Lecture notes on topological insulators

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II. CHARGE POLARIZATION, ANOMALOUS QUANTUM HALL EFFECT

In addition to the quantum Hall effect, Berry phase is essential to the calculation of charge polarization. It could also be a key ingredient in anomalous Hall effect. We illustrate these connections in this chapter.

A. Modern theory of charge polarization

The electric polarization $P$ of an infinite crystal, or a crystal with periodic boundary condition (PBC) is generally not well defined. The reason is that, in a periodic solid, the electric polarization depends on one’s choice of the unit cell. The theory of electric polarization in conventional textbooks applies only to solids consisting of well localized charges, such as ionic or molecular solids (Clausius-Mossotti theory). It fails, for example, in a covalent solid with bond charges such that no natural unit cell can be defined (see Fig. 1).

A crucial observation made by R. Resta is that, even though the value of $P$ may be ambiguous, its change is well defined (Resta, 1992). It was soon pointed out by King-Smith and Vanderbilt that $\Delta P$ has a deep connection with the Berry phase of the Bloch state (King-Smith and Vanderbilt, 1993).

To illustrate the modern theory of polarization, let’s consider a one-dimensional (1D) lattice with periodic boundary condition (PBC). There are $N$ lattice points located at $R_\ell = \ell a$ ($\ell \in \mathbb{Z}$), and $a$ is the lattice constant. The Fourier transformation of the Bloch state $\psi_{nk} = e^{ikx}u_{nk}$ is called the Wannier state,

$$|nR_\ell\rangle = \frac{1}{\sqrt{N}} \sum_{k=-\pi}^{\pi} e^{-ikR_\ell} |\psi_{nk}\rangle,$$

which is localized near a lattice point $R_\ell$. The Bloch states form an orthonormal basis,

$$\langle \psi_{n'k'} | \psi_{nk} \rangle = \delta_{n'n}\delta_{kk'}.$$

Likewise, the Wannier states are also orthonormal to each other,

$$\langle n'R|R\rangle = \delta_{nn'}\delta_{RR'}.$$

In an insulator, the electric polarization can be related to the charge center of the Wannier function,

$$P = q \sum_{\text{filled } n} \langle n0|x|n0\rangle, \quad q = -e$$

$$= \frac{q}{N} \sum_{n} \sum_{kk'} \langle u_{nk'}| e^{-ik'x} \frac{1}{i} \frac{\partial}{\partial k} (e^{ikx}) |u_{nk}\rangle$$

$$= \frac{q}{N} \sum_{n} \sum_{kk'} \langle u_{nk'}| e^{i(k-k')x} i \frac{\partial}{\partial k} |u_{nk}\rangle.$$

Decompose the $x$-integral as a sum of $N$ unit-cell integrals, and write $x = ma + x'$ ($x' \in [0, a]$), it can be shown that (see Nomura, 2013, p.85)

$$\langle u_{nk'}| e^{i(k-k')x} i \frac{\partial}{\partial k} |u_{nk}\rangle = N\delta_{k,k'} \langle u_{nk}| i \frac{\partial}{\partial k} |u_{nk}\rangle_{\text{cell}}$$

$$= \delta_{k,k'} \langle u_{nk}| i \frac{\partial}{\partial k} |u_{nk}\rangle,$$

where $\langle \cdot \cdot \cdot \rangle_{\text{cell}}$ integrates over only one unit cell, and $N\langle \cdot \cdot \cdot \rangle_{\text{cell}} = \langle \cdot \cdot \cdot \rangle$ is used in the second equation. Therefore,

$$P = \frac{q}{N} \sum_{n} \sum_{k} \langle u_{nk}| i \frac{\partial}{\partial k} |u_{nk}\rangle$$

$$= qa \sum_{n} \int_{-\pi}^{\pi} \frac{dk}{2\pi} A_n(k).$$
Under a gauge transformation, $|w'_{nk}\rangle = e^{i\chi_{nk}}|w_{nk}\rangle$, where $\chi_{nk}$ is single-valued (mod $2\pi$), the polarization contributed from band-$n$ is,

$$P_n' = P_n - qa \frac{\chi_{n+2\pi} - \chi_{n-\pi}}{2\pi}.$$  

(11.11)

Single-valuedness of $\chi_{nk}$ gives $\chi_{nk+2\pi} = \chi_{nk} + 2\pi ma$ ($m \in Z$), therefore,

$$P_n' = P_n - qma.$$  

(11.12)

The polarization could change by $qma$ under a gauge transformation. That is, only the fractional part of $P_n$ (and $P$) is physical.

