Topological Insulators - A review

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Central message: Do not stand on a block of topological insulator to change a light bulb.

These lecture notes were prepared for a mixed audience of students, postdocs and faculty from the Indian Institute of Technology Madras, India and neighboring institutions, particularly the Institute of Mathematical Sciences. I am not an expert on the subject and during the few years I spent working on the Quantum Hall effect, I had not fully appreciated that it was part of a family of topological insulators. It was a pleasure to dig a little deeper into this subject and to share its wonders with others. In preparing these lectures I relied heavily on the help of Ganpaty Murthy (UKy) and a very helpful conversation with Steve Kivelson (Stanford.) I am of course responsible any errors despite their efforts. I also relied on some excellent Powerpoint slides of various talks. I have furnished a few choice references at the end and very few references to original papers. I cover only $d=1$ and $d=2$.

Contents

I. Scalar and vector potentials
   A. Introducing $A$ and $\phi$ in classical electrodynamics 2
   B. $A$ and $\phi$ in quantum theory 3
   C. Aharanov-Bohm experiment 3
   D. Monopole problem 4
   E. Modern approach to the monopole problem 6

II. The Berry phase
   A. Berry phase affecting slow degree of freedom 9
   B. Berry monopole in parameter space 11

III. Time-reversal symmetry - TRS
   A. TRS in classical mechanics 13
   B. Time-reversal symmetry in quantum mechanics 14
   C. TRS in non-relativistic quantum mechanics 16
   D. TRS of the Schrödinger equation 17
   E. The $K$ operator 17
   F. General study of $\Theta$ and Kramers' degeneracy 18

IV. Symmetries in momentum space
   A. How symmetries of $H$ act on $H(k)$ 21
   B. Symmetry restrictions on Berry phase 22
   C. Examples of symmetries of $H(k)$ 24

V. Models on a lattice
   A. Fourier modes and bands in $k$-space 25
   B. Peierls instability 26
   C. Computation of Peierls distortion energy 27

VI. Su-Schrieffer-Heeger (SSH) model
   A. The band Hamiltonian 30

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I. SCALAR AND VECTOR POTENTIALS

A. Introducing $A$ and $\phi$ in classical electrodynamics

The following two Maxwell equations

$$\nabla \cdot B = 0$$  \hspace{1cm} (1) \\
$$\nabla \times E + \frac{\partial B}{\partial t} = 0$$  \hspace{1cm} (2)

can be satisfied as identities by setting

$$E = -\nabla \phi - \frac{\partial A}{\partial t}$$  \hspace{1cm} (3) \\
$$B = \nabla \times A$$  \hspace{1cm} (4)

where $A$ and $\phi$ are the vector and scalar potential respectively.

By writing the other two Maxwell equations involving the current density $j$, and the charge density $\rho$,

$$\nabla \cdot E = \frac{\rho}{\varepsilon_0}$$  \hspace{1cm} (5) \\
$$\nabla \times B = \mu_0 j + \mu_0 \varepsilon_0 \frac{\partial E}{\partial t}$$  \hspace{1cm} (6)

in terms of $(A, \phi)$ we can obtain equations that determine $(A, \phi)$ in terms of $(j, \rho)$.

In that process we invoke gauge freedom, which refers to the fact that $(A, \phi)$ can be traded for $(A', \phi')$ related by a gauge transformation:

$$A' = A + \nabla \chi$$  \hspace{1cm} (7) \\
$$\phi' = \phi - \frac{\partial \chi}{\partial t}$$  \hspace{1cm} (8)

without changing $(E, B)$. 
Exercise I.1 Verify this claim.

Even though $A$ is gauge-dependent, its line integral around a closed loop $C$ which is the boundary of a surface $S$ (i.e., $C = \partial S$) is gauge invariant:

$$\oint_{C=\partial S} A \cdot dr = \int_S (\nabla \times A) \cdot dS = \text{gauge invariant}.$$  

(9)

In classical physics we can work with either $(E, B)$ or $(A, \phi)$. Each version has its advantages. For example in electrostatics it is easier to solve for the scalar function $\phi$ rather than the vector field $E$ in terms of $\rho$. On the other hand one has the lingering feeling that the potentials are unphysical because they can be altered (by a gauge transformation) without changing the fields which are physical and can be measured by probes.

B. $A$ and $\phi$ in quantum theory

By "in quantum theory" I mean the particles are treated quantum mechanically, in contrast to quantum electrodynamics where even the electromagnetic fields are treated quantum mechanically.

Quantum theory gives us no choice: we have to work with the potentials from the outset.

In Feynman’s sum over paths each path is weighted by

$$e^{(i/h) \int L dt}$$  

(10)

where the Lagrangian for a particle of mass $m$ and charge $e$ in the presence of an electromagnetic field is expressed in terms of $(A, \phi)$:

$$L(r, v) = \frac{1}{2} mv^2 + ev \cdot A - e\phi.$$  

(11)

The same is true of the Hamiltonian approach where we have

$$H = \left(\frac{p - eA}{2m}\right)^2 + e\phi.$$  

(12)

Despite the appearance of potentials one can show that physical answers (say energy levels and probabilities) are gauge invariant.

Here is an example of gauge freedom and gauge invariance in the Hamiltonian formalism. Consider the eigenvalue equation

$$H\psi = \left(\frac{p - eA}{2m}\right)^2 \psi = E\psi.$$  

(13)

It is readily verified that

$$\left(\frac{p - eA'}{2m}\right)^2 \psi' = E\psi' \quad \text{where}$$

$$\psi'(r) = \exp \left[ \frac{ie}{\hbar} \chi(r) \right] \psi(r)$$

(14)

$$A' = A + \nabla \chi.$$  

(16)

In other words, a change of gauge and a corresponding change of phase of $\psi$ leave physical quantities like $E$ invariant.

In short, you have to chose some gauge to do the calculation but the physical quantities (e.g., $E$) will not depend on the choice. The wave function itself will change but probabilities or densities will be unaffected.

C. Aharanov-Bohm experiment

So far it looks like we are to work with $A$ but obtain results that depend only on $B$. But there is a celebrated example in which there is no $B$ acting on the particle and its behavior is modified by just $A$. Consider the double-slit experiment in Figure 1. Between the source of electrons and the screen is an impenetrable solenoid carrying flux $\Phi$ into the page. The interference pattern responds to the flux inside the solenoid. There is no $B$ outside the solenoid,
The end of Newtonian physics

FIG. 1 The double slit experiment with electrons. Between the source of electrons E and the screen is a solenoid carrying flux \( \Phi \) going into the page. The interference pattern responds to the flux inside the solenoid. There is no \( B \) outside the solenoid, but there is a concentric \( A \) everywhere, shown by a circle.

but there is an \( A \) everywhere. A classical particle excluded from the solenoid will not change its motion because \( B = \nabla \times A = 0 \) wherever it goes.

How does the electron respond to \( A \) and how does the response manage to be gauge-invariant? One way to see this is in the path integral approach where the electron goes along paths on either side of the solenoid.

Suppose without the \( A \) we had at a point \( r \) on the screen
\[
\psi(r) = \psi_{P1}(r) + \psi_{P2}(r)
\]
where the two contributions come from classical paths \( P1 \) and \( P2 \) and their neighbors with nearly the same action (i.e., within \( \hbar \)). Because of the \( e\mathbf{v} \cdot \mathbf{A} \) term in Eqn. 11, the contributions from the two classical paths \( P1 \) and \( P2 \) now get modified to yield
\[
\psi(r) = \psi_{P1}(r) \exp \left[ \frac{ie}{\hbar} \int_{P1} \mathbf{A} \cdot d\mathbf{r} \right] + \psi_{P2}(r) \exp \left[ \frac{ie}{\hbar} \int_{P2} \mathbf{A} \cdot d\mathbf{r} \right]
\]
\[
|\psi(r)|^2 = \left| \exp \left[ \frac{ie}{\hbar} \oint_{C=P1-P2} \mathbf{A} \cdot d\mathbf{r} \right] \psi_{P1} + \psi_{P2} \right|^2.
\]

Thus the usual phase difference \( \Delta \phi_{12} \) between the two paths is compounded by the line integral of the flux penetrating the closed loop made of path \( P1 \) and the reverse of path \( P2 \).

By going on both sides of the solenoid and comparing the phase difference, the electron is able to respond to the flux in the solenoid and respond gauge invariantly.

For future use note that if \( \Phi \), the enclosed flux in the solenoid, obeys
\[
\exp \left[ \frac{ie}{\hbar} \oint \mathbf{A} \cdot d\mathbf{l} \right] = \exp \left[ \frac{e\Phi}{\hbar} \right]
\]
\[
= \exp \left[ 2\pi im \right] \quad m = 0, \pm 1, \ldots \quad \text{or}
\]
\[
\Phi = m\Phi_0 \equiv \frac{2\pi \hbar}{e} \quad \text{where}
\]
\[
\Phi_0 \equiv \text{the flux quantum},
\]
the solenoid is unobservable.

D. Monopole problem

Imagine a particle moving in the field of a monopole of charge \( g \),
\[
B = \frac{ge_r}{r^2}.
\]
FIG. 2 Dirac string bringing in the flux to the monopole from infinity along an arbitrary path. Dirac’s quantization condition, Eqn. 32 ensures it is unobservable.

which emits a total magnetic flux $4\pi g$. We cannot describe this $B$ by a non-singular $A$. To see this consider a closed surface, which I take to be a sphere for convenience, enclosing the monopole and a closed loop $C$ surrounding the north pole in the sense of increasing azimuthal angle $\phi$. By Stokes’ theorem

$$\oint_C A \cdot dr = \Phi_{\text{enc}}$$

(24)

where $\Phi_{\text{enc}}$ is the flux enclosed in the region bounded by $C$. Now slowly increase the size of $C$ till it passes the equator and then starts to shrink and ends up as a point at the south pole. The flux enclosed now becomes $4\pi g$. On the other hand, it is not possible for an infinitesimal loop to enclose a finite amount of flux unless $A$ is singular.

Here is a concrete example

$$A = e_\phi \frac{g(1 - \cos \theta)}{r \sin \theta}$$

(25)

where $e_\phi$ is a unit vector along the azimuthal direction. If we integrate this $A$ around a circle at fixed latitude $\theta$ we find

$$\oint A \cdot dr = \int_0^{2\pi} A_\phi r \sin \theta d\phi = 2\pi g(1 - \cos \theta)$$

(26)

which is indeed the enclosed flux, which grows from 0 at $\theta = 0$ to $4\pi g$ at $\theta = \pi$. Notice that this $A$ is singular at $\theta = \pi$. We shall refer to it as $A_+$ because it good in the upper part of the sphere that excludes the south pole. Likewise

$$A_- = -e_\phi \frac{g(1 + \cos \theta)}{r \sin \theta}$$

(27)

is good everywhere except the north pole and yields the same $B$ because

$$A_+ - A_- = \frac{2g}{r \sin \theta} e_\phi$$

(28)

$$= \nabla \chi, \quad \text{where} \quad \chi(r, \theta, \phi) = 2g\phi.$$  

(29)

Dirac argued that an infinitesimally thin Dirac string was bringing in the flux $4\pi g$ at the singularities, (at the north or south pole in our example) and releasing them at the origin in a spherically symmetric manner, as indicated by
Figure 2. The location of the string can be changed by a change of gauge. (For example, by going from $A_+$ to $A_-$ we can move it from the south pole to the north.) Thus the string should not be observable, not just where it enters the sphere, but all the way to infinity, where it begins. A particle going around it would acquire a Bohm-Aharanov phase factor

$$\exp\left[\frac{ie\Phi}{\hbar}\right] = \exp\left[\frac{4\pi ie\theta}{\hbar}\right].$$

(30)

Dirac demanded that this be unobservable, i.e.

$$\frac{4\pi e\theta}{\hbar} = 2\pi m, \quad m = 0, \pm 1, \pm 2, \ldots$$

(31)

or

$$e\theta = \frac{1}{2}m\hbar.$$ 

(32)

This is a remarkable result: it implies that the presence of even a single monopole in the universe forces the electric charges of particles to be integral multiples of $\frac{\hbar}{2g}$. This gives a clue to why the electron and proton, which are so different, have charges of the same magnitude. I for one believe monopoles exist, if only for this reason.

E. Modern approach to the monopole problem

In the modern approach one abandons the notion of a single wave function for the particle or a single $A$ for the particle in the field of a monopole. Let us say the particle is moving on a sphere with the monopole at the center. One divides the sphere into two overlapping patches $S_+$ and $S_-$, one excluding the south pole and the other the north pole, as shown in Figure 3. In the two patches there will be vector potentials $A_{\pm}$ and wavefunctions $\psi_{\pm}$ which are called sections.

![Charged particle in a monopole field](image)

FIG. 3 One divides the sphere into two overlapping patches $S_+$ and $S_-$, one excluding the south pole and the other the north pole, with respective vector potentials $A_{\pm}$ and wavefunctions $\psi_{\pm}$ which are called sections. The overlap region is doubly shaded.

In the overlap region (say in a belt around the equator) the two potentials and corresponding wavefunctions will be related by a gauge transformation. Look at the contour $C$ in Figure 3. When traveled as shown we have

$$\oint_C A_+ \cdot dr = \Phi_+,$$ 

(33)

using Stokes’ theorem in a patch where $A$ is regular. If we now traverse $C$ the other way, i.e., along $-C$, and integrate $A_-$ we obtain

$$\oint_{-C} A_- \cdot dr = \Phi_-.$$ 

(34)
We add the two equations and manipulate as follows
\[ \oint_C (A_+ - A_-) \cdot dr = \text{total monopole flux} = 4\pi g. \] (35)

Since \( A_\pm \) describe the same \( B \) they must be related as follows
\[ A_+ - A_- = \nabla \chi, \] (36)
leading to
\[ \oint \nabla \chi \cdot dr = 4\pi g. \] (37)

(Recall our concrete example of \( A_\pm \)
\[ A_\pm = \pm \frac{g}{r \sin \theta} (1 \mp \cos \theta) e^\phi \] (38)
\[ A_+ - A_- = \frac{2g}{r \sin \theta} e^\phi = 2g \nabla \chi \text{ where } \chi(\theta, \phi) = \phi. \] (39)

Under this gauge transformation by \( \chi \) the wave functions are related by
\[ \psi_+ = \exp \left[ \frac{i e}{\hbar} \right] \psi_- . \] (40)

The requirement that \( \psi_+ \) be single valued assuming \( \psi_- \) is, means
\[ \frac{e}{\hbar} \oint \nabla \chi \cdot dr = 2\pi m, \text{ or, using Eqn. 37} \]
\[ eg = \frac{\hbar}{2}. \] (42)

II. THE BERRY PHASE

Consider a system whose Hamiltonian \( H \) is a function of time. Let \( |n(t)\rangle \) be an eigenket of \( H(t) \):
\[ H(t) |n(t)\rangle = E(t) |n(t)\rangle. \] (43)

What is the solution to
\[ i\hbar \frac{d|\psi(t)\rangle}{dt} = H(t) |\psi(t)\rangle \] (44)
assuming that the state never jumps to any other eigenstate (labeled by \( n' \neq n \)) as \( t \) is varied, i.e., the evolution is adiabatic? This is possible if there is a gap \( \hbar \omega \) in the spectrum and \( H \) changes sufficiently slowly, on a time scale \( 1/\omega \).

A reasonable guess is that if we started with \( |\psi(0)\rangle = |n(0)\rangle \) at \( t = 0 \), then at time \( t \)
\[ |\psi(t)\rangle = \exp \left[ -\frac{i}{\hbar} \int_0^t E(t') dt' \right] |n(t)\rangle, \] (45)
where \( \int_0^t E(t') dt' \) is the accumulated phase shift. You can verify that this does not work because \( |n(t)\rangle \) has its own time derivative. So we substitute
\[ |\psi(t)\rangle = e^{i\gamma(t)} \exp \left[ -\frac{i}{\hbar} \int_0^t E(t') dt' \right] |n(t)\rangle. \] (46)

into the Schrödinger equation, dot both sides with \( \langle n(t)| \) to find
\[ \dot{\gamma} = i \langle n| \frac{dn}{dt} \rangle \] (47)
with a solution

\[ \gamma(t) = \int_0^t A(t') dt' \]  
where

\[ A(t) = i \langle n | \frac{dn}{dt} \rangle. \]  

(48)

Thus we have

\[ |\psi(t)\rangle = \exp \left[ i \int_0^t A(t') dt' \right] \exp \left[ \frac{-i}{\hbar} \int_0^t E(t') dt' \right] |n(t)\rangle. \]  

(50)

One may be tempted to dismiss the extra phase due to \( A \), because the phase can always be changed by a change of phase of the kets \( |n(t)\rangle \) without affecting their defining property as instantaneous eigenkets of \( H(t) \). Under such a change

\[ |n(t)\rangle \rightarrow |n(t)\rangle e^{i\chi(t)} \]  
then \[ A(t) \rightarrow A(t) - \frac{d\chi}{dt}. \]  

(51)

(52)

But suppose \( H \) returns to the original starting point after some time \( T \), i.e., if \( H(0) = H(T) \), then the relationship

\[ \psi(T) = e^{i \oint_0^T A(t') dt'} |\psi(0)\rangle \]  

(53)

is unaltered by gauge transformations, given that \( \chi \) is single-valued: \( \chi(T) = \chi(0)2\pi m \). This is easier to visualize if we think that the space of parameters in \( H \) is labeled by a coordinate \( R \) and \( H \) varies with time because \( R \) does:

\[ H(t) = H(R(t)) \]  
\[ |n(t)\rangle = |n(R(t))\rangle. \]  

(54)

Then

\[ \int_0^t A(t') dt' = i \int_0^t \left\langle n | \frac{dn}{dt} + \frac{dR}{dt} \right\rangle dt' \]  

(55)

\[ = \int_0^t A(R) \frac{dR}{dt} dt' \]  

where \[ A(R) = i \left\langle n | \frac{dn}{dR} \right\rangle. \]  

(56)

(57)

In this form we see that \( A(R) \) couples to the velocity of the fictitious particle with coordinate \( R(t) \). Indeed we soon encounter problems where \( R \) is the coordinate of a real particle and \( A(R) \) affects its dynamics like a genuine vector potential, except that it is not of electromagnetic origin.

In this version it is readily seen that

\[ \exp \left[ i \oint_0^T A(t') dt' \right] = \exp \left[ i \oint_{R(0)}^{R(T)} A(R) dR \right] \]  

(58)

\[ = \exp \left[ i \int B \cdot dS \right] \]  

(59)

where

\[ B = \nabla \times A \]  

(60)

is called the Berry curvature and \( S \) the surface bounded by the loop traversed by the system in the time \( t = 0 - T \).

