbers \( m_j = 3/2 \) and \( m_j = -3/2 \).

We consider only the electron hopping between nearest neighbors. The relevant parameters are on-site energies \( \varepsilon_s, \varepsilon_p \), and hopping amplitudes \( t_{ss}, t_{pp}, \) and \( t_{sp} \) (and its complex conjugate \( t_{ps} \)), see Fig. 6. In a 2D square lattice, the vectors \( \mathbf{R} + a_p \) \((p = \pm x, \pm y) \) point to the four nearest neighbors of \( \mathbf{R} \). The tight-binding Hamiltonian is therefore given as,

\[
H = H_0 + H_1,
\]

\[
H_0 = \sum_{\mathbf{R} \sigma = \pm} (\varepsilon_s |\mathbf{R}s\sigma\rangle \langle \mathbf{R}s\sigma| + \varepsilon_p |\mathbf{R}p\sigma\rangle \langle \mathbf{R}p\sigma|),
\]

and \( (t_{ps} = t_{sp}) \)

\[
H_1 = -\sum_{\mathbf{R} \sigma} \sum_{\mu = \pm x, \pm y} (t_{ss}|\mathbf{R} + a_\mu s\sigma\rangle \langle \mathbf{R}s\sigma| - t_{pp}|\mathbf{R} + a_\mu p\sigma\rangle \langle \mathbf{R}p\sigma| + \varepsilon^{i\theta_{\mu}} t_{sp}|\mathbf{R} + a_\mu s\sigma\rangle \langle \mathbf{R}p\sigma| + \varepsilon^{-i\theta_{\mu}} t_{sp}|\mathbf{R}p\sigma\rangle \langle \mathbf{R} + a_\mu s\sigma|),
\]

where \( \theta_\mu = \angle(\hat{x}, a_\mu) \). That is, \( \theta_x = 0, \theta_y = \pi/2, \theta_{-x} = \pi, \theta_{-y} = 3\pi/2 \). Such a system has both TRS and SIS (details later).

Because of the lattice translation symmetry, the Hamiltonian can be diagonalized using the momentum basis. We therefore introduce the Fourier transformation \( (N \) is the total number of lattice sites),

\[
|R s\sigma\rangle = \frac{1}{\sqrt{N}} \sum_k e^{ik\mathbf{R}|k s\sigma\rangle},
\]

\[
|R p\sigma\rangle = \frac{1}{\sqrt{N}} \sum_k e^{ik\mathbf{R}|k p\sigma\rangle},
\]

and get (the lattice constant is set as one)

\[
H(k) = \begin{pmatrix}
\varepsilon_s - 2t_{ss}(\cos k_x + \cos k_y) & 2t_{sp}(\sigma_z \sin k_y - i \sin k_x) \\
2t_{sp}(\sigma_z \sin k_y + i \sin k_x) & \varepsilon_p + 2t_{pp}(\cos k_x + \cos k_y)
\end{pmatrix}.
\]
Or,
\[
H(k) = \left[ \frac{\varepsilon_s + \varepsilon_p}{2} - (t_{ss} - t_{pp})(\cos k_x + \cos k_y) \right] \tau_z \otimes 1 + \left[ \frac{\varepsilon_s - \varepsilon_p}{2} - (t_{ss} + t_{pp})(\cos k_x + \cos k_y) \right] \tau_z \otimes 1 + 2t_{sp} \sin k_x \tau_y \otimes 1 + 2t_{sp} \sin k_y \tau_x \otimes \sigma_z. \tag{1.45}
\]

The Pauli matrices \(\tau_{x,y,z}\) are for the orbital degree of freedom, and \(\sigma_{x,y,z}\) are for the spin degree of freedom.

1. Time reversal and space inversion

Time reversal flips spin, but not orbital, therefore it acts only on the spin degree of freedom. The TR operator is thus,
\[
\Theta = \begin{pmatrix}
i\sigma_y K & 0 \\
0 & i\sigma_y K
\end{pmatrix} = 1 \otimes i\sigma_y K. \tag{1.46}
\]

The \(s\)-orbital is even under space inversion, while the \(p\)-orbital is odd under SI. That is,
\[
\Pi|ks\sigma\rangle = |ks\sigma\rangle, \tag{1.47}
\]
\[
\Pi|kp\sigma\rangle = -|kp\sigma\rangle. \tag{1.48}
\]

Therefore,
\[
\Pi = \begin{pmatrix} 1 & 0 \\
0 & -1 \end{pmatrix} = \tau_z \otimes 1. \tag{1.49}
\]

One can check that the Hamiltonian \(H(k)\) is indeed invariant under these two transformations,
\[
\Theta H(k) \Theta^{-1} = H(-k), \tag{1.50}
\]
\[
\Pi H(k) \Pi^{-1} = H(-k). \tag{1.51}
\]