Note that the integral in Eq. (1.10) is nothing but the Berry phase divided by $2\pi$,

$$P = qa \sum_n \frac{\gamma_n}{2\pi}.$$  

(11.13)

The Berry phase of 1D Bloch states is first studied by Zak, 1989 and is called Zak phase. In addition to being gauge dependent, the value of Zak phase is also coordinate dependent (see Prob. 1), but the relative phases between energy bands are fixed. For a 1D lattice with space inversion symmetry, if the origin is at a symmetric point, then the Zak phase can only be $0$ or $\pi$, and $P_n$ can only be $0$ or $qa/2$. This can be understood as follows: It was shown earlier that if the lattice has space inversion symmetry, then (see Eq. (8))

$$A_n(-k) = -A_n(k).$$  

(11.14)

Therefore, after the inversion,

$$P_n \rightarrow P'_n = qa \int_{-\pi}^{\pi} \frac{dk}{2\pi} A_n(-k) = -P_n.$$  

(11.15)

Since $P_n$ is allowed to have the freedom of changing by $qma$, the constraint given by the inversion symmetry is

$$P_n = -P_n \mod qa$$  

(11.16)

$$\rightarrow P_n = 0 \mod a/2 \mod qa.$$  

(11.17)

Put it in another way, for a lattice with space-inversion symmetry, the charge center $\langle n|\rangle \langle x|\rangle \langle n|0\rangle$ in a unit cell can only be at $0$ or $a/2$ (on top of a lattice point or in the middle between two lattice points). On the other hand, if there is no inversion symmetry, then $\gamma_n$ (and $P_n$) can be any value. An experimental confirmation of the Zak phase with cold atoms can be found in Atala et al., 2013.

Even though $P_n$ is gauge dependent, the change of polarization $\Delta P_n$ under an adiabatic and continuous deformation is gauge invariant and well-defined. From here on we consider only one filled band, and use $A$ to label the degree of ion displacement. It varies from 0 to 1 as the ions shift adiabatically from an initial position to a final position. The difference of polarizations between these two states is,

$$P(\lambda_2) - P(\lambda_1) = qa \int_{-\pi}^{\pi} \frac{dk}{2\pi} [A(k, \lambda_2) - A(k, \lambda_1)].$$  

(1.18)

The parameter $\lambda$ defines a second dimension in addition to $k$. We can choose the parallel transport gauge, such that there is no phase accumulation along the $\lambda$-direction, then $\Delta P$ can be written as a (counter-clockwise) line integral around the rectangle in Fig. 2,

$$\Delta P = -\frac{qa}{2\pi} \int d\mathbf{k} \cdot A(\mathbf{k}), \quad \mathbf{k} \equiv (k, \lambda)$$  

(1.19)

$$= -\frac{qa}{2\pi} \int d^2k F_z(k),$$  

(1.20)

where $F_z(k) = \partial_k A_\lambda - \partial_\lambda A_k$, and $A_\lambda = i\langle u_k | \partial_\lambda | u_k \rangle$.

If $\lambda(1) = \lambda(0)$, then the rectangle is similar to a BZ, where opposite edges harbor the same states. Therefore, the integral of the Berry curvature is an integer ($\times 2\pi$), and

$$\Delta P = qaC_1.$$  

(1.21)

That is, under a periodic parametric variation, the charge transport is “quantized”. This fact can be utilized to build a quantized charge pump (Thouless et al., 1982). However, be aware that even though the quantization is precise in the adiabatic limit, it is no longer if the pumping is fast.