Next imagine a huge particle lumbering along in its configuration space with coordinate \( R \). Riding on it is a small but fast moving system. The small system experiences a Hamiltonian \( H(R) \). For example the small system could be a spin experiencing the magnetic field \( B(R) \) at the heavy particle’s location. (The heavy particle could be electrically
neutral and unaware of $B$.) We assume the small system stays in one particular state $|n(R)\rangle$ and does not jump to other states with a different $n$. The Berry phase it accumulates

$$
\exp \left[ i \int_0^{R(T)} A(R)dR \right]
$$

clearly affects the fate of the large particle as any vector potential would.

Or consider some electrons moving along with their parent nuclei. At a given location $R$ of the nuclei, the electrons settle down to some state $|n(R)\rangle$ and stay at fixed $n$ as $R$ slowly moves. The nimble electrons manage to find an eigenstate at each fixed $R$, which is a slowly varying parameter for them. This is the Born-Oppenheimer approximation. However Born and Oppenheimer did not consider the potential $A(R)$ that arises from the fast motion of the electrons.

We will now discuss a simpler example in which a Berry vector potential appears and modifies the dynamics.

**A. Berry phase affecting slow degree of freedom**

Consider the situation depicted in Figure 4. A massive particle is forced to move along a circle of radius $r$ lying in the $xy$ plane. There is a uniform magnetic field $B = kB_z$. In addition a wire passing through the center produces an azimuthal field $B_0 = B_0 e_\phi$. The particle, assumed neutral, does not feel $B$. Riding on the particle is a spin which sees the field

$$
B = kB_z + iB_0 \sin \phi + jB_0 \cos \phi.
$$

(The reason the sines and cosines seem interchanged is because the magnetic field at $\phi$ is the tangent to the circle.) The Hamiltonian for the combined system is

$$
H = \frac{L^2}{2I} - \sigma \cdot B.
$$

We will assume the spin is locked into the instantaneous ground state $|+\rangle$ (parallel to $B$). The naive expectation is that energy eigenstate and eigenvalue are

$$
|\Psi\rangle = e^{im\phi}|+\rangle \quad m = 0, \pm 1 \ldots
$$

$$
E_m = \frac{m^2\hbar^2}{2I} - \sqrt{B_0^2 + B_z^2}.
$$

But this result ignores the Berry phase which we will now incorporate. We first expand the combined state as

$$
|\Psi\rangle = \int \psi(\phi)|\phi \otimes n(\phi)\rangle d\phi
$$

Notice that $\phi$ is the only real degree of freedom: when the particle is at $\phi$, the spin is forced to be in $|n(\phi)\rangle$. This is why a single wavefunction $\psi(\phi)$ describes both. Just to make sure you got it:

$$
\langle \phi \otimes n(\phi)|\Psi\rangle = \int \psi(\phi') \langle \phi \otimes n(\phi)|\phi' \otimes n(\phi')\rangle d\phi' = \psi(\phi).
$$

Instead of directly jumping into the eigenvalue problem of $L^2$, let us deal with the eigenvalue problem of $L$ first.

$$
\langle \phi \otimes n(\phi)|L|\Psi\rangle = \int \langle \phi \otimes n(\phi)|L|\phi' \otimes n(\phi')\rangle \langle \phi' \otimes n(\phi')|\Psi\rangle d\phi' = \int \langle n(\phi)|n(\phi')\rangle \langle \phi|L|\phi'\rangle \psi(\phi') d\phi'
$$

$$
= -i\hbar \int \delta(\phi - \phi') \frac{d}{d\phi'} [\langle n(\phi)|n(\phi')\psi(\phi')\rangle]
$$

$$
= -i\hbar \int \delta(\phi - \phi') \frac{d}{d\phi'} [\langle n(\phi)|n(\phi')\psi(\phi')\rangle]
$$

$$
= -i\hbar \int \frac{dn(\phi)}{d\phi} \psi(\phi) - i\hbar \frac{d\psi}{d\phi}
$$

$$
= ( -i\hbar \frac{d}{d\phi} - \hbar A) \psi(\phi).
$$
FIG. 4 The heavy particle with moment of inertia $I$ moves slowly on a circle carrying a spin which evolves rapidly, i.e., is in the instantaneous eigenstate of the local magnetic field $B$ which is the sum of an azimuthal field due the current perpendicular to the plane of motion and a uniform field perpendicular to the plane of motion.

Choosing solutions of the form $e^{im\phi}$ we find that the eigenvalues of $L$ are

$$l = m\hbar - \hbar A.$$  \hspace{1cm} (71)

We see the spectrum is no longer the integers but shifted by $A$. Let us now compute $A$ for the spin whose ground state is

$$|n(\phi)\rangle = \left( \begin{array}{c} \cos \frac{\theta}{2} \\ i \sin \frac{\theta}{2} e^{i\phi} \end{array} \right),$$  \hspace{1cm} (72)

where $\tan \theta = \frac{B_0}{B_z}$. (The $i$ in the lower components is there because the field at $\phi$ is tangent to the circle at that point.) It is easily verified that

$$A = -\sin^2 \frac{\theta}{2}.$$  \hspace{1cm} (73)

Thus the spectrum of $L$ is

$$l = \hbar \left( m + \sin^2 \frac{\theta}{2} \right).$$  \hspace{1cm} (74)

Going back to

$$H = \frac{L^2}{2I} - \sigma \cdot B$$  \hspace{1cm} (75)

you may be tempted to conclude that the spectrum is

$$E_m = \frac{\hbar^2}{2I} \left( m + \sin^2 \frac{\theta}{2} \right)^2 - \sqrt{B_0^2 + B_z^2}.$$  \hspace{1cm} (76)

This is however incorrect: there is an extra constant $\frac{\hbar^2}{4} \sin^2 \theta$. The details are left to the following exercise.

**Exercise II.1** *Show that in addition to $A$, a scalar potential*

$$\Phi = \frac{\hbar^2}{4} [\langle dn|dn\rangle - \langle dn|n\rangle\langle n|dn\rangle]$$  \hspace{1cm} (77)

*arises when second derivatives enter $H$. Show that in our problem $\Phi = \frac{\hbar^2}{4} \sin^2 \theta$. In the above I use a compact notation in which $|dn\rangle = \frac{d|n(\phi)\rangle}{d\phi}$ etc.*
FIG. 5 The source of Berry flux is a monopole at $h = 0$, the origin of parameter space and the point of degeneracy. The figure shows a closed path on a sphere of radius $h$. The dynamical phase at time $t$ is $ht$. The Berry phase is the monopole flux penetrating the surface bounded by the closed loop, independent of how long it took to go around.

B. Berry monopole in parameter space

Where does the Berry flux come from? It has to do with degeneracies in parameter space where two levels $E_1$ and $E_2$ collapse to a common $E$. Consider a problem where two levels cross. Let us focus on them and ignore the rest. In the two-dimensional vector space the Hamiltonian has to have the following form

$$H = \begin{pmatrix} E + h_z & h_x - ih_y \\ h_x + ih + y & E - h_z \end{pmatrix} = EI + \sigma \cdot h$$

(78)

where

$$h = (ih_x + jh_y + kh_z)$$

(79)

are the three free parameters of the $2 \times 2$ traceless Hermitian Hamiltonian. We see that $h$ is the position vector in parameter space. (We can choose the degenerate energy $E = 0$.)

The energy levels of the two states $|n_\pm\rangle$ are

$$E_\pm = \pm |h|.$$  

(80)

The levels become degenerate at the origin in $h$ space. At every other point the levels are split.

This looks like a spin in magnetic field $B = h$ in $h$ space, which we previously referred to as $R$ space. Let us assume the system is in the spin up or $|n_+\rangle$ state. It has a dynamical phase factor

$$e^{i\gamma_d} = \exp \left[ \frac{i}{\hbar} \int_0^t E(t') dt' \right] = \exp \left[ \frac{i}{\hbar} \int_0^t |h(t')| dt' \right].$$

(81)

This phase depends on details of the motion. For example if it is a circle on a sphere of radius $h$ as shown in Figure 5, the accumulated dynamical phase at time $t$ is $ht$. It can be big or small depending on $t$.

But there is also a Berry phase, which is the focus of our discussion.

Let us say the system is in the spin up or $|n_+\rangle$ state. Then

$$A_+ \cdot dh = i \langle n_+ | dn_+ \rangle$$

(82)

$$= i \left( \cos \frac{\theta}{2}, \sin \frac{\theta}{2} e^{-i\phi} \right) \left( d\left( \sin \frac{\theta}{2} \right) e^{i\phi} + id\phi \sin \frac{\theta}{2} e^{i\phi} \right)$$

$$= -\frac{(1 - \cos \theta)}{2} d\phi \quad \text{so that}$$

$$A = -\frac{(1 - \cos \theta)}{2} e^{i\phi}.$$  

(83)
Consider a loop $C$ along a latitude $\theta$ on a sphere surrounding the origin, as shown in Figure 5. We find

$$\oint A_\phi d\phi = -\pi (1 - \cos \theta)$$

(85)

which we recognize as flux of a monopole of strength $g = -\frac{1}{2}$ at the origin. (When $\theta \to \pi$, the total flux enclosed is $-2\pi$.)

The Berry phase is thus due to a source which has a $\delta$-function divergence at the origin. Unlike the dynamical phase it does not depend on the “velocity” with which the path is traversed (as long as the adiabatic approximation is valid.)

**Note:** Some of you may be worried about the $\phi$ integral. We normally expect to integrate $A_\phi r \sin \theta d\phi$ but here we have just $A_\phi d\phi$. This is because we have defined

$$A_\phi = i \langle n | \frac{\partial n}{\partial \phi} \rangle.$$  

(86)

We could have instead used (remembering there is no $r$ dependence of $|n\rangle$)

$$A = i \langle n | \nabla n \rangle$$

(87)

$$= e_\theta \langle n | \frac{\partial n}{\partial \theta} \rangle + e_\phi \langle n | \frac{\partial n}{\partial \phi \sin \theta} \rangle,$$

(88)

in which case we would have integrated $A_\phi r \sin \theta d\phi$.

The point is that if we parametrize the curve on which the system moves by the variable $\eta$ and set

$$A_\eta = i \langle n | \frac{\partial n}{\partial \eta} \rangle,$$

(89)

then $A_\eta d\eta$ is the phase change when there is a change $d\eta$, while if we then proceed to re-parametrize the curve by $\zeta(\eta)$ and define

$$A_\zeta = i \langle n | \frac{\partial n}{\partial \zeta} \rangle,$$

(90)

then

$$A_\zeta d\zeta$$

(91)

is the change in phase over the same segment in the new parametrization. This all works out because of the transformation law

$$A_\eta = A_\zeta \frac{d\zeta}{d\eta}.$$  

(92)

To understand this better you should learn differential forms.

Back to the flux which seems to be due to a monopole of strength $-\frac{1}{2}$ at the origin. We demonstrate this as follows. Let $|n\rangle$ be the state the spin is in. (It was $|+\rangle$ in our example.)

$$A_\mu = i \langle n | \partial_\mu n \rangle \quad (\partial_\mu = \frac{\partial}{\partial h_\mu})$$

(93)

$$F_{\mu \nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

(94)

$$= i \langle \partial_\mu n | \partial_\nu n \rangle - \langle \partial_\nu n | \partial_\mu n \rangle$$

(95)

$$= \sum_{m \neq n} i \langle \partial_\mu n | m \rangle \langle m | \partial_\nu n \rangle - \langle \partial_\nu n | m \rangle \langle m | \partial_\mu n \rangle,$$

(96)

where $m \neq n$ because the $m = n$ term vanishes identically.

**Exercise II.2** Show that the $m = n$ vanishes identically using

$$0 = d\langle m | m \rangle = \langle dm | m \rangle + \langle m | dm \rangle.$$
Next we derive a very useful relation:

\[
\langle m|H|n \rangle = 0 \quad \text{(remember } m \neq n) \tag{97}
\]

\[
\langle dm|H|n \rangle + \langle m|dH|n \rangle + \langle m|H|dn \rangle = 0 \tag{98}
\]

\[
(E_m - E_n)\langle dm|n \rangle = \langle m|dH|n \rangle \quad \text{(use } (m|dn) = -(dm|n)) \tag{99}
\]

\[
\langle dm|n \rangle = \frac{\langle m|dH|n \rangle}{E_m - E_n} \tag{100}
\]

Consequently

\[
F_{\mu\nu} = i \sum_{m \neq n} \frac{1}{(E_n - E_m)^2} [\langle n|\partial_\mu H|m \rangle \langle m|\partial_\nu H|n \rangle - (\mu \leftrightarrow \nu)]
\]

\[
= i \sum_{m \neq n} \frac{1}{(2\hbar)^2} [\langle n|\partial_\mu H|m \rangle \langle m|\partial_\nu H|n \rangle - (\mu \leftrightarrow \nu)] \tag{101}
\]

Now put in the \( m = n \) term because it vanishes and use completeness and \( H = \sigma_\mu h_\mu \) to obtain

\[
F_{\mu\nu} = \frac{i}{4\hbar^2} \langle n|\partial_\mu H \partial_\nu H - \partial_\nu H \partial_\mu H \rangle \tag{102}
\]

\[
= \frac{i}{4\hbar^2} \langle n|\sigma_\mu \sigma_\nu - \sigma_\nu \sigma_\mu |n \rangle \tag{103}
\]

\[
= -\frac{1}{2\hbar^2} \epsilon_{\mu\nu\lambda} \langle n|\sigma_\lambda|n \rangle \tag{104}
\]

\[
B_\pm = \mp \frac{1}{2\hbar^2} \hbar \quad \text{for } |n\rangle = |\pm\rangle. \tag{105}
\]

Since \( \hbar^2 \) is the distance squared from the origin, this describes a monopole of strength \(-\frac{1}{4}\) sitting at the origin, the point of degeneracy.

Notice that the sign of \( B \) depends on which state (\( |n_+\rangle \) or \( |n_-\rangle \)) we are working with.

So the picture bear in mind is that there is a monopole with \( g = \mp \frac{1}{2} \) sitting at the origin in parameter space and as the system traverses a closed loop in the eigenstate \( |n_\pm\rangle \), the phase change is given by the flux intercepted by a surface bounded by this loop, as shown in Figure 5.

### III. TIME-REVERSAL SYMMETRY - TRS

Let us first meet this symmetry in classical mechanics.

#### A. TRS in classical mechanics

Suppose a planet moves from \( x(0) \) to \( x(T) \) with initial and final velocities \( \dot{x}(0) \) and \( \dot{x}(T) \) as shown in Figure 6 a. Say we make a movie of this and play it backwards starting at time \( T \). This time-reversed trajectory \( x_R(t) \) will have its velocity opposite to that of the original one on the way back and arrive at the starting point at time \( 2T \) with velocity \( \dot{x}_R(2T) = -\dot{x}(0) \). The reversed movie would appear perfectly regular, i.e., in accordance with Newton’s Laws, to a person viewing it. Indeed she will not know if the projector is running forward or backwards. In other words, what she sees can very well be the movie of a real planet obeying Newton’s laws, traveling along the trajectory \( x_R(t) \). This is an example of time-reversal symmetry (TRS) of Newton’s Laws and the gravitational force.

For cosmetic reasons let us change the initial time to \( t = -T \) so that the reversal takes place at \( t = 0 \) and the clip ends at time \( T \) as shown in Figure 6b. In this convention, the time-reversed path \( x_R(t) \) is related to the original one as follows:

\[
x_R(t) = x(-t). \tag{106}
\]

You can see this is true from the figure: if you slice it horizontally, you find \( x_R(t) = x(-t) \). Differentiating Eqn. 106 we find

\[
\dot{x}_R(t) = \frac{dx_R(t)}{dt} = \frac{dx(-t)}{dt} = \frac{dx(-t)}{d(-t)} = -\dot{x}(-t), \tag{107}
\]
FIG. 6 (a) A path and its reverse between times 0 and 2T. (b) The same paths with initial time changed to $-T$. The time reversal operation is done at $t = 0$. The original path $x(t)$ and its time-reversed version $x_R(t)$ obeying $x_R(t) = x(-t)$ and $\dot{x}_R(t) = -\dot{x}(-t)$. A time slice shows this relation between the two paths: at opposite times $x$ and $x_R$ have the same value and opposite derivatives.

again in accord with the figure. If you set $t = T$ in Eqns. 106, 107, you will find, as in Figure 6b, that after time-reversal the particle returns to its original location with opposite velocity.

Taking one more derivative we find

$$a_R(t) = \ddot{x}_R(t) = \ddot{x}(-t) = a(-t). \tag{108}$$

We are given that the trajectory $x(t)$ obeys

$$m\ddot{x}(t) = F(x(t)). \tag{109}$$

Using Eqn. 108

$$m\ddot{x}_R(t) = m\ddot{x}(-t) = F(x(-t)) = F(x_R(t)) \tag{110}$$

which means $x_R(t)$ also obeys Newton’s laws. In the present case this follows from the fact that because the law involves only acceleration, we may change $t$ to $-t$ and get a new solution from an existing one. This is not true if there is friction and there is a term in the equation of motion involving a single time-derivative.

B. Time-reversal symmetry in quantum mechanics

Wigner showed that there are two kinds of symmetries that leave the magnitude of the inner product invariant. Unitary symmetries $U$ represented by operators obeying

$$U^\dagger U = I, \tag{111}$$

and whose action is linear

$$U(\alpha|\psi\rangle + \beta|\chi\rangle) = \alpha U|\psi\rangle + \beta U|\chi\rangle \tag{112}$$

and preserve the inner product:

$$\langle U\phi|U\psi\rangle = \langle \phi|U^\dagger U|\psi\rangle = \langle \phi|\psi\rangle. \tag{113}$$

If $U$ is a symmetry operator, then

$$UHU^\dagger = H. \tag{114}$$
Consequently, if
\[ H|E\rangle = E|E\rangle \] (115)
then
\[ UHU^\dagger|E\rangle = EU|E\rangle \] (116)
\[ H|U\psi\rangle = E|U\psi\rangle, \] (117)
meaning \(|E\rangle\) and \(|UE\rangle\) are degenerate.

This is what we normally run into, when we consider symmetries like rotational or translational invariance. But now need a new beast.

Anti-unitary symmetries \(\Omega\) act as follows on any two generic kets \(|\phi\rangle\) and \(|\psi\rangle\):
\[ \langle\Omega\phi|\Omega\psi\rangle = \langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*. \] (118)
Thus they preserve only the absolute value of the inner product.

I bring them up because \(\Theta\), the operator which generates time-reversal is anti-unitary.