2. \(Z_2\) topological number

Since the BHZ model has SI symmetry, one can calculate the \(Z_2\) topological number from the parities of the Bloch states at TRIM (see Fig. 1(b)). At a TRIM, the first line of Eq. 1.45 contributes a constant energy shift and can be ignored, and the third line is zero. Therefore,
\[
H(\Lambda_1) = \left[ \frac{\varepsilon_s - \varepsilon_p}{2} - 2(t_{ss} + t_{pp}) \right] \tau_z \otimes 1, \tag{1.52}
\]
\[
H(\Lambda_2) = \left[ \frac{\varepsilon_s - \varepsilon_p}{2} \right] \tau_z \otimes 1, \tag{1.53}
\]
\[
H(\Lambda_3) = \left[ \frac{\varepsilon_s - \varepsilon_p}{2} \right] \tau_z \otimes 1, \tag{1.54}
\]
\[
H(\Lambda_4) = \left[ \frac{\varepsilon_s - \varepsilon_p}{2} + 2(t_{ss} + t_{pp}) \right] \tau_z \otimes 1. \tag{1.55}
\]

Since they are proportional to the parity operator \(\Pi = \tau_z \otimes 1\), an energy eigenstate at \(\Lambda_i\) is also a parity eigenstate.

Let’s assume \(\varepsilon_s > \varepsilon_p\) in the following discussion. If \(\varepsilon_s - \varepsilon_p > 4(t_{ss} + t_{pp}) > 0\), then the energies at \(\Lambda_1\) are
\[
\varepsilon_{1+} = \left[ \frac{\varepsilon_s - \varepsilon_p}{2} - 2(t_{ss} + t_{pp}) \right], \tag{1.56}
\]
\[
\varepsilon_{1-} = -\left[ \frac{\varepsilon_s - \varepsilon_p}{2} - 2(t_{ss} + t_{pp}) \right]. \tag{1.57}
\]

The degenerate eigenstates \(\psi_{1+}\) has even parity, while \(\psi_{1-}\) have odd parity. Only the state \(\psi_{1-}\) is filled instead. Therefore, \(\delta(\Lambda_1) = 1\). The other three parities are not changed. As a result,
\[
(-1)^\nu = 1, \text{ or } \nu = 0. \tag{1.58}
\]

This is a trivial insulator.

On the other hand, if \(\varepsilon_s - \varepsilon_p < 4(t_{ss} + t_{pp})\), then \(\varepsilon_{1-} > \varepsilon_{1+}\). Due to the band inversion, now the states \(\psi_{1-}\) are filled instead. Therefore, \(\delta(\Lambda_1) = -1\). The other three parities are not changed. As a result,
\[
(-1)^\nu = -1, \text{ or } \nu = 1. \tag{1.59}
\]

This is a topological insulator.

3. Orbital basis versus spin basis

Note that in Eq. 1.44, every 2 \(\times\) 2 block of the Hamiltonian matrix is diagonal. In this case, it is possible to block-diagonal the 4 \(\times\) 4 matrix by re-arranging the order of the basis,
\[
|s\uparrow\rangle, |s\downarrow\rangle, |p\uparrow\rangle, |p\downarrow\rangle \quad \rightarrow \quad |s\downarrow\rangle, |p\uparrow\rangle, |s\uparrow\rangle, |p\downarrow\rangle. \tag{1.60}
\]

For convenience, we call the first choice the orbital basis, and the second the spin basis.

Under the spin basis, the Hamiltonian becomes (first switch the 2nd and 3rd rows, then switch the 2nd and the 3rd columns of the matrix)
\[
H(k) = \begin{pmatrix}
h(k) & 0 \\
0 & h^*(-k)
\end{pmatrix}, \tag{1.62}
\]

where
\[
h(k) = \begin{pmatrix}
\varepsilon_s - 2t_{ss}(\cos k_x + \cos k_y) & 2t_{sp}(-i \sin k_x + \sin k_y) \\
2t_{sp}(i \sin k_x + \sin k_y) & \varepsilon_p + 2t_{pp}(\cos k_x + \cos k_y)
\end{pmatrix}
\]
\[
= \varepsilon_0(k) + 2t_{sp} \sin k_x \tau_y + 2t_{sp} \sin k_y \tau_x \tag{1.63}
\]
\[
+ \left[ \frac{\varepsilon_s - \varepsilon_p}{2} - (t_{ss} + t_{pp})(\cos k_x + \cos k_y) \right] \tau_z.
\]

Because of the block diagonalization, the up and down spins are explicitly decoupled.

Note that the TR and SI operators also are altered under the new basis. They now become
\[
\Theta = i\sigma_y K \otimes 1, \quad \Pi = 1 \otimes \tau_z. \tag{1.64}
\]
4. QWZ model versus BHZ model

When written in the block-diagonal form, the Hamiltonian $h(k)$ is similar to the QWZ model Hamiltonian for the QAHE (see ??). That is, the BHZ model is composed of two independent QWZ subsystems, $h(k)$ and $h^*(-k)$.