The analysis above is based on one-particle states in 1D. But the same scheme can be extended to real solids with electronic interactions in three dimensions. An essential alteration is to replace the one-particle states by Kohn-Sham orbitals in the density functional theory (King-Smith and Vanderbilt, 1993).

B. Rice-Mele model

To illustrate the parametric charge pumping, we consider a dimerized 1D lattice (Rice and Mele, 1982),

$$H = \frac{1}{2} \sum_{i=1}^{2N} \left( t_0 + (-1)^i \delta \right) (c_i^\dagger c_{i+1} + h.c.) - (-1)^i \Delta c_i^\dagger c_i,$$

(1.22)

where $t_0$ is the hopping amplitude between nearest neighbors, $\pm \delta$ modulate the hopping strength, $\pm \Delta$ are the onsite potentials for staggered sublattices, and $c_{2N+1} = c_1$. 

FIG. 2 The domain of Bloch momentum $k$ and parameter $\lambda$ is similar to a BZ of a two dimensional lattice.
(PBC). The famous Su-Shrieff-Heeger model (Su et al., 1979) for polyacetylene is a special case of the Rice-Mele model with $\Delta = 0$ (see Fig. 3).

Since the lattice is dimerized, it is convenient to write $c_{i=2j-1}$ as $c_j$, $c_{i=2j}$ as $d_j$, and double the size of the unit cell to $a$. The Hamiltonian becomes,

$$H = \frac{1}{2} \sum_{j=1}^{N} (t_0 - \delta) \left( c_j^\dagger d_j + h.c. \right) + \Delta c_j^\dagger c_j$$

$$+ \frac{1}{2} \sum_{j=1}^{N} (t_0 + \delta) \left( c_{j+1}^\dagger d_j + h.c. \right) - \Delta d_j^\dagger d_j.$$ (1.23)

Expand $c_j$ and $d_j$,

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{i(j-k)\delta} c_k,$$ (1.24)

$$d_j = \frac{1}{\sqrt{N}} \sum_k e^{i j \delta} d_k,$$ (1.25)

where $N$ is the total number of unit cells, then

$$H = \sum_k (c_k^\dagger d_k^\dagger) \left( t_0 \cos \frac{ka}{2} + i \delta \sin \frac{ka}{2} \right) \left( \begin{array}{c} c_k \\ d_k \end{array} \right).$$

$$= \sum_k (c_k^\dagger d_k^\dagger) H(k) \left( \begin{array}{c} c_k \\ d_k \end{array} \right).$$ (1.26)

(1.27)

\[FIG. 3\] Two different locations of double bonds in polyacetylene.

One can write $H(k) = h(k) \cdot \sigma$, in which

$$h(k) = \left( t_0 \cos \frac{ka}{2}, \delta \sin \frac{ka}{2}, \Delta \right).$$ (1.28)

The band energies are

$$\varepsilon_{\pm}(k) = \pm \left( \Delta^2 + t_0^2 \cos^2 \frac{ka}{2} + \delta^2 \sin^2 \frac{ka}{2} \right)^{1/2}.$$ (1.29)

The two energy bands touch at $(ka, \delta, \Delta) = (\pm \pi, 0, 0)$.

We now demonstrate the charge pumping under the periodic variation,

$$(\delta(t), \Delta(t)) = (\delta_0 \cos t, \Delta_0 \sin t).$$ (1.30)

Note that the Hamiltonian $H$ has the same structure as the one for the spin-1/2 system in Eq. (12). $h(k)$ plays the role of the magnetic field, and the two sublattices play the roles of the spin up/down degrees of freedom. Therefore, the Berry phase due to the variation of parameters can be determined by the solid angle extended by a closed path in the $h$-space.