I will now establish one central property of \(\Theta\) (or any anti-unitary operator), returning to others properties later. It is that they are anti-linear:
\[ \Theta \alpha|\psi\rangle = \Theta \alpha \Theta^{-1} \cdot \Theta |\psi\rangle = \alpha^* \Theta |\psi\rangle \equiv \alpha^* |\Theta \psi\rangle \] (119)
\[ \Theta \alpha \Theta^{-1} = \alpha^*, \] (120)
where \(\alpha\) is a c-number. In other words, when \(\Theta\) passes through a c-number it complex conjugates it. This property follows from the requirement Eqn. 118:
\[ \langle\Omega\phi|\Omega\psi\rangle = \langle\psi|\phi\rangle. \] (121)

We now establish Eqn. 120 by imposing this condition on two generic state vectors expanded in an orthonormal basis as follows:
\[ |\psi\rangle = \sum_n \psi_n |n\rangle \] (122)
\[ |\phi\rangle = \sum_m \phi_m |m\rangle \] (123)
\[ \Theta |\psi\rangle = \sum_n \Theta \psi_n \Theta^{-1} |n\rangle \] (124)
\[ \Theta |\phi\rangle = \sum_m \Theta \phi_m \Theta^{-1} |m\rangle \] (125)
\[ \langle\Theta\phi|\Theta\psi\rangle = \sum_{n,m}^{(n,m)\neq (m,n)} \langle\Theta\phi_n\Theta^{-1}|\Theta\psi_n\Theta^{-1}\rangle \] (126)
\[ = \sum_n (\Theta \phi_n \Theta^{-1})^* (\Theta \psi_n \Theta^{-1}) \] (127)
Since \(\phi_n\) and \(\phi_m\) are arbitrary, this means
\[ (\Theta \phi_n \Theta^{-1}) = \psi_n^* \] (128)
and likewise for \(\phi_m\).

If \(\Theta\) is a symmetry operation, it means
\[ \Theta H \Theta^{-1} = H. \] (129)

In this case
\[ H|E\rangle = E|E\rangle \] (130)
\[ \Theta H \Theta^{-1} \cdot \Theta |E\rangle = E \Theta |E\rangle \] (131)
\[ H(|\Theta E\rangle) = E(|\Theta E\rangle). \] (132)

Thus \(|E\rangle\) and its time-reversed partner \(|\Theta E\rangle\) are degenerate unless \(\Theta |E\rangle = c|E\rangle\). We will consider cases where this possibility is ruled out and a degeneracy is mandatory.
C. TRS in non-relativistic quantum mechanics

Let us consider the action of Θ in the non-relativistic quantum mechanics of a spinless particle. I discuss only one spatial dimension with coordinate $x$, but the extension to higher dimensions is obvious.

Consider the eigenkets of position and momentum:

$$X|x⟩ = x|x⟩ \quad (133)$$

$$P|p⟩ = p|p⟩ \quad (134)$$

The action of an anti-linear operator (like the linear operator) is fully defined by its action on a basis. We choose the $|x⟩$ basis. We demand, based on classical intuition that

$$Θ|x⟩ = |x⟩ \quad (135)$$

The action of Θ on the operator $X$ follows from Eqn. 135:

$$ΘXΘ^{-1} · Θ|x⟩ = xΘ|x⟩ \quad (136)$$

$$ΘXΘ^{-1}|x⟩ = x|x⟩ \quad (137)$$

which means

$$ΘXΘ^{-1} = X. \quad (138)$$

Consider the expansion

$$|ψ⟩ = \int dx|x⟩⟨x|ψ⟩ = \int dxψ(x)|x⟩ \quad (139)$$

$$Θ|ψ⟩ = \int dxψ^∗(x)|Θx⟩ = \int dxψ^∗(x)|x⟩ \quad (140)$$

which means the wavefunction get conjugated by Θ:

$$⟨x|Θψ⟩ = ψ^∗(x). \quad (141)$$

What does Θ do to $|p⟩$? This cannot be answered unless we specify what $|p⟩$ stands for. So we furnish its components in the $|x⟩$ basis:

$$⟨x|p⟩ = \exp \left[ \frac{ipx}{\hbar} \right]. \quad (142)$$

We may now deduce what Θ does to $|p⟩$

$$⟨Θx|Θp⟩ = ⟨p|x⟩ = \exp \left[ \frac{-ipx}{\hbar} \right] \quad (143)$$

$$⟨x|Θp⟩ = \exp \left[ \frac{-ipx}{\hbar} \right] \quad (144)$$

$$= ⟨x| − p⟩ \quad \text{which means} \quad (145)$$

$$Θ|p⟩ = | − p⟩. \quad (146)$$

It is now easy to show that

$$ΘPΘ^{-1} = −P. \quad (147)$$

Exercise III.1 Prove Eqn. 147.

The preceding results are consistent with the commutation relation:

$$XP − PX = i\hbar \quad \text{because} \quad (148)$$

$$ΘXΘ^{-1} ΘPΘ^{-1} − ΘPΘ^{-1}ΘXΘ^{-1} = ΘiΘ^{-1}h \quad (149)$$

$$−XP + PX = −i\hbar. \quad (150)$$
D. TRS of the Schrödinger equation

How does all this apply to the Schrödinger equation? Let us begin with the equation in the ket notation and act on both sides with $\Theta$:

\[ i\hbar \frac{d|\psi(t)\rangle}{dt} = H(X, P)|\psi(t)\rangle \]  

(151)

\[ (-i)\hbar \frac{d|\Theta\psi\rangle}{dt} = \Theta H(X, P)\Theta^{-1}|\Theta\psi\rangle \]  

(152)

\[ i\hbar \frac{d|\Theta\psi\rangle}{d(-t)} = \Theta H(X, P)\Theta^{-1}|\Theta\psi\rangle = H(X, -P)|\Theta\psi\rangle. \]  

(153)

Thus we find that $|\Theta\psi\rangle$ obeys the equation of motion with $t \rightarrow -t$ provided $H(X, -P) = H(X, P)$. This is the case if

\[ H = \frac{p^2}{2m} + V(X) \]  

(154)

but not if there is a magnetic field:

\[ H = \frac{(P - eA)^2}{2m} + V(X). \]  

(155)

Now we go to the $x$-basis by projecting Eqn. 153 on to the ket $\langle x |$ and recalling Eqn. 141, $\langle x | \Theta \psi \rangle = \psi^*(x)$:

\[ i\hbar \frac{\partial \psi^*(x, t)}{\partial (-t)} = \left( \left( i\hbar \frac{\partial}{\partial x} - eA \right)^2 + V(x) \right) \psi^*(x, t) \]  

(156)

\[ \Rightarrow \left[ \left( -i\hbar \frac{\partial}{\partial x} - eA \right)^2 + V(x) \right] \psi^*(x, t), \text{ i.e.,} \]  

(157)

\[ i\hbar \frac{\partial \psi^*(x, t)}{\partial (-t)} = H \left( -i\hbar \frac{\partial}{\partial x}, x \right) \psi^*(x, t). \]  

(158)

This means that $\psi^*(x, t)$ obeys the time-reversed equation if $H = H^*$ in the $x$-representation. (In particular only if $A = 0$.)

E. The $K$ operator

Limiting ourselves to the Schrödinger equation in the $x$-basis, we may set

\[ \Theta = K \]  

(159)

where $K$ is the complex conjugation operator on all $c$-numbers.

By definition,

\[ K^2 = I \quad \text{i.e.,} \]  

(160)

\[ K = K^{-1}. \]  

(161)

Let us see how $K$ acts:

\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = H \left( -i\hbar \frac{\partial}{\partial x}, x \right) \psi(x, t) \]  

(162)

\[ K i\hbar \frac{\partial \psi(x, t)}{\partial t} K = K H \left( -i\hbar \frac{\partial}{\partial x}, x \right) K \cdot K \psi(x, t) K \]  

(163)

\[ -i\hbar \frac{\partial \psi^*(x, t)}{\partial t} = H \left( -i\hbar \frac{\partial}{\partial x}, x \right)^* \psi^*(x, t) \]  

(164)

\[ i\hbar \frac{\partial \psi^*(x, t)}{\partial (-t)} = H \left( -i\hbar \frac{\partial}{\partial x}, x \right)^* \psi^*(x, t) \]  

(165)
from which it follows that $\psi^*(x, t)$ is the time-reversed solution provided $H^* = H$.

It is important to note that $\Theta = K$ only after going to the $x$-basis, whereupon only c-numbers (constants, functions and their derivatives) enter the picture.

When we have spin we must modify $\Theta = K$. Consider

$$H_{so} = s \cdot (r \times P) \quad (166)$$

which describes spin-orbit coupling. (Here we are obviously in higher dimensions and $x \to r$.) This $H_{so}$ should be TRI since both spin and angular momentum get reversed. However $\Theta = K$ does not do the job: it reverses $s_y$ (which is the pure imaginary Pauli matrix) but not the other two. The correct answer is

$$\Theta = is_yK \quad \Theta^{-1} = Ks_y(-i) \quad (167)$$

under which

$$\Theta s \Theta^{-1} = -s \quad (168)$$
$$\Theta r \Theta^{-1} = r \quad (169)$$
$$\Theta P \Theta^{-1} = -P \quad (170)$$
$$\Theta H_{so} \Theta^{-1} = H_{so}. \quad (171)$$

You may wonder how $K$ is to act on $s$: as a c-number or an operator? The answer is that it complex conjugates the matrix elements of $s$ as c-numbers that represent, in the $S_z$ basis, the abstract spin operator $S$ of Hilbert space, (just like $\psi(r)$ represents $|\psi\rangle$ in the $|r\rangle$ basis).

Once again $\Theta = is_yK$ is true only in the eigenbasis $|r, s_z\rangle$ of $R$ and $S_z$.

Here is a surprise. You might have expected that $\Theta^2 = I$ since a double reversal should be equal to no reversal. However we find

$$\Theta^2 = is_yKis_yK = is_y(-i(s_y)^*)K^2 = -1. \quad (172)$$

Indeed there are many problems where $\Theta^2 = -1$, which was shown by Kramers to imply the degeneracy of states related by $\Theta$. We will now discuss this at length.

F. General study of $\Theta$ and Kramers’ degeneracy

*Theorem*

$$\Theta = KU \quad \text{where } U \text{ is unitary.} \quad (173)$$

*Proof: Consider expanding $|\psi\rangle$ in an orthonormal basis and acting with $\Theta$:

$$|\psi\rangle = \sum_n \psi_n|n\rangle \quad (174)$$
$$\Theta|\psi\rangle = \sum_n \psi_n^*|\Theta n\rangle. \quad (175)$$

But

$$\langle \Theta n | \Theta m \rangle = \langle m | n \rangle = \delta_{mn}. \quad (176)$$

So $|\Theta n\rangle$ is also an orthonormal basis which must therefore be related to the basis $|n\rangle$ by a unitary transformation:

$$|\Theta n\rangle = \sum_m U_{nm}|m\rangle. \quad (177)$$

Substituting this in Eqn. 175,

$$\Theta|\psi\rangle = \sum_{mn} \psi_n^* U_{nm}|m\rangle \quad (178)$$
$$= K \sum_{mn} \psi_n U_{nm}^* |m\rangle \quad (179)$$
$$= K \sum_{mn} \psi_n U_{mn}^\dagger |m\rangle \quad (180)$$

(181)
Dotting both sides with $\langle k |$

$$\langle k | \Theta \psi \rangle = K \sum_{m n} \psi_n U^\dagger_{m n} \delta_{m k}$$  \hspace{1cm} (182)

$$= K \sum_{n} U^\dagger_{k n} \psi_n = K [U^\dagger \psi]^k$$ \hspace{1cm} (183) which means

$$|\Theta \psi \rangle = KU^\dagger |\psi \rangle.$$  \hspace{1cm} (184)

But $U^\dagger$ is also unitary and we have

$$\Theta = KU.$$  \hspace{1cm} (185)

Sometimes I may write $\Theta = UK$ which is just as good, with the elements of the new $U$ being the complex conjugate of the old $U$.

**Theorem** $\Theta^2 = \pm 1$.

**Proof**: We know that after two reversals we must get the same physical state:

$$\Theta^2 \psi \rangle = c |\psi \rangle.$$  \hspace{1cm} (186)

So

$$KUKU |\psi \rangle = c |\psi \rangle$$  \hspace{1cm} (187)

$$U^* U |\psi \rangle = c |\psi \rangle \hspace{1cm} \forall |\psi \rangle$$  \hspace{1cm} (188)

$$U^* U = c$$  \hspace{1cm} (189)

$$U^* = cU^\dagger = c(U^*)^T = c(cU^\dagger)^T = c^2 U^*$$  \hspace{1cm} (190)

$$c = \pm 1.$$  \hspace{1cm} (191)

Note for future use that since $U^* = c(U^*)^T$,

$$U^T = cU.$$  \hspace{1cm} (192)

**Theorem** If $\Theta^2 = -1$, it can’t have an eigenvector.

**Proof**: If

$$\Theta |\psi \rangle = \lambda |\psi \rangle$$  \hspace{1cm} (193)

then

$$\Theta^2 |\psi \rangle = \Theta \lambda |\psi \rangle = \lambda^* \Theta |\psi \rangle = |\lambda|^2 |\psi \rangle \neq -|\psi \rangle.$$  \hspace{1cm} (194)

Thus what we have are (at least) two degenerate states related by $\Theta$

$$\Theta |\psi \rangle = |\chi \rangle \hspace{1cm} \Theta |\chi \rangle = -|\psi \rangle.$$  \hspace{1cm} (195)

This is called a **Kramers doublet**. We can verify that $|\psi \rangle$ and $|\Theta \psi \rangle$ are orthogonal if $\Theta^2 = -1$:

$$\langle \psi | \Theta \psi \rangle = \langle \Theta^2 \psi | \Theta \psi \rangle = -\langle \psi | \Theta \psi \rangle.$$  \hspace{1cm} (196)

There is no $\Theta^\dagger$ in the usual sense:

$$\langle \chi | \Theta \psi \rangle \neq \langle \Theta^\dagger \chi | \psi \rangle$$  \hspace{1cm} (197)

because the expression would be anti-linear in $\psi$ and $\chi$ based on the left hand side but linear in both based on the right. This can be fixed by adding another complex conjugation in the definition, but we will not follow that route.
IV. SYMMETRIES IN MOMENTUM SPACE

Consider a single particle moving in a periodic potential with

\[ H = \frac{p^2}{2m} + V(x) \]  
\[ V(x + a) = V(x) \]

where \( a \) is the lattice spacing. Thus

\[ T(a)H T^{-1}(a) = H \]  
\[ T(a)\psi_k(x) = e^{ika}\psi_k(x) \]

This form respects the unitarity of \( T \) and ensures the group property that \( T(a)T(b) = T(a + b) \).

Bloch’s theorem says that we may choose energy eigenfunctions to be of the form

\[ \psi_k(x) = e^{ikx}u_k(x) \] where
\[ u_k(x + a) = u_k(x). \]

Let us check:

\[ T(a)\psi_k = \psi_k(x + a) = e^{ik(x+a)}u_k(x + a) = e^{ika}e^{ikx}u_k(x + a) = e^{ika}e^{ikx}u_k(x) = e^{ika}\psi_k(x). \]

The energy eigenvalue equation obeyed by \( u_k(x) \) is

\[ \begin{bmatrix} \frac{p^2}{2m} + V(x) \\ P + \hbar k \end{bmatrix} e^{ikx}u_k(x) = E_ke^{ikx}u_k(x) \]
\[ \begin{bmatrix} (P + \hbar k)^2/2m + V(x) \\ H(k) \end{bmatrix} u_k(x) = E_ku_k(x) \]

where I have defined \textit{in the x-representation}

\[ H(k) = e^{-ikx}He^{ikx}. \]

This discussion assumes that at each \( k \) there is just one eigenfunction. Generally, \( H(k) \) can have a tower of eigenfunctions \( u_{km} \) labeled by a \textit{band index} \( m \). In this larger space, \( H(k) \) will generally be a matrix with elements \( H_{mn} \). (That is \( u_{km} \) and \( \psi_{km} \) form a basis but not necessarily an eigenbasis of \( H \).)

I remind you of some basic facts about momentum space.

• If the system is periodic with length \( L = Na \), the allowed values of \( k \) obey

\[ e^{ikNa} = 1 \rightarrow k_m = \frac{2\pi m}{Na}, \quad m = 0, \ldots, N - 1. \]

It is more convenient (assuming \( N \) is even) to choose the allowed momenta symmetrically around 0

\[ k = k_m = \frac{2\pi m}{Na} \quad \text{where} \quad m = \left[ 0, \pm 1, \pm 2, \ldots, \frac{N}{2} \right]. \]

Note that 0 and \( \frac{N}{2} \) are equal to minus themselves because \( e^{\pm i0} = 1 \) and \( e^{\pm i\pi} = -1 \).
• The momenta lie in the interval

\[-\frac{\pi}{a} \leq k < \frac{\pi}{a}\].

(211)

From now on I will use \( a = 1 \). Thus

\[-\pi \leq k < \pi\].

(212)

When \( N \to \infty \), the allowed values of \( k \) get closer and closer, the spacing between adjacent ones (labeled \( m \) and \( m + 1 \)) being

\[ \Delta k = \frac{2\pi}{N} \].

(213)

Then a sum over \( m \) of any function of \( k_m \) can be turned into an integral over \( k \) as follows:

\[ \sum_m f(k_m) = \frac{N}{2\pi} \sum_m f(k_m) \frac{2\pi}{N} = N \int \frac{dk}{2\pi} f(k). \]

(214)

A. How symmetries of \( \mathcal{H} \) act on \( H(k) \).

I will begin with the toughest example of TRS, implemented by the antilinear operator \( \Theta \). Unitary symmetries will be then be a breeze.

Let us define time-reversed Hamiltonian

\[ \mathcal{H}_\Theta = \Theta \mathcal{H} \Theta^{-1}. \]

(215)

If there is TRS, then

\[ \Theta \mathcal{H} \Theta^{-1} = \mathcal{H}. \]

(216)

Let

\[ H_{nm}(k) = \langle \psi_{kn}|\mathcal{H}|\psi_{km}\rangle = \langle u_{kn}|e^{-ikx}\mathcal{H}e^{ikx}|u_{km}\rangle \equiv \langle u_{kn}|H(k)|u_{km}\rangle. \]

(217)

(218)

In the above \( k \) labels the conserved momentum index and \( n \) and \( m \) label the band. We want to know what restrictions \( \mathcal{H}_\Theta = \mathcal{H} \) places on the matrix element of \( H(k) \).