One can write
\[ h(k) = \varepsilon_0(k) + d(k) \cdot \tau, \]  
then the Hall conductivity of the subsystem is,
\[ \sigma_{xy} = -\frac{e^2}{4\pi} \int_{BZ} d^2k \frac{1}{d^4} \frac{\partial d}{\partial k_x} \times \frac{\partial d}{\partial k_y}. \]  

One can check that if $\varepsilon_s - \varepsilon_p > 4(t_{ss} + t_{pp})$, then the signs of $d_z(\varepsilon)$ are all positive at the TRIM (analogous to Fig. ??(a)). If $\varepsilon_s - \varepsilon_p < 4(t_{ss} + t_{pp})$, then $d_z(\Lambda_1)$ becomes negative, while the other three signs remain the same (see Fig. ??(b)). According to the analysis of the QAHE in ??, the first case has $\sigma_{xy} = 0$, while the second case has $\sigma_{xy} = e^2/h$.

When the subsystem is in the QAHE phase, according to the discussion in ??, it has chiral edge states. Since this subsystem consists only of spin-up electrons (see Eq. 1.61), the edge-state electrons are spin-up. On the other hand, the conjugate subsystem $h^*(-k)$ has $\sigma_{xy} = -e^2/h$. Its edge electrons transport along the opposite direction and the spins are down (see Fig. 7(a)).

In momentum space, the energy dispersion of the edge state is linear in the small $k$-limit. One has positive slope (positive velocity), and the other has negative slope (negative velocity). Because of the Kramer degeneracy, these two dispersion curves have to cross each other at a TRIM (see Fig. 7(b)). This point degeneracy can be lifted only if the TRS is broken.

The topological phase of the BHZ model is called a 2D TI phase, aka a quantum spin Hall (QSH) phase. Its edge state, with one spin moving along one direction, and the opposite spin moving along the opposite direction, is called a helical edge state. It is robust in the sense that, even if there is a non-magnetic impurity $V_{imp}(r)$ blocking the way, the electron will not be back scattered since that requires a spin flip. In the Born approximation, the transition amplitude for backscattering is zero since $\langle \psi_e | V_{imp}(r) | \theta \psi_e \rangle = 0$. See Prob. 2 of Chap ??.

If there is a magnetic impurity that breaks TRS, then an electron could be backscattered, accompanied by a spin flip. Also, in the presence of electron interaction, there is a possibility that the edge is spontaneously magnetized. Should this happen, then the edge state is no longer protected by the TRS.

Even though several materials are predicted to be 2D TI, few has been verified in experiments due to small band gap. Some candidates proposed in recent years are 2D transition metal dichalcogenides (such as the 1T’ form of WTe$_2$) (Cazalilla et al., 2014, Qian et al., 2014), and single-layer ZrTe$_5$ (Weng et al., 2014, Li et al., 2016).

Exercise
1. Start from the tight-binding Hamiltonian in Eqs. (1.40) and (1.41), switch to the momentum basis, and verify Eq. (1.44).
2. In addition to $w$, $s$, and $v$, a fourth type of sewing matrix is defined as
\[ m_{\alpha\beta}(k) = \langle u_{k\alpha} | \Theta | u_{k\beta} \rangle. \]

Consider the case with only one Kramer pair ($\alpha, \beta = \pm$):
(a) Show that the matrix $m$ is unitary and antisymmetric.
(b) Show that
\[ m(-k) = w(k)m^*(k)w^T(k). \]
(c) With the help of the identity $\text{pf}(BA) = (\text{det } B)(\text{pf } A)$, show that
\[ \log[\text{det } w(k)] = \log[\text{pf } m(-k)] - \log[\text{pf } m^*(k)] \]
\[ = \log[\text{pf } m(-k)] + \log[\text{pf } m(k)]. \]
(d) Let $\Lambda_x$ and $\Lambda_y$ be 0 or $\pi$. Write $\text{pf } m(k_x, \Lambda_y)$ as $m(k_x); \text{pf } w(k_x, \Lambda_y)$ as $w(k_x)$. Show that $(k_y = \Lambda_y)$,
\[ P_0 = \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk_y \partial_k \log m(k_x) + \frac{i}{\pi} \log \frac{m(\pi)}{m(0)} \]
Note that $w(\Lambda_x) = m(\Lambda_x) = \pm 1$.
(e) Finally, show that
\[ \Delta P_0 = P_0(k_y = \pi) - P_0(k_y = 0) \]
\[ = \frac{1}{2\pi i} \int_{EBZ} dk \cdot \partial_k \log[\text{pf } m(k)] \mod 2, \]
where $EBZ = [-\pi, \pi] \times [0, \pi]$ is the upper half of the BZ. That is, the $Z_2$ topological invariant is the total vorticity of the zeros of $\text{pf}[m(k)]$ in the effective BZ. For more details, see Fu and Kane, 2006 and Sec. 4.5 of Fruchart and Carpentier, 2013.

References