First, consider the case with $\Delta = 0$, then

$$h(k) = \left( t_0 \cos \frac{ka}{2}, \delta \sin \frac{ka}{2}, 0 \right).$$ (1.31)

Expand $c_j$ and $d_j$,

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{i(j-k)\delta} c_k,$$ (1.24)

$$d_j = \frac{1}{\sqrt{N}} \sum_k e^{i j \delta} d_k,$$ (1.25)

where $N$ is the total number of unit cells, then

$$H = \sum_k (c_k^\dagger d_k^\dagger) \left( t_0 \cos \frac{ka}{2} + i \delta \sin \frac{ka}{2} \right) \left( \begin{array}{c} c_k \\ d_k \end{array} \right).$$

$$= \sum_k (c_k^\dagger d_k^\dagger) H(k) \left( \begin{array}{c} c_k \\ d_k \end{array} \right).$$ (1.26)

(1.27)

\[FIG. 4\] (a) Two semi-circle paths due to the increasing of $ka$ from $0$ to $2\pi$. Path-1 is for $\delta > 0$; path-2 is for $\delta < 0$. (b) A closed path on the $\delta - \Delta$ plane.

If $\delta > 0$, then when $ka$ increases from $0$ to $2\pi$, $h$ follows the path-1 in Fig. 4(a). On the other hand, if $\delta < 0$, when $ka$ increases from $0$ to $2\pi$, $h$ follows the path-2 in Fig. 4(a). The two paths together extends a solid angle $\Omega = 2\pi$. Therefore, the difference of polarizations,

$$P(\delta_0, 0) - P(-\delta_0, 0) = qa \gamma \Omega = q a \Omega \gamma \frac{1}{2}.$$ (1.32)

This is a sensible result since a chain with modulation $-\delta$ can be obtained from shifting a chain with modulation $\delta$ by $a/2$ (Xiao et al., 2010).

We now consider the cyclic variation,

$$h(k) = \left( t_0 \cos \frac{ka}{2}, \delta_0 \sin \frac{ka}{2} \cos t, \Delta_0 \sin t \right).$$ (1.33)

When $\Delta \neq 0$, the size of the loop traversed in Fig. 4(a) shrinks. It shrinks to $0$ when $\Delta(t) = \pm \Delta_0$ and $P(\delta, \pm \Delta_0) - P(-\delta, \pm \Delta_0) = 0$. Maximum difference is reached when $\Delta$ is zero.
Start from \( t = 0 \), then (see Fig. 4(b)) under appropriate gauge choice, one could expect to have

\[
P(\delta_0, 0) = q\frac{a}{4}.
\]

(1.34)

Next, at \( t = \pi / 2 \),

\[
P(0, \Delta_0) = 0.
\]

(1.35)

Also, at \( t = \pi \),

\[
P(-\delta_0, 0) = -q\frac{a}{4},
\]

(1.36)

and so no. This is consistent with the result in Eq. (1.32).

After a full cycle in Fig. 4(b), the polarization changes by 0 or \( qa \). In the latter case, a quantized charge has been transported. Recent confirmations of the charge pumping related to the Rice-Mele model are reported in Lohse et al., 2015, and Nakajima et al., 2016.

C. Qi-Wu-Zhang model

In this section, we introduce a simple 2D model proposed by Qi, Wu and Zhang to illustrate the connection between Berry phase and quantized Hall conductivity (Qi et al., 2006). The fermions are living on a 2D square lattice, and each lattice point is allowed to have two degrees of freedom (quasi-spin). The quasi-spin typically refers to the valence band with \( s \)-orbitals and the conduction band with \( p \)-orbitals. The QWZ Hamiltonian is given as,

\[
\begin{align*}
H(k) &= H_0 + H_m + H_{by}, \\
H_0 &= \varepsilon_0(k) + \\
t \begin{pmatrix}
2 - \cos k_x a - \cos k_y a & 0 \\
0 & -(2 - \cos k_x a - \cos k_y a)
\end{pmatrix}, \\
H_m &= m \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}, \\
H_{by} &= \lambda \begin{pmatrix}
0 & \sin k_x a - i \sin k_y a \\
\sin k_x a + i \sin k_y a & 0
\end{pmatrix}.
\end{align*}
\]

(1.37)

\( H_m \) is a mass term that breaks parity symmetry (see p.12 of Hugh’s thesis), and \( H_{by} \) is the hybridization between \( s \) - and \( p \)-bands.