In the abridged notation

\[ |\psi_{nk}\rangle = |k,n\rangle, \]

(219)

\[ H_{nm}(k) = \langle k,n|\mathcal{H}|k,m\rangle. \]

(220)

Before proceeding we need to define the action of \( \Theta \) on the states \( |k,n\rangle \). We assume that \( \Theta \) reverses \( k \) and then possibly scrambles up the band index by a unitary transformation:

\[ \Theta|k,n\rangle = \sum_r U_{rn}|r\rangle = \sum_r U_{rn}| - k, r\rangle. \]

(221)

Now we systematically assemble the matrix elements of \( \mathcal{H}_\Theta \):

\[ \mathcal{H}|k,i\rangle = \sum_j |k,j\rangle\langle k,j|\mathcal{H}|k,i\rangle = \sum_j |k,j\rangle H_{ji}(k) \]

(222)

\[ \Theta \mathcal{H}|k,i\rangle = \sum_j H_{ji}^*(k)\Theta|k,j\rangle \]

(223)

(224)
\[ \sum_j H^*_{ji}(k) U_{rj} \mid -k, r \rangle = \sum_j H^*_{ji}(k) U_{rj} \mid -k, r \rangle \]  
(225)

\[ \Theta \mathcal{H} \Theta^{-1} \Theta \mid k, i \rangle = \sum_{j,r} H^*_{ji}(k) U_{rj} \mid -k, r \rangle \]  
(226)

\[ \mathcal{H}_\Theta \sum_s U_{si} \mid -k, s \rangle = \sum_{j,r} H^*_{ji}(k) U_{rj} \mid -k, r \rangle \]  
(227)

\[ \sum_s (\mid -k, r \rangle \mathcal{H}_\Theta \mid -k, s \rangle U_{si} = \sum_j H^*_{ji}(k) U_{rj} \]  
(228)

But if \( \mathcal{H}_\Theta = \mathcal{H} \), we have then

\[ [H(-k) U]_{ri} = [U H^*(k)]_{ri} \]  
(229)

\[ H(-k) = U H^*(k) U^\dagger \]  
(230)

Using \( K \) to produce the complex conjugation, we rewrite

\[ H(-k) = U K H(k) K^\dagger = \Theta H(k) \Theta^{-1} \]  
where

\[ \Theta = U K = K \cdot KUK = KU^* \equiv KU' \]  
(231)

Since \( U' = u^* \) is also unitary we will refer to it also as \( U \) so that \( \Theta = KU \). (I denote by \( \Theta \) both the time-reversal operator in Hilbert space and its matrix counterpart that conjugates the matrix \( H_{mn} \).)

**In words:** if \( \Theta \) is a symmetry there must exist a matrix \( \Theta = KU \) such that \( \Theta H(k) \Theta^{-1} = H(-k) \).

If parity \( \Pi = \Pi^{-1} = \Pi^1 \) is a symmetry, the same arguments lead to

\[ \Pi H(k) \Pi = H(-k) \]  
(233)

where \( \Pi \) is unitary, there being no need for complex conjugation of \( H \) by an anti-linear operator.

**Exercise IV.1** Derive Eqn. 233 assuming \( \Pi \mid k, n \rangle = \sum_r U_{rn} \mid -k, r \rangle \).

**B. Symmetry restrictions on Berry phase**

What are the implications for the Berry phase \( A(k) \) if the problem is symmetric under the action of \( \Theta \) or \( \Pi \)? Consider parity first. We reason as follows:

\[ H(k) \mid k \rangle = E \mid k \rangle \]  
(234)

\[ \Pi H(k) \Pi \mid k \rangle = E \Pi \mid k \rangle \]  
(235)

\[ H(-k) \Pi \mid k \rangle = E \Pi \mid k \rangle \]  
(236)

In the simple case where there is just one state at each \( k \), this means

\[ \Pi \mid k \rangle = \mid -k \rangle \]  
(237)

\[ \mid k \rangle = \Pi \mid -k \rangle \]  
(238)

\[ A(k) = i \langle k | \frac{d}{dk} \mid k \rangle \]  
(239)

\[ = i \langle \Pi \cdot (-k) | \frac{d}{dk} \Pi \cdot (-k) \rangle \]  
(240)

\[ = i \langle (-k) \Pi | \frac{d}{dk} \Pi \rangle (-k) \]  
(241)

\[ = i \langle (-k) \frac{d}{dk} (-k) \rangle ( \text{as } \Pi^2 = I) \]  
(242)

\[ = -i \langle (-k) \frac{d}{d(-k)} \rangle (-k) \]  
(243)

\[ = -A(-k). \]  
(244)
In general we will have to add a gradient \(-d\chi/dk\) to the right hand side: although \(\Pi\) will always reverse \(k\), the state vector it produces could have a different phase from the one initially chosen in forming the basis:

\[
\Pi|k\rangle = e^{i\chi(k)}|−k\rangle.
\]

(245)

I will ignore this gradient \(d\chi/dk\) since it will drop out of gauge invariant quantities.

With this caveat, we may say \(A(k)\) is an odd function of \(k\). This result is true in higher spatial dimensions where \(k \rightarrow −k\). One consequence is that \(B\), its curl in the 2-dimensional BZ with coordinate \(k\) is an even function:

\[
A(k) = −A(−k)
\]

(246)

\[
B(k) = \nabla_k \times A(k) = −\nabla_k \times A(−k) = \nabla_k \times A(−k) = B(−k).
\]

(247)

If at each \(k\) there are many states \(|k,m\rangle\) labeled by a band index \(m\), we will write in place of Eqn. 237

\[
\Pi|km\rangle = \sum_n U_{mn} |−k,n\rangle
\]

(248)

and you may verify that this \(k\)-independent unitary operator \(U\) will meet its \(U^\dagger\) and disappear in the calculation.

**Exercise IV.2** Verify that \(U\) drops out as claimed.

Consider now TRS. Start with Eqn. 221:

\[
\Theta|k,n\rangle = \sum_r U_{rn} |−k,r\rangle
\]

(249)

\[
\Theta^2|k,n\rangle = \sum_r \Theta U_{rn} |−k,r\rangle
\]

(250)

\[
±1|k,n\rangle = \sum_r U_{rn}^\dagger (\Theta(−k)r) = \sum_r U_{nr}^\dagger (\Theta(−k)r)
\]

(251)

which we can write more compactly as

\[
|k\rangle = ±U^\dagger (\Theta(−k)).
\]

(252)

(In this notation \(|k\rangle\), for example, is a column vector whose entries are kets \(|k,n\rangle\) while \((k)|\) is a row vector whose entries are obtained by complex conjugating c-number coefficients and turning kets into corresponding bras.)

Now plug this into the expression for \(A\), set \((±1)^2 = 1\), and proceed as we did with \(\Pi\):

\[
A(k) = i\langle k|\frac{d}{dk}|k\rangle
\]

(253)

\[
= i\langle U^\dagger \Theta(−k)|\frac{d}{dk}|U^\dagger \Theta(−k)⟩
\]

(254)

\[
= i\langle \Theta(−k)|U|\frac{d}{dk}|U^\dagger \Theta(−k)⟩
\]

(255)

\[
= i\langle \Theta(−k)|\frac{d}{dk} \Theta(−k)⟩
\]

(256)

\[
= i\langle d_k(−k)|(−k)⟩
\]

(257)

\[
= −i\langle (−k)|d_k(−k)⟩
\]

(258)

\[
= i\langle (−k)|d_{−k}(−k)⟩
\]

(259)

\[
= A(−k).
\]

(260)

Thus if we have TRS

\[
A(k) = A(−k) \quad \text{and} \quad B(k) = −B(−k).
\]

(261)

It follows that if both \(\Theta\) and \(\Pi\) are symmetries,

\[
\frac{B(−k)}{\Pi} - B(−k) = 0.
\]

(262)
C. Examples of symmetries of $H(k)$.

Example 1: Spinless Bernevig-Hughes -Zhang (SBHZ) model

$$H(k) = \sigma_1 \sin k_x + \sigma_2 \sin k_y + \sigma_3 (\Delta - \cos k_x - \cos k_y).$$  \hspace{1cm} (263)

(In this context $\sigma$ are matrices in internal space and do not correspond to actual spin.) Let $\Theta = K$. Then

$$\Theta H(k) \Theta^{-1} = KHK$$  \hspace{1cm} (264)

$$= \sigma_1 \sin k_x + \sigma_2^* \sin k_y + \sigma_3 (\Delta - \cos k_x - \cos k_y)$$  \hspace{1cm} (265)

$$= \sigma_1 \sin k_x - \sigma_2 \sin k_y + \sigma_3 (\Delta - \cos k_x - \cos k_y)$$  \hspace{1cm} (266)

$$= \sigma_1 \sin k_x + \sigma_2 \sin (-k_y) + \sigma_3 (\Delta - \cos (-k_x) - \cos (-k_y))$$  \hspace{1cm} (267)

It seems to be invariant under $\Pi$ because

$$(i\sigma_3)H(k)(-i\sigma_3) = H(-k).$$  \hspace{1cm} (268)

However this is just invariance under a $\pi$ rotation around the $z$-axis. In $d = 2$ the effect of reflecting both coordinates through the origin coincides with a $\pi$ rotation in the plane. So by parity one means flipping just one coordinate. This is not a symmetry of our $H$. In $d = 3$ parity defined as flipping all three coordinates cannot be accomplished by any rotation.

Our $H$ does have an anti-unitary charge conjugation symmetry $C$ where

$$C = i\sigma_2 K$$  \hspace{1cm} and

$$CH(k)C^{-1} = -H(k).$$  \hspace{1cm} (270)

Example 2:

Say we drop the $\sigma_3$ term in the SBHZ model so that

$$H(k) = \sigma_1 \sin k_x + \sigma_2 \sin k_y.$$  \hspace{1cm} (271)

Let $\Theta = i\sigma_2 K$. Clearly $\Theta^2 = -1$. Then, using $\Theta \sigma \Theta^{-1} = -\sigma$,

$$\Theta H(k) \Theta^{-1} = -\sigma_1 \sin k_x - \sigma_2 \sin k_y$$  \hspace{1cm} (272)

$$= H(-k).$$  \hspace{1cm} (273)

Thus our $H$ is TRS. But there is another unitary choice

$$\Theta = \sigma_3, \quad \Theta^2 = +1.$$  \hspace{1cm} (274)

In Chapter VI we will find that the unitary choice places the more relevant restriction on the Hamiltonian.

Example 3: Kane-Mele model

$$H(k) = \sum_{a=1}^{5} \Gamma_a d_a(k) + \sum_{a<b=1}^{5} \Gamma_{ab} d_{ab}(k)$$  \hspace{1cm} where

$$\Gamma_a = (\sigma_x \otimes I, \sigma_z \otimes I, \sigma_y \otimes s_x, \sigma_y \otimes s_y, \sigma_y \otimes s_z)$$  \hspace{1cm} (276)

$$\Gamma_{ab} = \frac{i}{2} [\Gamma_a, \Gamma_b] = i\Gamma_a \Gamma_b \quad (\Gamma's \text{ anticommute.})$$  \hspace{1cm} (277)

Here the $s$’s are spin matrices. The $\Gamma$’s obey the algebra of Dirac matrices in 5 dimensions and $\Gamma_{ab}$ are generators of rotations acting on the spinors.
We choose
\[ \Theta = iI \otimes s_y K. \]  
(278)

Note that \( \Theta^2 = -1 \) here. Given this definition of \( \Theta \),
\begin{align*}
\Theta \Gamma_a \Theta^{-1} &= \Gamma_a \quad \text{(279)} \\
\Theta \Gamma_{ab} \Theta^{-1} &= -\Gamma_{ab} \quad \text{(280)}
\end{align*}

Exercise IV.4 Verify this.

Next, if the functions \( d \) are real and obey
\[ d_a(k) = d_a(-k) \quad \text{(281)} \]
\[ d_{ab}(k) = -d_{ab}(-k) \quad \text{then} \]
\[ \Theta H(k) \Theta^{-1} = \sum_{a=1}^{5} \Gamma_s d_a(k) + \sum_{a<b=1}^{5} (-\Gamma_{ab})d_{ab}(k) \quad \text{(283)} \]
\[ = \sum_{a=1}^{5} \Gamma_s d_a(-k) + \sum_{a<b=1}^{5} (-\Gamma_{ab})(-d_{ab}(-k)) \quad \text{(284)} \]
\[ = H(-k) \quad \text{(285)} \]

The functions \( d \) may be found in the Kane-Mele paper.

V. MODELS ON A LATTICE

We begin with some preliminaries.

A. Fourier modes and bands in k-space

Consider a fermion (say an electron) that lives on the sites of a lattice labeled by an integer \( n \). For now ignore spin or assume it is frozen. In terms of the lattice spacing \( a \), the site labeled \( n \) is at \( x = na \).

I will set \( a = 1 \). Thus the allowed values of position are just \( x = n \).

Suppose the lattice has only two sites and that the fermion can stay in either site with energy \( E \) or hop to the other with an amplitude \(-t\). The Hamiltonian is
\[ H = \begin{pmatrix} E & -t \\ -t & E \end{pmatrix}. \]  
(286)

The eigenstates and eigen-energies are
\[ \psi_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad E_+ = E - t, \text{ bonding state} \quad \text{(287)} \]
\[ \psi_- = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad E_- = E + t, \text{ anti-bonding state.} \quad \text{(288)} \]

Notice that hopping has split a degenerate level at \( E \) to two distinct levels \( E_\pm \). If we now consider a chain of \( N \) atoms there will be \( N \) non-degenerate levels. This is the valence band.

If there is another atomic level separated by an amount \( \Delta >> t \), it will form another distinct band. In real life such bands may cross.

The second-quantized Hamiltonian is
\[ H = -t \sum_n (c_{n+1}^\dagger c_n + h.c). \quad \text{(289)} \]

We now expand
\[ c_n = \frac{1}{\sqrt{N}} \sum_k c_k e^{ikn} \]  
(290)
and its adjoint in terms of plane wave operators. Using
\[ \sum_{N} e^{ikn} e^{-ik'n} = N\delta_{nn'}, \] (291)
we find
\[ H = -t \sum_{k} c_{k}^\dagger c_{k}(e^{-ik} + e^{ik}) \] (292)
\[ = -2t \sum_{k} c_{k}^\dagger c_{k}(\cos k). \] (293)

If we assume the system forms a ring of \( N \) sites then the allowed momenta are
\[ k = \frac{2\pi m}{N}, \quad m = 1, \ldots, N \quad \text{or} \quad m = 0, \pm 1, \ldots, \frac{N}{2}. \] (294)

The range of energies, going from \(-2t\) to \(+2t\) has a width \( 4t \), called the bandwidth.

In the ground state we want to occupy all negative energy states. These correspond to
\[ -K_{F} < k \leq K_{F} \quad \text{where} \quad K_{F} = \frac{\pi}{2}. \] (295)

Since only half the states are filled, we are at half-filling. This is depicted in Figure 7.

B. Peierls instability

So far we imagined the atoms to be at fixed locations \( x_n = n \). In reality the atoms can also be found in nearby locations \( x_n + \phi_n \) in the course of vibrations about the stable configuration of lowest energy. The elastic energy cost for this deformation is
\[ V_{el} = \lambda \sum_{n} (\phi_{n+1} - \phi_n)^2, \] (296)
which vanishes when all \( \phi \)'s are equal, as it should, for this just corresponds to translating the whole lattice. The continuum form of \( V_{el} \), dropping constants, is
\[ V_{el} = \int dx \left( \frac{d\phi}{dx} \right)^2. \] (297)

Including \( \pi(x) \), the momentum conjugate to \( \phi \), we arrive at the phonon Hamiltonian (dropping constants):
\[ H_{ph} = \int \left[ \pi^2(x) + \phi^2(x) \right] dx \] (298)
When quantized, the excitations at each $k$ are called *phonons*. These are to lattice vibrations what photons are to electromagnetism.

The lowest energy configuration has $\phi_n = 0$ for all $n$, i.e., each atom is at its assigned place $x_n = n$. Peierls pointed out that the system would choose to be in a new ground state in which there is a non-zero, non-constant $\phi_n$:

$$\phi_n = (-1)^n u$$  \hspace{1cm} (299)

or, where

$$x_{n+1} - x_n = 1 + (-1)^n u.$$  \hspace{1cm} (300)

In this configuration the distance between atoms would alternate between two values $1 \pm u$. Why would a system do this given that the energy cost per unit volume would go up as $u^2$? The answer lies in the electronic sector. In the presence of this Peierls distortion, the drop in the ground state energy of the electrons exceeds the increase in lattice energy at small $u$. More precisely one finds the energy density for small $u$ is of the form

$$E(u) = \alpha u^2 + \beta u^2 \ln u$$  \hspace{1cm} (301)

where the first part is from the lattice distortion and the second from the modified electronic energy. Due to the logarithm, which is arbitrarily large and negative as $u \to 0$, the origin is guaranteed to be a local maximum. As we move away, $E(u)$ will fall symmetrically to two degenerate minima at opposite values of $u$ and then rise up to form a double-well potential. This spontaneous symmetry breaking is called the *Peierls instability*.

### C. Computation of Peierls distortion energy

Let us see how the electrons respond to the lattice distortion and lower their energy. Since the distance between atoms now oscillate between two values in the Peierls state, so would the hopping amplitude oscillate:

$$t = t + (-1)^n u = t + e^{i\pi n} u.$$  \hspace{1cm} (302)

(The alternating part of $t$ vanishes at $u = 0$. I assuming that it will be linear in $u$ for small $u$.) The Hamiltonian is now

$$H = -t \sum_n (c_{n+1}^\dagger c_n + h.c) - u \sum_n (c_{n+1}^\dagger c_n e^{i\pi n} + h.c)$$  \hspace{1cm} (303)

Since a momentum of $\pi$ (i.e., the factor $e^{i\pi n}$) connects $k$ and $k + \pi$, we pair the operators so connected into a column vector. Since the BZ is a ring of circumference $2\pi$, any interval of width $\pi$ will do. We choose it symmetrically around $k = 0$ and write in obvious notation

$$\frac{H}{N} = \int_{-\pi/2}^{\pi/2} \frac{dk}{2\pi} \begin{bmatrix} c_k & c_{k+\pi} \end{bmatrix} \begin{pmatrix} -t \cos k & -u & -u t \cos k \\ -u & t \cos k \end{pmatrix} \begin{bmatrix} c_k \\ c_{k+\pi} \end{bmatrix}.$$  \hspace{1cm} (304)

Though $k$ runs over half the values as before, there are two states at each $k$ with equal and opposite energies:

$$\frac{E_{\pm}}{N} = \pm \sqrt{t^2 \cos^2 k + u^2}$$  \hspace{1cm} (305)

Notice the gap $2u$ in the spectrum at $\pm \frac{\pi}{2}$. At half-filling, the lower branch is totally filled and the upper branch is empty. Without the gap, the system would have been a conductor, while with the gap it would be an insulator. By this I mean that a DC voltage cannot excite an electron from the filled state to an empty state, while in a gapless ground state, there are states arbitrarily close the Fermi energy and a DC voltage can produce a DC current. (Of course a an AC voltage of sufficiently high $\omega$ can bridge the gap.)

Figure 8 shows the spectrum after the distortion. We see that all the occupied levels are pushed down as a result. This is what lowers the electronic energy. Of course to know by how much, we need to do the integral over $k$ to find
The energy spectrum of fermions after the Peierls distortion. There is now a gap $2u$ separating the occupied and empty bands. The occupied states all get pushed down, thereby lowering the electronic energy.

the ground state energy due to occupied negative energy states. This we do ignoring constants and focusing on just the $u$-dependence:

$$E_g \simeq -\int_0^{\frac{\pi}{2}} \sqrt{t^2 \cos^2 k + u^2} dk \quad (306)$$

$$\frac{dE_g}{du} \simeq -\int_0^{\frac{\pi}{2}} \frac{u}{\sqrt{t^2 \cos^2 k + u^2}} dk. \quad (307)$$

For small $u$, the integrand diverges near $k = \frac{\pi}{2}$. Integrating over an interval of width $\Lambda$ near $K_F = \frac{\pi}{2}$ we find (upon focusing on the leading divergence),

$$\frac{dE_g}{du} \simeq -\int_0^{\Lambda} \frac{u}{\sqrt{t^2 q^2 + u^2}} dq; \quad q = \frac{\pi}{2} - k \quad (308)$$

$$\simeq u \ln \frac{u}{\Lambda} + \text{less singular terms}, \quad (309)$$

$$E_g \simeq u^2 \ln \frac{u}{\Lambda} + \text{less singular terms}. \quad (310)$$

as advertised earlier.

VI. SU-SCHRIEFFER-HEEGER (SSH) MODEL

The SSH model is a wonderful tool for explaining many features of topological insulators: a topological index tied to the band structure, edge states, a Berry phase that affects the dynamics, and charge fractionalization. Consider the following chain depicted in Figure 9. It has undergone Peierls distortion. The inequivalent sites are labeled A and B. The degenerate symmetry-breaking solutions shown one below the other are called the A-vacuum and B-vacuum. In the A-vacuum the bond going from A to B as we move to the right is shown by a double line while the one from B to A is shown by a single line. The saw-tooth and linear depictions are completely equivalent, except in the latter the double (single) bonds are inclined upwards (downwards) in the A-vacuum and oppositely inclined in the B-vacuum. In the B-vacuum the pattern is displaced by one lattice unit relative to the A vacuum and corresponds to reversing $u$, the order parameter.

The single and double lines connecting the atoms signify two things.

First, the double line means the atoms are closer and the hopping is stronger. A single line means the atoms are further and the hopping is weaker. The symbols $v$ and $w$ shall denote intracell and intercell amplitudes. In the A-vacuum $v > w$ while it is the other way in the B -vacuum.

Second, the (single) double lines denote (single) double covalent bonds, and each bond corresponds to two electrons in a singlet state shared by the atoms at either end. To properly interpret the diagram, we need to dig a little deeper into the underlying chemistry. Look at Figure 10. Each carbon atom has 4 electrons in its outer shell and it would like to have 8 to form a full shell. To this end it reaches out to its neighbors which are also looking for an electron to share. One covalent bond is with a H atom outside the chain, and one with each of its carbon neighbors in the
FIG. 9 The Peierls distorted lattice. The inequivalent sites are labeled A and B. The degenerate symmetry-breaking vacua are also called A-vacuum and B-vacuum. The single (double) bonds denote atoms which are further (closer) and share one (two) electrons in the covalent bond.

FIG. 10 Each carbon atom wants to form four covalent bonds to fill up its outer shell. One is with a H atom outside the chain, and one with each of its neighbors. These are very strong bonds due to strongly overlapping wavefunctions. They are inert and can be ignored in consideration of excitations. The last and fourth bond is weaker and is what concerns us. It shown with the neighbor which is closer although the hybridization with the other neighbor is not negligible. Thus the fourth bond can be with the neighbor on either side, although only the bond with the closer neighbor is shown. In the A (B) vacuum this happens to lie within (between) the unit cells.

These three bonds are very strong due to the strong overlap of wavefunctions. The bonds are frozen and form the inert background as far as the excitations of interest are concerned. We can forget about them and focus on the fourth bond that this chapter is all about. It is substantially weaker than the other three (due to weaker overlap of orbitals) and preferentially formed with the neighbor which is closer. In the A (B) vacuum this happens to be within (between) the unit cells. Although I show only the stronger bond in the figures, they are to be viewed as an extreme caricatures of the A and B phases in which the weaker bond, smaller but by no means negligible, is ignored. (This is like figures that depict the ordered phase of the Ising model with all spins perfectly aligned.)

For our purposes, we can ignore the inert bonds, and view the single line as denoting a single bond with the more distant neighbor and a weaker hopping amplitude and the double line as the stronger bond with the closer neighbor and larger hopping. Thus in the following discussions, both single and double lines represent just one bond (weak or strong) with one pair of spin-singlet electrons.

Since the hopping amplitude is spin-independent and there will be no interactions in the model, we can treat each
spin separately. This is what one means by the model with spinless fermions. We will not consider that option here.

A. The band Hamiltonian

Consider the A-vacuum. The unit cell has two sites with A and B atoms as shown. We will set \( a = 1 \), where \( a \) is the distance from one A atom to the next A atom. The Hamiltonian is

\[
H = v \sum_n (A_n^\dagger B_n + B_n^\dagger A_n) + w \sum_n (A_{n+1}^\dagger B_n + B_n^\dagger A_{n+1}).
\]  

(311)

We can choose \( v \) and \( w \) to be positive. If they are not, we can make them positive by the following change of operators:

| sign of \( v \) | sign of \( w \) | transformation |
|----------------|----------------|---------------|
| +              | +              | do nothing    |
| +              | −              | \( A_n \to (-1)^n A_n, B_n \to (-1)^n B_n \) |
| −              | +              | \( A_n \to (-1)^n A_n, B_n \to (-1)^n B_n \) |
| −              | −              | \( A_n \to -A_n \) |

(312)

Upon Fourier transformation

\[
H(k) = \int_0^{2\pi} \frac{dk}{2\pi} \left[ (v + we^{-ik})A_k^\dagger B_k + (v + we^{ik})B_k^\dagger A_k \right]
\]  

(313)

\[
= \int_0^{2\pi} \frac{dk}{2\pi} \left[ A_k^\dagger, B_k^\dagger \right] \left[ \begin{array}{cc} 0 & v + we^{-ik} \\ v + we^{ik} & 0 \end{array} \right] \left[ A_k \right]
\]

(314)

\[
\equiv \int_0^{2\pi} \frac{dk}{2\pi} \Psi_k^\dagger [(v + w \cos k) \sigma_1 + w \sin k \sigma_2] \Psi_k.
\]

(315)

Consider

\[
H(k) = (v + w \cos k)\sigma_1 + w \sin k \sigma_2 \equiv \hbar \cdot \sigma.
\]

(316)

It has charge conjugation symmetry:

\[
\mathcal{CHC}^{-1} = -H \quad \mathcal{C} = \sigma_3
\]

(317)

where we have chosen the unitary option with \( \mathcal{C}^2 = +1 \).

There is also the antiunitary option \( \mathcal{C} = iK\sigma_2 \), with \( \mathcal{C}^2 = -1 \).

The difference between the two choices is that \( \mathcal{C} = \sigma_1 \) will not allow any term of the form \( f(k)\sigma_3 \), by forcing \( f(k) = -f(-k) \), whereas \( \mathcal{C} = iK\sigma_2 \) (which is just the “spin-flip” operator) will allow such a term.

We shall see that it is \( \mathcal{C} = \sigma_1 \) that is more relevant to us because it keeps \( \hbar \) in the \( 1 - 2 \) plane, which in turn is essential in isolating different topological sectors.

This \( H \) also has TRS:

\[
\Theta H(k)\Theta^{-1} = H(-k) \quad \Theta = K.
\]

(318)

TRI does not forbid an \( \sigma_3 \) term if it is multiplied by an even function of \( k \).

This \( H \) also has parity or \( x \to -x \) invariance

\[
\Pi H(k)\Pi = H(-k) \quad \Pi = \sigma_1
\]

(319)

because \( \Pi = \sigma_1 \) exchanges A and B atoms which is what should happen when we reflect through their midpoint.

The ground state of \( H \) is

\[
\Psi_- = \frac{1}{\sqrt{2}} \left[ \begin{array}{c} 1 \\ -e^{i\phi} \end{array} \right],
\]

(320)

\[
\tan \phi = \frac{w \sin k}{v + w \cos k}.
\]

(321)
FIG. 11 The ground state spinor at each momentum $k$ follows the field $h$ which undergoes a $2\pi$ rotation when $w > v$ (left half) but not so when $w < v$ as in the right half.

The "magnetic field" $h$ that couples to $\sigma$ in Eqn. 316 lies in the $h_1 - h_2$ plane at an angle $\phi$ with respect to the $h_1$-axis. As the momentum $k$ varies from 0 to $2\pi$, the tip of $h$ moves along a circle of radius $w$ centered at $x = v$. For $w > v$, the circle encloses the origin and the tip of the $h$ vector rotates by $2\pi$ as shown in the left half of Figure 6.3. On the other hand, as shown in the right half, when $w < v$, the tip of $h$ does not go around a full circle. These two possibilities are topologically distinct. Since $\hat{h}$ is the direction of the expectation value of $\sigma$ in the ground state, these statements also apply to it.

When the topology changes, the circle representing $k$ crosses the origin, where $h = 0$. Here the Hamiltonian is degenerate, and indeed vanishes entirely. This closing of the band gap is needed for any topology change, which signifies singular behavior.

The word "topological" is apt because whether or not $h$ encircles the origin is a binary question, not affected by small changes in $v$ or $w$, changes which would affect all other quantity like energies, wavefunctions etc.

In the presence of a $\sigma_3$ term, this would no longer be true because the spinor can leave the $h_1 - h_2$ plane and there is no real sense to the loop encircling the origin. Thus the topological classification relies on charge-conjugation symmetry corresponding to $C = \sigma_3$.

The topology can also be described in terms of the Berry potential

$$A(k) = i \left< \Psi_- \frac{d\Psi_-}{dk} \right> = -\frac{1}{2} \frac{d\phi}{dk}. \quad (322)$$

The gauge-invariant result is

$$\oint A(k) dk = -\pi \quad \text{if} \quad w > v, \quad \text{else} \quad 0. \quad (323)$$

This is an example of the Zak phase.

**Exercise VI.1** Verify by evaluating $\frac{d\phi}{dk}$ that $A(k) = A(-k)$, as required by TRS.

**B. Effect of the Berry phase on dynamics**

Say we apply an electric field $E$ along our linear system. For this purpose let us treat the $x$ coordinate as a continuum and imagine a momentum-space wavepacket centered at $k$ slowly (adiabatically) drifting in response. (The adiabatic condition means that the system will never jump to the states in the upper positive-energy band.) The field enters the Hamiltonian as a potential $-eE x$ in real space or as the operator $i\hbar eE \frac{d}{dk}$ in momentum space. The Schrödinger equation

$$\left( i\hbar eE \frac{d}{dk} + \varepsilon(k) \right) \psi(k) = E \psi(k) \quad \text{where}$$

$$\varepsilon(k) = -\sqrt{v^2 + w^2 + 2vw \cos k} \quad (324)$$

can be simply integrated to give

$$\psi(k) = \psi(0) \exp \left[ -\frac{i}{\hbar eE} \int_{0}^{k} (E - \varepsilon(k')) dk' \right]. \quad (326)$$
The single valued condition \( \psi(0) = \psi(2\pi) \) or
\[
\frac{i}{\hbar \mathcal{E}} \left[ 2\pi E - \int_0^{2\pi} \varepsilon(k')dk' \right] = 2\pi im \implies (327)
\]
\[
E = E_m = \bar{\varepsilon} + m\hbar \mathcal{E} \text{ where}\ (328)
\]
\[
\bar{\varepsilon} = \frac{1}{2\pi} \int_0^{2\pi} \varepsilon(k)dk
\]
is the average energy of the occupied band. This calculation however ignores the Berry phase of \(-\pi\) that arises in the slow transport in \(k\) and makes a measurable change in the spectrum. Upon including it we find
\[
E_m = \bar{\varepsilon} + \left( m + \frac{1}{2} \right) \hbar \mathcal{E}. \tag{330}
\]

### C. Topological index \( Q \) and edge states

A salient feature of topological insulators is that gapless or zero energy states appear at the interface of the insulator and the vacuum or another insulator with a different value of the topological index, which is also called the winding number. The adjective winding arises as follows. The Brillouin zone (BZ) is a circle parametrized by \( k \) which ranges from 0 to \( 2\pi \). The expectation value of \( \sigma \) in the state \( \Psi_\pm \) also lies on the unit circle parametrized by the angle \( \phi \). Thus the the ground state spinor defines map from a circle \( S_1 \), the BZ, to the circle \( \hat{\mathfrak{h}} \). Such a map is indexed by an integer which counts the number of times \( \hat{\mathfrak{h}} \) goes around as \( k \) goes around once. The winding number is
\[
Q = \int_0^{2\pi} \frac{dk d\phi(k)}{2\pi dk}\tag{331}
\]
which meant \( Q = -1 \) when \( w > v \) and \( Q = 0 \) when \( w < v \). (One can cook up band structures when the non-zero index is +1 or some other integer.)

Suppose we chop off the \( Q \neq 0 \) insulator at some point, i.e., there is just the vacuum beyond this. Then \( Q \) has to jump from non-zero to zero at the edge. Since \( Q \) is restricted to integer values, the jump cannot take place as long as everything is analytic, i.e., as long there is a gap. Hence gapless edge states are mandatory when \( Q \) jumps. In our example, instead of the vacuum we could also have a \( Q = 0 \) insulator i.e., with \( w < v \) at the interface and a gapless edge state would have to arise there as well.

Since particle hole symmetry \( CHC^{-1} = -H \) implies that each energy \( E \) is accompanied by \(-E\), the edge state, if alone, must be at \( E = 0 \). (Without particle-hole symmetry, \( E = 0 \) does not have any significance since \( E \) can be moved up and down by adding a constant to \( H \).)

Let us now verify the existence of such an edge state when we have the vacuum to the left of the origin and the \( w > v \) system to the right. It is easier to do this in first-quantization. We rewrite \( H \) in Eqn. 6.1 as
\[
H = \sum_{m=1}^{\infty} \left( v |A_m\rangle \langle B_m| + |B_m\rangle \langle A_m| \right) + w \left[ |A_{m+1}\rangle \langle B_m| + |B_m\rangle \langle A_{m+1}| \right] \tag{332}
\]
where \( |A_m\rangle \) and \( |B_m\rangle \) denote particles of type A or B sitting at site \( m \). Notice that there are no sites to the left of \( m = 1 \). Thus the \( m = 1 \) term in the sum multiplied by \( w \) which invokes \( |B_0\rangle \) is actually 0.

Let us demand that
\[
|\Psi\rangle = \sum_n \left( a_n|A_n\rangle + b_n|B_n\rangle \right) \tag{333}
\]
be a zero-energy eigenket of \( H \):
\[
0 = H|\Psi\rangle \tag{334}
\]
\[
= v \left[ \sum_n (a_n|B_n\rangle + b_n|A_n\rangle) \right] + w \left[ \sum_n (a_n|B_{n-1}\rangle + b_n|A_{n+1}\rangle) \right] \tag{335}
\]
FIG. 12 The first and third lines show that $A$ and $B$ vacua while the second and fourth the extreme case when only $v$ or $w$ is non-zero. In the former case all electrons are locked into bonding orbitals and there is a gap to the anti-bonding state. The latter case describes two loose electrons at the ends of the chain not bonding with any other.

Setting the coefficients of $|A_m\rangle$ and $|B_m\rangle$ to 0, we obtain the recursion relations

$$a_{n+1} = -\frac{v}{w}a_n \quad (336)$$

$$b_n = -\frac{w}{v}b_{n-1}. \quad (337)$$

While these are the equations away from the ends, there is one equation

$$vb_1 = -wb_0 \quad (338)$$

which, because there is no $b_0$, forces $b_1$ and all higher $b$’s to be zero.

(I suggest you explicitly write out the first few terms to see that $b_1$ has to vanish and hence so must all its descendants.)

Next,

$$a_n = \left(-\frac{v}{w}\right)^{n-1}a_1. \quad (339)$$

This is a normalizable (exponentially falling) solution if $v < w$, i.e., the system is topologically non-trivial and has a non-zero $Q$.

We can see the distinction between the two phases if we go to the extreme ends of each phase where only $v$ or $w$ alone is non-zero, as in Figure 12. In the former case all electrons are locked into bonding orbitals and there is a gap to the anti-bonding state. The latter case describes two loose electrons at the ends of the chain not bonding with any other. The unpaired spins can point up or down, which implies degeneracy.

Notice that in an infinite lattice you would not know if you were in the $A$ or $B$ vacuum because the atoms, also called $A$ and $B$, are identical. We need the edges to define the distinction: in the finite system first and last bonds are strong (weak) in the $A$ ($B$) vacuum. Thus edges or boundaries are essential in fully characterizing topological insulators.

D. Continuum theory

When the gap is small or zero, we can approximate the lattice problem by one in the continuum, which may be more tractable mathematically. Let us begin with

$$H(k) = (v + w \cos k)\sigma_1 + \sin k\sigma_2. \quad (340)$$
The gap vanishes when $H = 0$ i.e.,

\begin{align}
  v + w \cos k &= 0 \\
  w \sin k &= 0.
\end{align}

(341) (342)

The options are

\begin{align}
  k &= 0 \quad v + w = 0 \quad \text{not possible as both are positive} \\
  k &= \pi \quad v = w \quad \text{possible}.
\end{align}

(343) (344)

(Look at Figure 11 which displays where the circle crosses the origin.) So let us go near the second point and set

\begin{align}
  k &= \pi + q, \quad \cos k \simeq -1 \quad \sin k \simeq -q
\end{align}

so that

\begin{equation}
  H = (v-w)\sigma_1 - wq\sigma_2 \equiv m\sigma_1 - wq\sigma_2.
\end{equation}

(346)

Remember that when $m = v - w > 0$, the topological index is 0 while if $m = v - w < 0$, the index is 1. Let us set $w = 1$ which merely affects the overall energy scale. In real space we obtain the Dirac equation

\begin{equation}
  i\hbar \sigma_2 \frac{d\psi}{dx} + m \sigma_1 \psi = E\psi, \quad m = v - 1.
\end{equation}

(347)

In this long-wavelength theory we have the continuum Dirac equation. We replace the sharp edge where $m$ changes sign by a smooth edge in which $m = m(x)$ is a function that slowly changes from some large positive value $m_0$ at negative $x$ to a large negative value $-m_0$ for large positive $x$, crossing zero linearly at $x = 0$, as shown in Figure 13. Thus to the far left we have the system with $m = v - w \gg 0$, the trivial phase, and to the far right the system with $v \ll w$, the non-trivial phase. The varying $m(x)$ is a smooth interpolation between the phases. Multiplying Eqn. 347 by $\sigma_2$ we obtain, when $E = 0$, the equation

\begin{equation}
  i\hbar \frac{d\psi}{dx} - im\sigma_3\psi = 0.
\end{equation}

(348)

We cleverly choose $\sigma_3\psi = +\psi$ and solve for $\psi$ by integration:

\begin{equation}
  \psi(x) = \psi(0) \exp \left[ \frac{1}{\hbar} \int_0^x m(x')dx' \right].
\end{equation}

(349)

Notice that the $x$ integral falls off in either direction as we move away from $x = 0$. (Consider $m(x') = -x'$.) Had we chosen $\sigma_3\psi = -\psi$ the wavefunction would have been non-normalizable. This solution is a special case of the Jackiw-Rebbi prediction that fermions always form a zero mode in the presence of a kink or soliton which interpolates...
FIG. 14 At the top are a pair of solitons that lead to a change from A to B and back. At the bottom we see an extreme case when the weak bonds are set to zero. Now you can see two atoms disconnected from everything else. The text and the Figure 15 explain the associated charges.

between two different vacua. The kink here is in $m(x)$. Their result in turn is a special case of what are called Index Theorems.