It is also possible to interpret the quasi-spins as true spins, then \( H_m \) is a magnetization term that breaks time-reversal symmetry, and \( H_{by} \) is a spin-orbit coupling.

In short,

\[
H(k) = \varepsilon_0(k) + h(k) \cdot \sigma,
\]

(1.38)

where

\[
h(k) = \begin{pmatrix}
\lambda \sin k_x a, \lambda \sin k_y a, m + t \sum_{j=1}^{2}(1 - \cos k_j a)
\end{pmatrix}.
\]

(1.39)

The eigen-energies are,

\[
\varepsilon_{\pm}(k) = \varepsilon_0(k) \pm |h(k)|.
\]

(1.40)

For simplification, we will set \( t, a, \lambda = 1 \). It is not difficult to see that there are energy gaps at

\[
\begin{align*}
k_0 &= 0 \rightarrow \varepsilon_{\pm}(k_0) = \varepsilon_0 \pm m, \\
k_0 &= (\pi, 0), (0, \pi) \rightarrow \varepsilon_{\pm}(k_0) = \varepsilon_0 \pm |m + 2|, \\
k_0 &= (\pi, \pi) \rightarrow \varepsilon_{\pm}(k_0) = \varepsilon_0 \pm |m + 4|.
\end{align*}
\]

(1.41-1.43)

The energy gap closes at \( m = 0, -2, \) and -4. We will see that the topology of the Bloch states changes at these critical points, when the energy gap closes.

The distribution of the \( h(k) \) vectors in the BZ changes when an energy gap closes, see Fig. 5. Depending on the value of \( m \), there are four different regimes:

1. \( m > 0 : h_z(k) > 0 \) over the whole BZ.
2. \( -2 < m < 0 : h_z(k) < 0 \) near \( k = 0 \).
3. \( -4 < m < -2 : h_z(k) > 0 \) near \( k = (\pi, \pi) \) (and its equivalent points).
4. \( m < -4 : h_z(k) < 0 \) over the whole BZ.

The \( h \) in Eq. (1.38) is the “magnetic field” for the quasi-spin. In case (1), the magnetic field only sweeps over the northern hemisphere when \( k \) scans over the BZ. According to the analysis in ??, one needs only to choose one gauge \( A^N(k) \) over the whole BZ. Therefore, the topology is expected to be trivial and the Hall conductivity \( \sigma_H = 0 \).

In cases (2) and (3), \( h_z \) changes sign, and two gauges, \( A^N \) and \( A^S \) are required to avoid the singularity. Therefore the topology is non-trivial and \( \sigma_H \neq 0 \).

Case (4) is similar to Case (1), but \( h \) sweeps over the southern hemisphere only. The topology is again trivial and \( \sigma_H = 0 \).

The simple picture presented above can be verified by actual calculation of \( \sigma_H \). First, we show that (Nomura,
\[ F^\pm_z(k) = ± \frac{1}{2\hbar^3} \mathbf{h} \cdot \frac{\partial \mathbf{h}}{\partial k_x} \times \frac{\partial \mathbf{h}}{\partial k_y} \]  \hspace{1cm} (1.44)

**Pf.** The Berry connections in \( k \)-space are,

\[ A^\pm_x(k) = i\langle \mathbf{h}, \pm | \frac{\partial}{\partial k} | \mathbf{h}, \pm \rangle \]  \hspace{1cm} (1.45)

\[ = \frac{\partial h_{k\alpha}}{\partial k_{\ell}} i\langle \mathbf{h}, \pm | \frac{\partial}{\partial h_{k\alpha}} | \mathbf{h}, \pm \rangle \]  \hspace{1cm} (1.46)

\[ = \frac{\partial h_{k\alpha}}{\partial k_{\ell}} a^\pm_{\alpha \beta}(\mathbf{h}), \]  \hspace{1cm} (1.47)

where \( a^\pm \) are the Berry connections in \( h \)-space. Therefore, the Berry curvatures in \( k \)-space are,