This solution shows a universal feature: there are only half as many states at the $d-1$ dimensional boundary of a $d$ dimensional TI as in an isolated $d-1$ dimensional system. Here $d = 1$, and the boundary is a point which, in isolation, could have had both eigenvalues of $\sigma_3$.

The fact that the “spin” is restricted $\sigma_3 = +$ means that the wave function has support only in one sub-lattice (A), as was the case for our solution on the lattice which had only $a_n \neq 0$.

E. Charge fractionalization

This model provides one of the simplest examples of charge fractionalization: where the spin and charge of the electron separate. (If we worked with spinless fermions, the excitations would have half-integer charge.)

Recall the two Peierls states called A-and B-vacua. A soliton is a configuration that interpolates between the two. Look at Figure 14. We see at the top a switch from A to B vacuum when we run into two adjacent single bonds. This is a soliton. A few sites later we run into another repeated single bond and soliton. The lower line shows the extreme case where weak bonds are set to zero.

To find the charge associated with these solitonic excitations look at the extreme case shown in Figure 15. Now all weak bonds have been set to zero in the two kinds of vacuums in the top two lines. We then pluck out the bond circled by an oval from the A vacuum as shown in the top line. The eliminated bond leaves behind charge $2e$ because it used to contain a pair of electrons in a spin-singlet. This actually creates a double soliton and leaves behind two vacancies which corresponds to charge $2e$ as shown in the third line. Now we slowly flip the bonds to the left as shown in the third line so that the double soliton is now split into two, each of charge $e$. The conversion of single to double lines is assumed to be accompanied by the corresponding change in atomic spacing from large to small. Ideally we want to separate the solitons not by just three but a very large number of sites so they correspond to well defined excitations.

The charge $e$ excitation is not the usual hole because it carries no spin, since we removed a spin singlet. If we add an electron at either soliton location, the soliton would now have spin but no charge. In either case the quantum numbers are not those of an electron or hole. This is called spin-charge separation.

VII. CHERN BANDS

We now extend many of the ideas of the SSH model to two spatial dimensions.
FIG. 15  The first two rows show the A and B vacua in the extreme limit where weak bonds are set to zero. In the third row the bond marked by an oval in the top line is eliminated, removing the two electrons. This creates two vacancies. The curly arrows in the third line show how bonds (and atoms) are moved to the left to reach the fourth line in which the two vacancies and the solitons are separated. The lone sites carry charge +e and no spin. If we put an electron (charge −e) there, the soliton would have spin but no charge. These soliton quantum number correspond neither to standard electrons nor holes.

A. Preview

Let us recall the highlights of the SSH topological insulator. It was defined by a Hamiltonian

\[ H(k) = \hbar \cdot \sigma. \] (350)

The ground-state spinor at each \( k \) had an expectation value \( \langle \sigma \rangle = -\hat{h} \) which lay on the unit circle. The BZ was also a circle with coordinate \( k \) that ranged from 0 to \( 2\pi \). As \( k \) varied over the circular BZ, we could follow either \( h(k) \) or \( \langle \sigma \rangle = -\hat{h} \) around the origin. In the nontrivial case \( \langle \sigma \rangle = -\hat{h} \) wound around the origin once while in the trivial case it wound part of the way and then unwound. The topologically non-trivial system had an index \( Q \) equal to the winding number alluded to above.

Equivalently we could define a Berry vector potential

\[ A(k) = i \langle n | \frac{dn}{dk} \rangle \] (351)

where \( |n\rangle \) was the ground state spinor \( |\Psi_-\rangle \). Its line integral around the BZ was gauge invariant and yielded \( -\pi \) in the non-trivial phase and 0 in the trivial phase. This difference had measurable consequences.

We now extend these ideas to two spatial dimension. Here is a preview with details to follow.

At each \( k \) there will a basis of wavefunctions \( \Psi_{k\alpha} \) (where \( \alpha \) is the band index) and the corresponding Bloch functions \( u_{k\alpha} \):

\[ \Psi_{k\alpha} = e^{ik \cdot r} u_{k\alpha} \] (352)

with the usual relation between the Hamiltonians \( H(k) \) and \( \mathcal{H} \):

\[ H(k) = e^{-ik \cdot r} \mathcal{H} e^{ik \cdot r}. \] (353)

The Berry potential in any occupied band will be

\[ A = i \langle u | \nabla u \rangle \] (354)

where \( |u\rangle \) is the eigenspinor at that \( k \) and \( \nabla \) is the gradient in \( k \)-space. The curl of \( A \) is the Berry flux or Berry curvature

\[ B = \nabla \times A. \] (355)
The Chern number will be defined as
\[ C = \frac{1}{2\pi} \int B d^2 k. \] (356)

We will show that \( C \) is an integer for any filled band with a gap. A band with \( C \neq 0 \) will be called a Chern band. We have shown (Eqn. 261) that
\[ B(k) = -B(-k) \] if there is TRS. Therefore
\[ C = \frac{1}{2\pi} \int B d^2 k = 0 \] if there is TRS. (358)

We can have a non-zero Chern number only if there is no TRS.

A Chern band is assured to have gapless edge states at the boundary with the vacuum or another band with a different \( C \) for the reason given earlier: an integer like \( C \) cannot change smoothly from one value to another value unless there is a some non-analyticity due to gap closing. A surprising result due to Thouless, Kohmoto, Nightingale and den Nijs (TKNN) is that a Chern band will have a Hall conductance
\[ \sigma_{xy} = \frac{e^2}{2\pi\hbar} C. \] (359)

This was a surprise for people (like me) who were under the impression that you needed to put the sample in a perpendicular magnetic field to obtain a non-zero \( \sigma_{xy} \). It turns out you just have to break TRS. A concrete example on the honeycomb lattice was provided by Haldane.

B. The Kubo formula and the TKNN result

The rest of this chapter is dedicated to the derivation of the TKNN formula relating the Chern number to Hall conductance.

The Hall conductance of a sample in the \( x - y \) plane is the ratio
\[ \sigma_{xy} = \frac{j_y}{E_x} \] (360)

of the current density and applied field.

One way to compute it is as follows.

1. Consider a system in the distant past in its ground state, \( |0\rangle \), a filled band wherein every single-particle state \( |k, \alpha\rangle \) is occupied. Imagine there is just one unoccupied band of single-particle states \( |k, \beta\rangle \).
2. Couple the system to a spatially uniform external electric field produced by a spatially uniform, time-dependent transverse vector potential \( A_x \):
\[ E_x = -\frac{\partial A_x}{\partial t} \] (361)
\[ E_x(\omega) = i\omega A_x(\omega). \] (362)

(We prefer \( A \) to a scalar potential with a gradient in order to keep the system translationally invariant.)

3. In the interaction picture let the initial state with \( \langle j_y \rangle = 0 \) evolve, working to first order in the perturbation
\[ H_I = -e j_x A_x \] (363)

where \( e \) is the charge of the particle. (The sign of \( e \) will drop out.)

4. Compute the expectation of \( \langle j_y(\omega) \rangle \) in the distant future and evaluate
\[ \sigma_{xy} = \lim_{\omega \to 0} \frac{\langle j_y(\omega) \rangle}{E_x(\omega)}. \] (364)
The result of standard first-order time-dependent perturbation theory is:

\[
\sigma_{xy}(\omega) = -\frac{e^2}{i\omega\hbar^2} \sum_{n\neq 0} \left[ \frac{\langle 0|j_x|n\rangle\langle n|j_y|0\rangle}{E_n - E_0 + \hbar\omega} + \frac{\langle 0|j_y|n\rangle\langle n|j_x|0\rangle}{E_n - E_0 - \hbar\omega} \right]
\]  

(365)

where \(|n\rangle\) is an exact eigenstate of the unperturbed Hamiltonian.

It can be shown that the sum in Eqn. 365 vanishes at \(\omega = 0\).

**Exercise VII.1** Prove this claim. Be ready for some serious juggling.

Since, since \(\omega \to 0\), we expand

\[
\frac{1}{E_n - E_0 \pm \hbar\omega} = \frac{1}{E_n - E_0} \left( 1 \mp \frac{\hbar\omega}{E_n - E_0} + \ldots \right).
\]  

(366)

to arrive at

\[
\sigma_{xy}(0) = \frac{i e^2}{\hbar} \sum_{n\neq 0} \left[ \frac{\langle 0|j_x|n\rangle\langle n|j_y|0\rangle}{(E_n - E_0)^2} - \frac{\langle 0|j_y|n\rangle\langle n|j_x|0\rangle}{(E_n - E_0)^2} \right].
\]  

(367)

Here is one way to approach the matrix elements of \(j_x\) and \(j_y\). The current operator in second quantization is

\[
j_x = \int \Psi^\dagger(r) \frac{(-i\hbar \nabla)}{m} \Psi(r) dr
\]  

(368)

Now we expand

\[
\Psi(r) = \sum_\alpha \int \frac{d^2k}{4\pi^2} e^{ik\cdot r} u_\alpha c_{k\alpha}
\]  

(369)

and find, after using the orthogonality properties of \(u\),

\[
j_x = \int \frac{d^2k}{4\pi^2} \sum_\beta c_{k\beta} \left[ \frac{(-i\hbar \nabla + \hbar k)_x}{m} \right] c_{k\alpha}
\]  

(370)

\[
= \int \frac{d^2k}{4\pi^2} \sum_\beta c_{k\beta} \left[ \frac{\partial H(k)}{\partial k_x} \right] c_{k\alpha}
\]  

(371)

where

\[
\left[ \frac{\partial H(k)}{\partial k_x} \right]_{\beta\alpha} = \int_{\text{unit cell}} dr u_{k\beta}^\ast(r) \frac{(-i\hbar \nabla + \hbar k)_x}{m} u_{k\alpha}
\]  

(372)

and similarly for \(j_y\).

**Exercise VII.2** Here is a sample exercise in orthogonality in a finite system in one spatial dimension. Consider a system of length \(N\) and unit cell size \(a = 1\) and assume that

\[
H(x) = H(x + 1)
\]  

(373)

\[
u_{k\alpha}(x + 1) = u_{k\alpha}(x)
\]  

(374)

\[
\psi_{k\alpha}(x) = \frac{1}{\sqrt{N}} e^{ikx} u_{k\alpha}
\]  

(375)

\[
\int_0^1 u_{k\alpha}^\ast(y) u_{k\beta}(y) dy = \delta_{\alpha\beta} \quad (u_{k\alpha} \text{ orthonormal})
\]  

(376)

Show that

\[
\int_0^N \psi_{k\alpha}^\ast(x) \psi_{k\beta}(x) dx = \delta_{k\alpha} \delta_{\alpha\beta}.
\]  

(377)

**Hint:** Let \(x = nx + y, 0 \leq y \leq 1\) and break the integral over \(x\) into \(N\) integrals over adjacent unit intervals \(n \leq x \leq n+1\). First do the sum over \(n = 0, 1, 2..N - 1\) to extract a \(\delta_{kk'}\). Then do the \(y\) integral over \(0 \leq y \leq 1\). Remember \(u\) is periodic.
FIG. 16 The transition out of the $\alpha$ band to the $\beta$ band at the same $\mathbf{k}$ using $j_y$ and back to $\alpha$ using $j_x$.

In Eqn. 367 $j_y$ will transform the single-particle state $|k\alpha\rangle$ to the state $|k\beta\rangle$ with matrix element $\langle k|\frac{\partial H}{\partial y}|k\alpha\rangle$ and then $j_x$ will similarly bring it back to $|k\alpha\rangle$, so that the many-body state returns to the filled band $|0\rangle$. Figure 16 describes this process. The $\mathbf{k}$ label will be suppressed in the kets from now on.

Applying Eqn. 370 through 372 to Eqn. 367 we find

$$\sigma_{xy}(0) = \frac{ie^2}{\hbar} \int \frac{d^2k}{4\pi^2} \sum_{\alpha \neq \beta} \left[ \langle \alpha|\partial_x H|\beta \rangle \langle \beta|\partial_y H|\alpha \rangle - \langle \alpha|\partial_y H|\beta \rangle \langle \beta|\partial_x H|\alpha \rangle \right] \cdot (E_\beta - E_\alpha)^2.$$

(378)

Next we call repeatedly on relations like

$$\langle \alpha|\partial_x H|\beta \rangle = (E_\alpha - E_\beta)\langle \partial_x \alpha|\beta \rangle$$

(379)

to arrive at

$$\sigma_{xy}(0) = \frac{ie^2}{\hbar} \int \frac{d^2k}{4\pi^2} \sum_{\alpha \neq \beta} \left[ \langle \partial_x \alpha|\partial_y \beta \rangle \langle \beta|\partial_x \alpha \rangle - \langle \partial_y \alpha|\partial_x \beta \rangle \langle \beta|\partial_x \alpha \rangle \right]$$

$$= \frac{ie^2}{\hbar} \int \frac{d^2k}{4\pi^2} \sum_{\alpha} \left[ \langle \partial_x \alpha|\partial_y \alpha \rangle - \langle \partial_y \alpha|\partial_x \alpha \rangle \right].$$

(380)

where to get to the last line I have inserted the $\alpha = \beta$ term because its contribution vanishes and then used completeness.

**Exercise VII.3** Verify that the $\alpha = \beta$ term vanishes.

I will now show that the Berry flux $\mathcal{B}$ enters the formula above:

$$A_x = i\langle k|\alpha|\frac{d}{dk_x}|k,\alpha\rangle \equiv i\langle \alpha|\partial_x \alpha \rangle$$

(381)

$$\mathcal{B} = \partial_y A_x - \partial_x A_y$$

(382)

$$= i \left[ \partial_x \langle \alpha|\partial_y \alpha \rangle - \partial_y \langle \alpha|\partial_x \alpha \rangle \right]$$

(383)

$$= i \left[ \langle \partial_x \alpha|\partial_y \alpha \rangle - \langle \partial_y \alpha|\partial_x \alpha \rangle \right].$$

(384)

Inserting this into Eqn 380, finally we arrive at the celebrated TKNN result relating $\sigma_{xy}$ to the Chern number:

$$\sigma_{xy} = \frac{e^2}{2\pi\hbar} \int \frac{d^2k}{2\pi} \mathcal{B}$$

(385)

$$= \frac{e^2}{2\pi\hbar} \mathcal{C}$$

(386)

where the definition of the Chern number

$$\mathcal{C} = \int \frac{d^2k}{2\pi} \mathcal{B}$$

(387)

has been recalled.
C. Quantization of $C$ in the BZ

We prove that $C$ is quantized to integral values pretty much along the same lines we used to show Dirac’s condition $eg = m\hbar/2$. Consider a closed two-dimensional surface $S$ (which represents the BZ) as shown in Figure 17. Let $C_1$ be a loop enclosing an area $S_I$ within which is a well defined non-singular $A_I$. The complimentary region is $S_{II}$ and the potential there is $A_{II}$. (We have seen in the monopole problem that when there is non-trivial topology, we will need more than one patch.) We know that

$$A_I - A_{II} = \nabla \chi.$$  \hfill (388)

Then we follow the well known path

$$\exp \left[ i \oint_{C_1} A \cdot dk \right] = \exp \left[ i \int_{S_I} B \right],$$  \hfill (389)

$$\exp \left[ i \oint_{-C_1} A_{II} \cdot dk \right] = \exp \left[ i \int_{S_{II}} B \right],$$  \hfill (390)

$$\exp \left[ i \oint_{C_1} (A_I - A_{II}) \cdot dk \right] = \exp \left[ i \int_{S} B \right],$$  \hfill (391)

$$\exp \left[ i \oint_{C_1} \nabla \chi \cdot dk \right] = \exp \left[ i \int_{S} B \right],$$  \hfill (392)

$$\exp [2\pi im] = \exp \left[ i \int_{S} B \right].$$  \hfill (393)

$$m = \frac{1}{2\pi} \int B = C.$$  \hfill (394)

D. Hall conductance of the filled Dirac sea

We will establish that

$$\sigma_{xy} = \frac{1}{2} \frac{m}{|m|}$$  \hfill (395)

for the filled sea of a Dirac fermion of mass $m$. The procedure is once again to apply an electric field

$$E_y(\omega) = i\omega A_y(\omega),$$  \hfill (396)

find $\langle j^y \rangle$ and take the ratio.

By definition

$$\langle j^\mu(x) \rangle = \frac{e}{Z} \int [D\phi D\bar{\phi}] \bar{\psi} \gamma^\mu \psi(x) \exp \left[ \frac{iS}{\hbar} \right] \text{ where}$$  \hfill (397)
\[ S = \int \bar{\psi}(y)(i\partial_y - eA - m)\psi(y)d^3y \tag{398} \]
\[ Z = \int \left[ D\psi D\bar{\psi} \right] \exp \left( \frac{iS}{\hbar} \right). \tag{399} \]

If we bring down the interaction to first order in \( e \) we find
\[ \langle j^\mu(x) \rangle = -\frac{ie^2}{\hbar} \left( \int d^3y \bar{\psi}(x)\gamma^\mu(x)\psi(y)A^\nu(y) \right). \tag{400} \]

where the average is taken with respect to \( Z_0 \), the partition function with \( A = 0 \). Notice that \( j^x \) (and not \( j_x = -j^x \)) is the current we want and \( A^y \) is the vector potential we want, which is why I have chosen \( \gamma_\nu \) with the lower index.

Let us now go to momentum space
\[ F(t, r) = \int F(\omega, \mathbf{q}) \exp \left( i\omega t - i\mathbf{q} \cdot \mathbf{r} \right) \frac{d\omega d^2\mathbf{q}}{8\pi^3} \tag{401} \]
and use the Feynman rules to arrive at
\[ j^\mu(q) = \frac{-ie^2}{\hbar} \left( -1 \right) \int \frac{d\omega d^2\mathbf{q}}{8\pi^3} \text{Tr} \left[ \frac{i}{\hat{p} - m + i\varepsilon} \gamma^\nu \frac{i}{\hat{q} + \hat{\sigma} - m + i\varepsilon} \right] A^\nu(q) \tag{402} \]

We want to set \( \mu = x, \nu = y \) and extract just the part of the trace proportional to \( q_0 = \omega \), setting \( q = 0 \) everywhere else:
\[ \text{“Tr”} = \text{Tr} \left[ \gamma^0 \gamma^x \frac{\hat{p} + m}{p^2 - m^2 + i\varepsilon} \gamma^y \frac{\hat{p} + \hat{q} + m}{(p + q)^2 - m^2 + i\varepsilon} \right] A^y(q) \tag{403} \]
\[ \text{“Tr”} = \frac{2im\omega A^y}{(p^2 - m^2 + i\varepsilon)^2} + \text{terms that do not matter} \]

Now we are going to choose our \( \gamma \) matrices in a particular way. Suppose our single-particle Hamiltonian is
\[ H = \mathbf{\sigma} \cdot (\mathbf{p} - e\mathbf{A}) \tag{404} \]
then we will find, upon following the usual route to the path integral, (see my book on QFT and CMT) that
\[ \gamma^0 = \sigma_z \quad \gamma^x = i\sigma_y \quad \gamma^y = i\sigma_x = -\gamma^y. \tag{405} \]
and
\[ \text{“Tr”} = \frac{2im\omega A^y}{2m^2 + i\varepsilon} \tag{406} \]
So we need to evaluate
\[ \sigma_{xy} = \frac{-ie^2(2m)}{\hbar} \left( -1 \right) \int \frac{d\omega d^2\mathbf{q}}{8\pi^3} \frac{1}{(\omega^2 - |\mathbf{p}|^2 - m^2 + i\varepsilon)^2}. \tag{407} \]

There are poles at
\[ \omega = \pm(E - i\varepsilon) \quad \text{where} \quad E = \sqrt{|\mathbf{p}|^2 + m^2} \tag{408} \]
which lie just below (above) the real axis for \( \omega \) positive (negative). This allows us to do a Wick-rotation of the \( \omega \)-axis by \( \frac{1}{2}\pi \) without encountering any singularities, set
\[ \omega = ip_0 \tag{409} \]
and integrate up the $y$-axis from $-\infty$ to $+\infty$ to arrive at the final result

$$\sigma_{xy} = \frac{e^2 2m}{\hbar} \frac{2\pi^3}{n^4} \int_0^\infty \frac{|p|^2 dp}{(|p|^2 + m^2)^2}$$

$$= \frac{e^2}{2\pi \hbar} \frac{1}{2|m|}$$

Suppose in a filled band we have a *Dirac point* near which $H$ takes the form in Eqn. 404, and $m$ changes sign. Then the change in Chern number (due to the Dirac point) will be

$$\Delta C = \frac{1}{2} \Delta \left( \frac{m}{|m|} \right)$$

Thus if $m$ changes from positive to negative values, $\Delta C = -1$.

**E. An alternate expression for the Chern number**

When there are just two bands, there is a very appealing way to express the Chern number.

Let the one-body Hamiltonian at any $k$ be written as

$$H = \sigma \cdot \hbar(k)$$

This follows from hermiticity and the freedom to shift the energies of the two bands so that they add up to zero and $H$ becomes traceless.

*Theorem:*

$$C = \frac{1}{4\pi} \int \hbar \cdot (\partial_x \hbar \times \partial_y \hbar) d^2 k$$

$$= \frac{1}{4\pi} \int \varepsilon_{abc} \hat{h}_a \partial_x \hat{h}_b \partial_y \hat{h}_c d^2 k$$

$$\partial_j = \frac{\partial}{\partial k_j} \text{ etc.}$$

*Proof:* Let the occupied band be called $n$, the empty one $m$ and let $l$ run over both. Remember in the ground state

$$\langle n|\sigma|n \rangle = -\hat{h}.$$  \hspace{1cm} (417)

Now,

$$A_x = i\langle n|\partial_x n \rangle \quad A_y = i\langle n|\partial_y n \rangle$$

$$B = i \left[ \langle \partial_x n|\partial_y n \rangle - \langle \partial_y n|\partial_x n \rangle \right]$$

$$= i \sum_l \left[ \langle \partial_x n|l \rangle \langle l|\partial_y n \rangle - \langle \partial_y n|l \rangle \langle l|\partial_x n \rangle \right].$$

The $l = n$ term vanishes (check this). So we may sum over $m \neq n$ and use old results like

$$\langle \partial_x n|m \rangle = \frac{\langle n|\partial_x H|m \rangle}{E_n - E_m} \quad \text{if } m \neq n$$

and

$$(E_m - E_n)^2 = 4\hbar^2,$$

there being just one state with $m \neq n$ with a gap $2\hbar$. We now arrive at

$$B = \frac{i}{4\hbar^2} \sum_{m \neq n} \left[ \langle n|\partial_x H|m \rangle \langle m|\partial_y H|n \rangle - \langle n|\partial_y H|m \rangle \langle m|\partial_x H|n \rangle \right].$$
FIG. 18 Under the map $BZ \rightarrow h$ a patch of sides $dk_x \cdot dk_y$ maps into a parallelogram of area $\frac{1}{h^2} \h \cdot (\partial_x h \times \partial_y h)$. Projecting along $\h$ and dividing by $h^2$ gives $d\Omega$, the solid angle subtended at the origin of $h$ space.

Now we can put back the term with $m = n$ because its contribution vanishes. (Check this!) Then, using completeness,

$$B = \frac{i}{4h^2} \langle n | \partial_x H \partial_y H - \partial_y H \partial_x H | n \rangle. \quad (424)$$

Now we use

$$\partial_x H = \sigma_a \partial_x h_a \quad \partial_y H = \sigma_b \partial_y h_b$$

to arrive at

$$B = \frac{i}{4h^2} \langle n | \partial_x h_a \partial_y h_b (\sigma_a \sigma_b - \sigma_b \sigma_a) | n \rangle \quad (426)$$

$$= \frac{1}{2h^2} \partial_x h_a \partial_y h_b \epsilon_{abc} \langle n | \sigma_c | n \rangle \quad (427)$$

$$= \frac{1}{2h^2} \h \cdot (\partial_x h \times \partial_y h) \quad \text{using} \ \langle n | \sigma_c | n \rangle = -\hat{h}_c. \text{ So} \quad (428)$$

$$C = \frac{1}{2\pi} \int d^2k \ B = \frac{1}{4\pi} \int \frac{\h \cdot (\partial_x h \times \partial_y h)}{h^2} \ dk_x dk_y. \quad (429)$$

We are now going to interpret Eqn. 428 geometrically.

Consider a patch of size $dk_x dk_y$ in the BZ as shown in Figure 18. Under the map $BZ \rightarrow h$ this patch maps into a parallelogram of area $\frac{\h \cdot (\partial_x h \times \partial_y h)}{h^2}$. Projecting the area vector along $\h$ and dividing by $h^2$ gives

$$\frac{1}{h^2} \h \cdot (\partial_x h \times \partial_y h) = d\Omega \quad (430)$$

the solid angle subtended by the patch at the origin of $h$ space. Thus

$$B \ dk_x dk_y = \frac{1}{2} d\Omega. \quad (431)$$

If the totality of patches representing the BZ surround the origin,

$$C = \frac{1}{2\pi} \int B \ dk_x dk_y = \frac{1}{4\pi} \int d\Omega = 1. \quad (432)$$

otherwise $C = 0$. 
FIG. 19 Two possible maps of the BZ to $h$ space: one which encloses the monopole and corresponds to $C = 1$, and one which does not, corresponding to $C = 0$. It is clear from the figure that if $C$ is to change, the monopole has to enter or exit the BZ-torus and that will be a Dirac point.

This same solid angle $d\Omega$ can be measured on the unit sphere if we map $BZ \rightarrow h/h = \hat{h}$. So we may rewrite Eqn. 429 as an integral over the unit sphere $S^2$: $|h| = 1$.

\[
C = \frac{1}{2\pi} \int_{S^2} d^2k B = \frac{1}{4\pi} \int \hat{h} \cdot \left[ \partial_x \hat{h} \times \partial_y \hat{h} \right] dk_x dk_y
\]

which establishes the theorem.

**Exercise VII.4** Starting with $h = h\hat{h}$ show by direct computation that Eqn. 429 leads to Eqn. 433 above.

These result Eqn. 431 has another interpretation. Imagine a monopole of strength $\frac{1}{2}$ at the origin of $h$ space. It creates a radial field

\[
B = \frac{1}{2} \frac{\hat{h}}{h^2}.
\]

The flux intercepted by an area $dS$ is

\[
d\Phi = B \cdot dS = \frac{1}{2} \frac{\hat{h} \cdot dS}{h^2} = \frac{1}{2} d\Omega
\]

Comparing to Eqn. 431 we find that:

The Berry flux piercing a small area in the BZ equals the monopole flux piercing its image in $h$ space under the map $BZ \rightarrow h$.

I depict this situation in Figure 19. It shows a monopole sitting at the origin and two possible maps of the BZ to $h$ space. In one, the monopole is enclosed by the image of the BZ (also depicted as a torus) and $C = 1$, while in the other the monopole lies outside and $C = 0$.

It is clear from the figure that if $C$ is to change, the monopole has to enter or exit the BZ-torus. That point of entry or exit will be a point of degeneracy since $h = 0$ at the location of the monopole.

We may re-express these ideas involving Berry flux into corresponding statements about vector potentials. The Berry potential produces a phase change

\[
d\chi = A(k) \cdot dk
\]

over an infinitesimal line segment $dk$ in the BZ. Under the map $BZ \rightarrow h$ the line segment goes into the line segment $dh$ and the same phase change is produced there by a vector potential $A(h)$:

\[
A(k) \cdot dk = A(h) \cdot dh.
\]

The curl of $A(k)$ is $B$ and the curl of $A(h)$ is $B$, the monopole field.

The line integral of $A(k) \cdot dk$ around a closed loop in the BZ will equal that of $A(h) \cdot dh$ around the image of the loop under the map. (These statements can be made more precise in the language of differential forms.)

**Exercise VII.5** Show that the Chern number of the two bands adds up to zero. Generalize to many bands. (Consider a pair at a time.)
VIII. THE SPINLESS-BERNEVIG-HUGHES-ZHANG (SBZH) MODEL.

The Hamiltonian is

\[
H(k) = \sigma_x \sin k_x + \sigma_y \sin k_y + \sigma_z (\Delta - \cos k_x - \cos k_y) \equiv h \cdot \sigma
\]

\[
E = \pm \sqrt{\Delta^2 + 2(1 - \Delta(\cos k_x + \cos k_y) + \cos k_x \cos k_y)}
\]

Here are the questions we will ask and answer:

- Where does the gap close?
- What is \( C \) as a function of \( \Delta \)?
- How do the Dirac points mediate the change in \( C \)?

**Where does the gap close?**
The gap closes when \( h = 0 \). This means we must kill the sin terms that multiply \( \sigma_x \) and \( \sigma_y \) and then handle the \( \sigma_z \) term. There are four options:

\[
\begin{array}{ccc}
  k_x & k_y & \Delta \\
  0 & 0 & 2 \\
  \pi & \pi & -2 \\
  0 & \pi & 0 \\
  \pi & 0 & 0 \\
\end{array}
\]

**What is \( C \) as a function of \( \Delta \)?**
First consider \( \Delta \gg 2 \). Then \( H \simeq \sigma_z \Delta \quad \forall k \) and the BZ maps into a speck way up the \( h_z \) axis. It does not come close to enclosing the monopole, which sits at \( h = 0 \). Indeed for any \( \Delta > 2 \), we know \( h_z > 0 \) and the image torus cannot wrap around the origin. This region must have \( C = 0 \).

For the same reason \( \Delta < -2 \) also corresponds to \( C = 0 \).

Consider the transition at \( \Delta = 2 \), where \( k \) vanishes. Near this point let

\[
k = 0 + p.
\]

Near the transition, and to first order in \( p \),

\[
H(p) = \sigma_x p_x + \sigma_y p_y + \sigma_z (\Delta - 2) m.
\]

When \( \Delta > 2 \) and \( m = 0^+0 \) the Dirac point contributes (in its immediate neighborhood)

\[
C_{DP} = \frac{1}{2} \frac{m}{|m|} = \frac{1}{2}
\]

Since the band as a whole has \( C = 0 \), the rest of the BZ must contribute

\[
C_{\text{band}} = \frac{1}{2} \frac{m}{|m|} = \frac{1}{2}
\]

When we cross over to \( \Delta < 2 \) or \( m < 0^- \), the Dirac contribution to \( C \) changes by \(-1\) while the band contribution, being smooth stays the same. So we have \( C = -1 \) for \( \Delta < 2 \) till we hit the Dirac point at \( \Delta = 0 \).

Before going to the next transition, I will show you that as \( m \to 0 \), the Dirac point contribution \( C_{DP} \) is essentially a \( \delta \)-function in \( \mathcal{B} \) at the origin.

The lower energy eigenspinor \(|n\rangle\) satisfies

\[
\begin{pmatrix}
  m + E & p_x - ip_y \\
  p_x + ip_y & m - E
\end{pmatrix}
\begin{pmatrix}
  u \\
  v
\end{pmatrix} = 0.
\]

The solution which is regular at the origin as \( m \to 0^+ \) is

\[
|n\rangle = \frac{1}{\sqrt{2E(E + m)}} \begin{pmatrix}
  -p e^{-i\phi} \\
  E + m
\end{pmatrix}.
\]

where \( \phi \) is the angle in the \( p_x - p_y \) plane. You can see that as even though \( e^{-i\phi} \) is ill defined at the origin, it is multiplied by \( p \) and so approaches 0. The normalization factor becomes \( 1/(2m) \) as \( p \to 0 \).
Exercise VIII.1 Show that if \( m \to 0^- \), you should multiply both components by \( e^{i\phi} \) to get a regular solution.

As for the Berry potential,
\[
A_\phi d\phi = i \langle n | \partial_\phi n \rangle d\phi
\]
\[
= \frac{p^2 d\phi}{2E(E + m)}
\]
\[
\simeq \frac{1}{2} \left( 1 - \frac{m}{E} \right) d\phi \quad \text{when} \quad m \to 0.
\]
When integrated over a small circle of radius \( p >> m \), when \( m \to 0 \),
\[
\oint A_\phi d\phi = \pi \left( 1 - \frac{m}{p} \right)
\]
(451)

(Remember \( A_\phi \) is defined such that \( A_\phi d\phi \) is the phase change.) As \( m \to 0 \), the entire contribution of \( \pi \) comes from an arbitrarily small circle surrounding the origin. The Berry flux density \( B \) is therefore a \( \delta \)-function with coefficient \( \pi \). The Chern number is
\[
C = \frac{1}{2\pi} \oint A_\phi d\phi = \frac{1}{2}.
\]
(452)

Of course the full band has to have an integral value for \( C \) and the balance \((-\frac{1}{2} \text{ in this case})\) comes from the non-singular contribution over the rest of the BZ.

We can now jump to the transition at \( \Delta = -2 \) at \((\pi, \pi)\). Denoting by \( p \) the deviation from \((\pi, \pi)\),
\[
H(p) = -\sigma_x p_x - \sigma_y p_y + \sigma_z (\Delta + 2). \quad \text{(453)}
\]

We can reverse the sign of both \( p_x \) and \( p_y \) (or \( k_x \) and \( k_y \)) or \( h_x \) and \( h_y \) in formula Eqn. 429 for \( C_{DP} \), without any effect.

When \( \Delta < -2 \) or \( m < 0 \), the total \( C = 0 \) with \( C_{DP} = -\frac{1}{2} \) and \( C_{\text{band}} = \frac{1}{2} \). When we cross over to \( m > 0 \), \( C = 1 \) due to the jump in \( C_{DP} \).

The situation is depicted in Figure 20.

We finally confront the point \( \Delta = 0 \) where \( C \) changes by 2. Consider first the Dirac point at \((0, \pi)\). Near it
\[
H = p_x \sigma_x - p_y \sigma_y + \Delta \sigma_z.
\]
(454)
If we flip \( k_y \to -k_y \) or \( p_y \to -p_y \) to bring \( H \) to the standard form, we reverse the formula for \( C \):
\[
C_{DP} = -\frac{1}{2} \frac{m}{|m|} \quad \text{(455)}
\]
The same applies to the point \((\pi, 0)\). So when \( \Delta \) goes from positive to negative at the origin, \( C_{DP} \) goes up by +2.
FIG. 21. As we scan the BZ at $\Delta = 0$ as a function of $k_x$ at fixed $k_y$, we get a slice of the torus in $h$ space. As we vary $k_y$ from 0 to $\pi$ the image starts at the page (lower circle), goes into the page and then returns at $k_y = \pi$ after twisting and turning inside out. The points $(0, \pi)$ and $(\pi, 0)$ touch as shown. The orientations of the outward normals are opposite so that when the monopole crosses over it increases the flux entering at both points.

How can the monopole hit two points of the torus at the same time? The answer is that the torus is actually twisted and turned inside out before its ends are glued and at $\Delta = 0$ two points $(0, \pi)$ and $(\pi, 0)$ touch. As the monopole crosses this point, it increases the net flux because the orientation of the surface (for computing the flux with proper sign) is opposite at these points, as shown in Figure 21.

Exercise VIII.2 Start with

$$C = \frac{1}{4\pi h^3} \int d^2k \left( \frac{\partial h_x}{\partial k_x} \frac{\partial h_y}{\partial k_y} - \frac{\partial h_x}{\partial k_y} \frac{\partial h_y}{\partial k_x} \right)$$

where

$$h = (\sin k_x, \sin k_y, \Delta - \cos k_x - \cos k_y)$$

and show that

$$C = \frac{1}{4\pi} \int d^2k \frac{\Delta \cos k_x \cos k_y - \cos k_x - \cos k_y}{(\Delta^2 + 2(1 + \cos k_x \cos k_y - \Delta(\cos k_x + \cos k_y))^{3/2}}.$$

Integrate this numerically and show that

$$C = 0 \quad |\Delta| > 2$$

$$= -1 \quad 0 < \Delta < 2$$

$$= +1 \quad -2 < \Delta < 0.$$

A. Edge states of the SBHZ model

Consider the sample (with negative $x$) terminated by an edge at $x = 0$ separating the $C = -1$ region with $m = \Delta - 2 < 0$ from the $C = 0$ region with $m = \Delta - 2 > 0$. The continuum limit of the Dirac equation for energy is

$$(p_x \sigma_x + p_y \sigma_y + m(x)\sigma_z)\psi(x, y) = E\psi(x, y)$$

$$(m(x) \lim_{|x| \to \infty} = \mp M$$
We may exploit translation invariance in $y$ to choose
\[ \psi(x, y) = e^{i k y} u_k(x). \] (464)

Then we may write
\[ (p_x \sigma_x + k \sigma_y + m(x) \sigma_z) u(x) = Eu(x) \] (465)

Let us first set $k = 0$ and look for a solution at $E = 0$. The equation to solve is
\[ (p_x \sigma_x + m(x) \sigma_z) u(x) = 0. \] (466)

Multiplying by $\sigma_x$ and rearranging we find
\[ \frac{du}{dx} = -m(x) \sigma_y u. \] (467)

With some foresight we choose
\[ \sigma_y u = +u \] (468)

Then Eqn. 467 has a solution
\[ u_k(x) = \exp \left[ - \int_x^0 m(x') dx' \right] |+. \] (469)

You may verify that the exponential falls like a Gaussian in both sides of the interface $x = 0$. (Consider an approximation $m(x) = x$.)