\[ F^\pm_z(k) = \frac{\partial A^\pm_x}{\partial k_x} - \frac{\partial A^\pm_y}{\partial k_y} \]  \hspace{1cm} (1.48)

\[ = \frac{\partial}{\partial k_x} \left( \frac{\partial h_{k\alpha}}{\partial k_{\beta}} a^\pm_{\alpha \beta} \right) - \frac{\partial}{\partial k_y} \left( \frac{\partial h_{k\alpha}}{\partial k_{\beta}} a^\pm_{\alpha \beta} \right) \]  \hspace{1cm} (1.49)

\[ = \frac{\partial h_{k\alpha}}{\partial k_x} \frac{\partial h_{k\beta}}{\partial k_{\gamma}} \varepsilon_{\alpha \beta \gamma} b^\pm \]  \hspace{1cm} (1.50)

\[ = \frac{\partial h_{k\alpha}}{\partial k_x} \frac{\partial h_{k\beta}}{\partial k_{\gamma}} \varepsilon_{\alpha \beta \gamma} b^\pm \]  \hspace{1cm} (1.51)

\[ = \pm \frac{1}{2\hbar^3} \mathbf{h} \cdot \frac{\partial h_{k\alpha}}{\partial k_x} \times \frac{\partial h_{k\beta}}{\partial k_y} \]  \hspace{1cm} (1.52)

in which \( b^\pm = \mp h_z/2\hbar^3 \) are the Berry curvatures in \( h \)-space. End of proof.

Suppose the lower band is completely filled, and the upper band is empty, then

\[ \sigma_H = \frac{e^2}{\hbar} \frac{1}{2\pi} \int_{BZ} d\mathbf{k} F^-_z(k) \]  \hspace{1cm} (1.53)

\[ = \frac{e^2}{\hbar} \frac{1}{4\pi} \int_{BZ} d\mathbf{k} \frac{1}{\hbar} \mathbf{h} \cdot \frac{\partial \mathbf{h}}{\partial k_x} \times \frac{\partial \mathbf{h}}{\partial k_y} \]  \hspace{1cm} (1.54)

In the integrand, \( \mathbf{h} \cdot \left( \frac{\partial h_{k\alpha}}{\partial k_x} d\mathbf{k} \right) \times \left( \frac{\partial h_{k\beta}}{\partial k_y} d\mathbf{k} \right) \) is actually the area \( d^2S \) on the \( h \)-surface in Fig. 6. After being divided by \( \hbar^2 \), it becomes the solid angle \( d\Omega \) extended by that area. Since the BZ is a closed surface (a 2D torus, or \( T^2 \)), under a continuous mapping, it would map to a closed surface in \( h \)-space (see Fig. 7). The integral in Eq. (1.54) gives the total solid angle extended by that \( h \)-surface. For a closed surface, it must be an integer multiple of \( 4\pi \), thus

\[ \sigma_H = w \frac{e^2}{\hbar^2} \]  \hspace{1cm} (1.55)

The integer \( w \), which is equal to the first Chern number \( C_1 \), is the number of times the \( h \)-surface wraps over a unit sphere \( S^2 \). It characterizes the topology of the mapping (and the Bloch states) and is called the winding number (or the wrapping number). We emphasize that \( w \) is an integer only if the base space is a close surface (in this case, \( T^2 \)), which requires the valence band to be completely filled (that is, an insulator).

The quantized Hall conductance in the QWZ model is a result of the “magnetization” \( m \), not an external magnetic field (as in the case of the quantum Hall effect). It is called alternatively as the quantum anomalous Hall effect (QAHE). Their difference is that, in the QHE, the electron orbitals are quantized due to the external magnetic field; in the QAHE there is no orbital quantization,
FIG. 8 (a) A topological phase occupies the left side of the space. (b) A finite sample with two boundaries. The edge states move in a definite direction along an edge.

but only spin re-orientation due to \( m \). A recent confirmation of the QAHE can be found in Chang et al., 2013.

One could apply an external magnetic field to the QAH insulator (aka Chern insulator). Then there will be orbital quantization and Landau levels in energy spectrum. Interested readers can consult p. 103 of Bernevig and Hughes, 2013 for more details.

D. Edge state in the Qi-Wu-Zhang model

Topological materials (insulators) have an important property: their surface states are stable against perturbations. They can be destroyed only if the energy gap of the bulk bands closes so that the topology of the electronic states is trivialized. In general, the interface between two materials with different topologies would have robust interface states. A heuristic explanation is as follows: to go from one material to another, the spatial-dependent interface states. A heuristic explanation is as follows: to go from one material to another, the spatial-dependent energy gap (in the sense of the Thomas-Fermi approximation) needs to close near the interface, otherwise it is simply impossible for the topology to change. This gapless region is where the surface states reside.

Take the 2D QWZ model as an example. Divide the space to two parts where

\[
m(x) = \begin{cases} 
> 0 & \text{for } x > 0, \\
< 0 & \text{for } x < 0,
\end{cases}
\]

so that there is a 1D boundary along the \( y \)-axis (see Fig. 8(a)). For simplicity, consider only the small \( k \) limit,

\[
H(k) = \varepsilon_0 + \left( \frac{m(x)}{\lambda(k_x - ik_y)} \right) + O(k^2).
\]

The exact profile of \( m(x) \) does not matter, as long as it is monotonic and smooth (compared to the electron wavelength \( \lambda \)). To solve for the surface states, one needs to re-quantize the Hamiltonian using the substitution \( k \rightarrow \frac{1}{\lambda} \frac{\partial}{\partial x} \), such that

\[
H(p) = \varepsilon_0 + \left( \frac{m(x)}{\lambda} \right) \left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) - m(x).
\]

The \( x \)-directions extend to infinity on both ends, and PBC is imposed along the \( y \)-direction.

We now solve the differential equation,

\[
H(p)\psi(x, y) = \varepsilon\psi(x, y).
\]

Use the method of separation of variables and write

\[
\psi(x, y) = \phi_1(x)\phi_2(y).
\]

Since the \( y \)-direction is invariant under translation, a trivial solution is \( \phi_2(y) = e^{ik_yy} \), a plane wave. Therefore, the equation for \( \phi_1(x) \) is

\[
\left( \frac{m(x)}{\lambda} \right) \left( \frac{\partial}{\partial x} - m(x) \right) \phi_1(x) = \varepsilon\phi_1(x).
\]

We can take a guess at a solution that is localized near the boundary,

\[
\phi_1(x) = e^{-\frac{i}{\lambda} \int_0^x dx' m(x')} \begin{pmatrix} a \\ b \end{pmatrix}.
\]

It can be verified as an eigenstate with eigenvalue \( \varepsilon = \lambda k_y \) if \((a, b) = (1, i)\). Furthermore, it decays to zero at \( x \ll 0 \) and \( x \gg 0 \), and has a peak at \( x = 0 \).

On the other hand, if

\[
m(x) \begin{cases} 
> 0 & \text{for } x < 0, \\
< 0 & \text{for } x > 0,
\end{cases}
\]

then

\[
\phi_1(x) = e^{\frac{i}{\lambda} \int_0^x dx' m(x')} \begin{pmatrix} 1 \\ i \end{pmatrix}.
\]

is a localized eigenstate with \( \varepsilon = -\lambda k_y \).

Therefore, in a sample with finite width (see Fig. 8(b)), the electrons on the right edge move with velocity \( \frac{\partial}{\partial x} = \lambda/y \); the ones on the left move with velocity \( -\lambda/y \). They are called chiral edge states. The two edges can be treated as independent only if the strip is wide enough (compared to the decay length of the edge state) so that the edge states on two sides do not couple with each other. In the small \( k_y \) limit, the energy dispersion \( \varepsilon(k_y) \) of the edge states are linear in \( k_y \). This is not so for larger \( k_y \)'s, where numerical calculation is required.

Exercise

1. The value of Zak phase depends on the choice of the origin. Under a shift of the origin,

\[
\psi_k(x) \rightarrow \psi'_k(x) = \psi_k(x-d).
\]

This leads to

\[
u_k(x) \rightarrow u'_k(x) = u_k(x-d)e^{-ikd}.
\]

Show that

\[
\gamma \rightarrow \gamma' = \gamma + 2\pi \frac{d}{a}.
\]
where $a$ is the lattice constant.

2. Consider the Rice-Mele model with $\Delta = 0$, i.e., the Su-Schrieffer-Heeger (SSH) model.

(a) *Instead of Eq. (1.25)*, use the following expansion,

$$
c_j = \frac{1}{\sqrt{N}} \sum_k e^{i j a k} c_k,
$$

$$
d_j = \frac{1}{\sqrt{N}} \sum_k e^{i j a k} d_k.
$$

Find out the Hamiltonian in momentum-space, $H(k) = \hbar k \cdot \sigma$.

(b) Find out the winding number of $h(k)$ around the origin when $k$ runs through the 1D Brillouin zone. Consider the cases with $\delta > 0$ and $\delta < 0$ respectively. They represent two phases with different topologies.

Note: The winding number can be written as,

$$
\text{winding number} = \int_{\text{BZ}} dB \cdot h \times \frac{dh}{dk}.
$$

But you do not need to rely on this expression, just draw the trajectory of $h(k)$ to find out $w$.

(c) The SSH Hamiltonian can be written as

$$
H(k) = \begin{pmatrix} 0 & Q(k) \\ Q^*(k) & 0 \end{pmatrix}.
$$

Find out $Q(k)$ and show that the following expression also gives the winding number:

$$
w = \frac{i}{2\pi} \int_{\text{BZ}} dk \frac{d}{dk} \ln Q(k).
$$

3. Assume a SSH chain has two domains: $\delta(x) = -\delta_0 < 0$ for $x < 0$, $\delta(x) = \delta_0$ for $x \geq 0$, and $\delta(x)$ varies smoothly and monotonically from $-\delta_0$ to $\delta_0$ in between. We will find out a localized state that is trapped in this domain wall.

(a) The low-energy states are located near $ka = \pm \pi$. Write $k$ as $\pi/a + q$, and expand $H(k)$ to linear order in $q$. This is the Hamiltonian in the continuum limit.

(b) Replace $q$ with $(1/i)\partial/\partial x$ to requantize the $H$ in (a), and find out the eigenstate $\psi_0(x)$ with zero energy. (This problem is first studied in Jackiw and Rebbi, 1976)

4. In Prob. 3 of Chap 2, we derived the effective Hamiltonian of an electron moving in a non-uniform magnetic field $B(r,t) = B_0 \hat{m}(r,t)$,

$$
\left[ \frac{1}{2m} (p - \hbar \mathbf{A}_n)^2 - \hbar V_n + \varepsilon_n \right] \psi_n = i\hbar \frac{\partial \psi_n}{\partial t},
$$

where $V_n$ and $\mathbf{A}_n$ can be found there.

(a) Show that an electron with spin up/down feels an effective electromagnetic field,

$$
\tilde{E}_n = \frac{1}{2} \frac{\partial \hat{m}}{\partial \alpha} \times \frac{\partial \hat{m}}{\partial \beta},
$$

$$
\tilde{B}_n = \frac{1}{4} \frac{\partial \hat{m}}{\partial \alpha} \times \frac{\partial \hat{m}}{\partial \beta}.
$$

As a result, an electron with velocity $v$ is subject to a force $\mathbf{F} = \mathbf{v} \times \mathbf{B}$.

(b) A magnetic skyrmion is a topological spin texture in magnetic materials. Because of the exchange interaction, the spin texture has an associated magnetic field that can be identified with the $\mathbf{B}(r,t)$-field above. Show that a skyrmion moving rigidly (no change of shape) with velocity $\mathbf{v}_s$ generates an effective electric field,

$$
\tilde{E} = -\mathbf{v}_s \times \tilde{B},
$$

where $\tilde{B}$ is the effective magnetic field of a static skyrmion.

References