Now go back to Eqn. 465 and restore the $\sigma_y k$. It simply adds to the energy an amount $k$ because of Eqn. 468. Thus

\[ E = k. \] (470)

The group velocity is
\[ v_y = \frac{dE}{dk} = +1 \] (471)

as indicated in the Figure 22.

Notice that the edge carries current only in one direction. It thus differs from a one-dimensional wire in that it supports only half the number of modes as the latter. It is true of all $d$-dimensional topological insulators that their $d-1$-dimensional boundaries support only half as many states as an isolated $d-1$ dimensional system.

When we discuss the Hall effect, we will find that the edge current in the Figure has the opposite direction to what you in the Hall effect at the interface of a $C = -1$ sample and the vacuum. The reason is that the Dirac particle is confined by a mass term $m \sigma_z$ whereas the usual Hall sample is confined by a scalar potential $V$.

Consider the transition which occurs at $\Delta = -2$ when $C = 1$ and $m = \Delta + 2 > 0$ changes to $C = 0, m < 0$ as we cross the interface in the direction of increasing $x$. The situation is depicted in Figure 23. Now we find that
\[ E = -k \] (472)
\[ v = -1 \] (473)

as shown in the figure.
FIG. 23 Localized normalizable zero-energy edge state with indicated velocity \(v_y\) separating \(C = 1\) from \(C = 0\).

FIG. 24 Localized normalizable zero-energy edge states with indicated velocities \(v_y\) separating \(C = 1\) from \(C = -1\). The edges are due to the Dirac points at \((0, \pi)\) and \((\pi, 0)\) which are responsible for the transition at \(\Delta = 0\).

**Exercise VIII.3** Furnish the details leading to the result above. Remember that near \((\pi, \pi)\) the equation to solve is

\[
(-p_x \sigma_x - p_y \sigma_y + m(x) \sigma_z) \psi(x, y) = E \psi(x, y).
\]  

Finally consider the edge states separating \(C = 1\) from \(C = -1\). That is, we have glued a sample with \(m < 0\) to one with \(m > 0\) at \(x = 0\). The function \(m(x)\) rises from negative to positive values, crossing the origin at \(x = 0\). The Dirac points at \((0, \pi)\) and \((\pi, 0)\) each contribute an edge state. We just need to find \(E\) as a function of \(k\) and determine the direction of the edge currents.

The equations are

\[
(p_x \sigma_x - p_y \sigma_y + m(x) \sigma_z) \psi(x, y) = E \psi(x, y) \quad (0, \pi) \\
(-p_x \sigma_x + p_y \sigma_y + m(x) \sigma_z) \psi(x, y) = E \psi(x, y) \quad (\pi, 0)
\]

The profile of \(m(x)\) is the same as in Figure 22 and so is the normalizable solution which must again obey \(\sigma_y u = +u\). This is an eigenfunction also of \(-p_y \sigma_y = -k \sigma_y\) with eigenvalue \(-k\). Thus, for the \((0, \pi)\) Dirac point

\[
E = -k \quad v = -1.
\]

Now consider the case \((\pi, 0)\). This differs from the standard form by reversal of \(x\). The normalizable solution must now have \(\sigma_y = -1\). This is an eigenfunction also of \(p_y \sigma_y = k \sigma_y\) with eigenvalue \(-k\). So once again \(E = -k, v = -1\). Consequently there will be two edge states running down the \(y\)-axis as shown in Figure 24.

**IX. GRAPHENE**

Graphene is the two-dimensional version of graphite. It has the lattice structure shown in Figure 25. The unit cell (enclosed by an oval) has two atoms labeled \(A\) and \(B\). Let hopping be allowed only between nearest neighbors, i.e., members of opposite sublattices. The Hamiltonian is

\[
\mathcal{H} = -t \sum_{<A,B>} c_B^\dagger(r')c_A(r) + h.c.
\]

The coordinates \(r\) and \(r'\) refer to that of the \(A\) atom in that unit cell. The \(B\) atom in each unit cell is assigned the same spatial coordinate as the \(A\) even though it is off by an amount in the vertical direction. That information is contained in our calling it a \(B\) atom.
The basis vectors are $e_1$ and $e_2$ and their length is set to unity. The $A$ atom from which these are measured in the figure will be called the central $A$ atom. We now perform a Fourier transform and obtain

$$H(k) = -t \sum_k \left[ (c_B^\dagger(k)c_A(k))(1 + e^{ik \cdot e_1} + e^{ik \cdot (e_1 - e_2)}) \right] + h.c.$$  

(480)

In matrix notation

$$H(k) = \sum_{i,j=A,B} c_i^\dagger(k) H_{ij} c_j(k)$$  

(481)

$$H_{ij}(k) = -t \begin{pmatrix} 0 & 1 + e^{ik \cdot e_1} + e^{ik \cdot (e_1 - e_2)} \\ 1 + e^{ik \cdot e_1} + e^{ik \cdot (e_1 - e_2)} & 0 \end{pmatrix}$$  

(482)

$$E_\pm = \pm |1 + e^{ik \cdot e_1} + e^{ik \cdot (e_1 - e_2)}|$$  

(483)

The matrix elements need some explanation. Consider all the jumps out of the central $A$ site (at the origin $r = 0$) to its three neighbors. If they are at the cell with coordinate $r'$, the matrix elements in momentum space will be as follows

$$c_B^\dagger c_A e^{ik \cdot (r - r')} = c_B^\dagger c_A e^{ik \cdot (-r')}$$  

(484)

The central atom jumps to its companion in the same cell (at $r' = 0$) or to its neighbors in the southeast and southwest in cell located at $r' = -e_1 + e_2$ and $r' = -e_1$ respectively. The corresponding $e^{-ik \cdot r'}$ appear in the second row first column. The conjugates appears in the transposed location.

From Eqn 482 we see the problem has TRS with $\Theta = K$:

$$KH(k)K = H(-k).$$  

(485)

We need to find the zero’s of $E$ to locate the Dirac points. We want three unimodular numbers to add to zero. As one of them is +1, the other two must be complex conjugates and add up to -1. They must be at angles $2\pi/3$ and $4\pi/3$.

Here are the relevant equations for finding $K$ and $K'$ the two Dirac points. (All others we find will differ by a reciprocal lattice vector and thus equivalent.)

$$e_1 = \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \quad e_2 = (1, 0)$$  

(486)

$$k \cdot e_1 = \frac{4\pi}{3} \quad k \cdot (e_1 - e_2) = \frac{2\pi}{3} \quad \text{K point}$$  

(487)

$$K = \left( \frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}} \right) \quad \text{K point}$$  

(488)

FIG. 25 The graphene lattice. The basis vectors are $e_1$ and $e_2$ and their length is set to 1. The unit cell (marked by an oval) has two atoms labeled $A$ and $B$. 
\[ k \cdot e_1 = \frac{2\pi}{3} \quad k \cdot (e_1 - e_2) = \frac{4\pi}{3} \quad \text{K' point} \quad (489) \]

\[ K' = \left( -\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}} \right) \quad (490) \]

**Exercise IX.1** Provide the steps leading to the determination of \( K \) and \( K' \).

### A. The BZ

This is a two-step process.

- Find the reciprocal lattice vectors \( \mathbf{G}_1 \) and \( \mathbf{G}_2 \) such that
  \[ \mathbf{G}_i \cdot e_j = 2\pi \delta_{ij} \quad (491) \]

- Find the unit cell by drawing perpendicular bisectors of reciprocal lattice vectors.

The reciprocal vectors are given by

\[ \mathbf{G}_1 = 2\pi \frac{e_2 \times \hat{z}}{\hat{z} \cdot (e_1 \times e_2)} = \left( 0, \frac{4\pi}{\sqrt{3}} \right) \quad (492) \]

\[ \mathbf{G}_2 = 2\pi \frac{\hat{z} \times e_1}{\hat{z} \cdot (e_1 \times e_2)} = \left( 2\pi, -\frac{2\pi}{\sqrt{3}} \right) \quad (493) \]

As for the perpendicular bisectors, the one for \( \mathbf{G}_1 \), which is purely along the \( y \)-direction is just a horizontal line passing through \((0, \frac{2\pi}{\sqrt{3}})\).

Next consider

\[ \mathbf{G}_1 + \mathbf{G}_2 = 2\pi \left( 1, \frac{1}{\sqrt{3}} \right) \quad (494) \]

The equation of the perpendicular bisector is

\[ y = -\sqrt{3}x + \frac{4\pi}{\sqrt{3}} \quad (495) \]

and it cuts the bisector of \( \mathbf{G}_1 \) at

\[ \left( \frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}} \right) = \mathbf{K}. \quad (496) \]

Thus one Dirac point lies at a corner of the BZ. The bisector of \( \mathbf{G}_2 \) cuts bisector of \( \mathbf{G}_1 + \mathbf{G}_2 \) at \((\frac{4\pi}{3}, 0)\). The rest of the BZ may be deduced by symmetry. It too is hexagonal and the \( K' \) Dirac point lies at the corner obtained by reflecting \( K \) on the \( y \)-axis as shown in figure 26.

**Exercise IX.2** Derive the coordinates of the corners of the BZ.

For a square lattice the BZ has area \((2\pi)^2\). The unit cell in real space has unit area (upon setting the lattice constant \( a = 1 \)). So we have the result

\[ \text{Area of cell in real space} \times \text{Area of BZ} = 4\pi^2. \quad (497) \]

This is also true in the graphene problem.

**Exercise IX.3** Verify Eqn. 497.
B. Dirac points of graphene

Let us consider $H_{ab}$ near $K$. Writing

$$k = K + p$$

and expanding to first order in $p$ we find

$$\frac{H_{ba}}{-t} = 1 + e^{i(K+p) \cdot e_1} + e^{i(K+p) \cdot (e_1-e_2)}$$

$$= 1 + e^{iK \cdot e_1} (1 + i p \cdot e_1) + e^{i(K-e_2)(1 + i p \cdot (e_1 - e_2))} \text{to order } p$$

$$= \frac{\sqrt{3}}{2} (p_x - i p_y).$$

Exercise IX.4 Furnish the steps between the last two equations.

This means

$$H(K + p) = -t\frac{\sqrt{3}}{2} (\sigma_x p_x - \sigma_y p_y).$$

If we repeat the calculation at $K'$ we find

$$H(K' + p) = -t\frac{\sqrt{3}}{2} (-\sigma_x p_x - \sigma_y p_y).$$

The Chern densities are not defined for this gapless system. To produce a gap we need to add

$$\Delta H = m \sum_n (c_{An}^\dagger c_{An} - c_{Bn}^\dagger c_{Bn}) = m \sum_n \sigma_z(n)$$

which in turn will add an $m\sigma_z$ term to the Dirac Hamiltonian. This term denotes a chemical potential that alternates with the sub-lattice. The model still has TRS with $\Theta = K$. However it does not have inversion symmetry, or symmetry under reflection with respect to the horizontal line that bisects the bond joining $A$ and $B$ sites of a unit cell. If we call this operation $\mathcal{I}$, with

$$\mathcal{I} = \sigma_x, \text{ we want}$$

$$\mathcal{I}H(k_x, k_y)\mathcal{I}^{-1} = H(-k_x, -k_y)$$

This is true true without the $\sigma_z$ term but not with it. If we open a gap using a non-zero $m$, $C$ is defined and the two Dirac points contribute oppositely to it because they have opposite coefficients of $\sigma_x p_x$. This had to be so because of TRS of the Graphene Hamiltonian (Eqn. 482:)

$$\Theta H(k)\Theta^{-1} = H(-k)$$

where $\Theta$, is the complex conjugation operator, which I do not want to refer to as $K$ for obvious reasons.
X. QUANTUM HALL STATE AS A TOPOLOGICAL INSULATOR

This is the most studied example of a TI. I will limit myself to introducing the Integer Quantum Hall problem, focusing on how $\sigma_{xy}$ is computed. The Hamiltonian is

$$H = \frac{P_x^2}{2m} + \frac{(P_y - eB_0x)^2}{2m}$$

where

$$A = B_0(0, x) \quad \text{Landau gauge}$$

$$B = zB_0$$

We choose the Landau gauge because $P_y$ is conserved. Consequently

$$\psi_k(x, y) = e^{iky} u(x)$$

$$\left[ \frac{P_x^2}{2m} + \frac{(\hbar - eB_0x)^2}{2m} \right] u_n(x) = E_n$$

$$\left[ \frac{P_x^2}{2m} + \frac{e^2B_0^2(x - kl)^2}{2m} \right] u_n(x) = E_n \quad \text{where}$$

$$l^2 = \frac{\hbar}{eB_0}$$

is the square of the magnetic length.

This is just a harmonic oscillator at the cyclotron frequency

$$\omega_0 = \sqrt{\frac{\omega}{m'}} = \sqrt{\frac{\hbar^2}{m'^2l^4}} = \frac{eB}{m}$$

centered at

$$x_0 = kl^2.$$ 

In the Lowest Landau Level (LLL) which we shall focus on, we have $n = 0$ and the solution is

$$\psi = e^{iky} \phi_0(x - kl^2)$$

where $\phi_0$ is the familiar Gaussian.

You should visualize the wave functions as strips along $y$ of width $\simeq l$ centered at $x_0$. There is a large degeneracy because $E$ is independent of $k$. Let us compute this for an $L_x \times L_y$ sample where the $y$ direction is periodic i.e., $y = 0$ and $y = L_y$ are joined.

The allowed momenta are

$$k_y = \frac{2\pi m}{L_y} \quad m = 1, 2, \ldots$$

The largest allowed value for $m$ is determined by the sample width $L_y$. Since the solution is centered at $x = kl^2$ and $x \leq L_x$ we demand that $M$, the largest value of $m$, satisfies

$$\frac{2\pi M}{L_y} l^2 = L_x$$

$$M = \frac{L_x L_y}{2\pi l^2} = \frac{L_x L_y eB_0}{2\pi \hbar} = \frac{\Phi}{\Phi_0}$$

which states that the degeneracy of the LLL (or any LL) is the flux penetrating the sample in units of the flux quantum.

A. Hall conductance computation

Following Laughlin we roll up the system into a cylinder of circumference $L_y$ in the $y$-direction. Now we thread some flux along the axis of the cylinder as shown in Figure 27. We choose a vector potential
Finite sample with a normal magnetic field rolled up into a cylinder threaded by axial flux

FIG. 27 A finite sample rolled up into a cylinder and threaded by a flux that grows from 0 to $\Phi_0$ adiabatically. At the end one particle of charge $e$ is transported from one end to the other. Relating the integral of the current to $e$ and the changing $A_y$ to an electric field along $y$ one finds $\sigma_{xy} = e^2/2\pi\hbar$.

\[ A_y = \frac{2\pi\hbar}{eL_y}\lambda \]  

(520)

where $\lambda$ is a parameter that will be slowly raised from $\lambda = 0$ to $\lambda = 1$. The flux along the cylinder follows from Stokes's theorem:

\[ \Phi = \oint A_y dy = A_y L_y = -\frac{2\pi\hbar}{e\lambda} = -\Phi_0\lambda. \]  

(521)

At some intermediate value of $\lambda$

\[ H = \frac{p_x^2}{2m} + \left(\hbar k - eB_0x + \frac{2\pi\hbar\lambda}{L_y}\right). \]  

(522)

When $\lambda$ rises from 0 to 1,

\[ k = \frac{2\pi m}{L_y} \rightarrow \frac{2\pi (m + 1)}{L_y} \]  

(523)

The particles follow the states they are in (in the adiabatic limit) and at the end of the process, the particles have moved over by one strip: the leftmost is empty and there is an extra particle at the right end. Thus charge $e$ has been transported from one end of the sample to the other. From this we can deduce the Hall conductance as follows. When $A_y$ grows there is an electric field

\[ E_y = -\frac{\partial A_y}{\partial t} = -\frac{\partial A_y}{\partial \lambda} \frac{d\lambda}{dt} = \frac{2\pi\hbar}{eL_y} \frac{d\lambda}{dt}. \]  

(524)

If $\sigma_{xy}$ is the Hall conductance, it will produce a current density

\[ j_x = \sigma_{xy} E_y \quad \text{and a current} \]

\[ I_x = \sigma_{xy} E_y L_y = \sigma_{xy} \frac{2\pi\hbar}{e} \frac{d\lambda}{dt}. \]  

(525)

(526)

Since the time-integral of $I_x$ is $e$, the charge transported across the sample, we may write

\[ e = \int I(x) dt = \sigma_{xy} \int_0^1 \frac{2\pi\hbar}{e} \frac{d\lambda}{e} = \sigma_{xy} \frac{2\pi\hbar}{e} \]  

(527)

which leads to

\[ \sigma_{xy} = \frac{e^2}{2\pi\hbar}. \]  

(528)
B. Hall conductance: another look

If you take a wire with just one conducting channel it will have the conductance \( \sigma_{xy} = \frac{e^2}{2\pi h} \). How can a sheet have the same conductance? This is what we want to understand now by computing the Hall current when a voltage is applied.

Consider any one strip with the wave function peaked at \( x_0(k) = kl^2 \). By applying a tiny \( A \) and taking the derivative at \( A = 0 \), we find

\[
\dot{j}_y = -\frac{\partial H}{\partial (eA_y)} = \frac{\hbar k - eB_0 x}{m} \simeq (x - x_0(k)) \quad \text{(Eqn. 515.) (529)}
\]

The current density changes sign as we cross the strip. The oppositely moving currents from two adjacent strips cancel and we are left with just the two uncancelled edge currents. Thus all the action (conduction) is at the boundary in the Hall state. If there is no voltage across the sample, these edge currents will be equal and opposite. Let us see what happens when a bias is applied.

Suppose we apply a tiny potential difference \( \Delta V = V_R - V_L \) between the two edges. The Landau level which used to be flat now get a little tilt. Starting with

\[
\langle v \rangle = \langle \frac{dE}{\hbar dk} \rangle \quad \text{(530)}
\]

we find the current due to the wave function at each \( k \):

\[
I_y(k) = \frac{e}{\hbar} \int |\psi_k(x)|^2 \frac{dE}{dk} dx \quad \text{(531)}
\]

In the presence of the potential \( V(x) = V(kl^2) \), \( \frac{dE}{dk} \) acquires a non-cancelling part \( e \frac{dV}{dk} \). Continuing,

\[
\psi_k(x) = \frac{1}{\sqrt{L_y}} e^{iky} u_k(x) \quad \text{(532)}
\]

so that

\[
I_y(k) = \frac{e}{\hbar L_y} \frac{dE}{dk} \quad \text{using } \int |\psi_k(x)|^2 dx = \frac{1}{L_y} \quad \text{(533)}
\]

assuming \( dE/dk \) is constant over the narrow Gaussian wavefunction.

The contributions from all \( k \) values is obtained by integrating with a measure \( \frac{L}{2\pi} dk \):

\[
I_y = \int \frac{dk}{2\pi} I_y(k) \quad \text{(534)}
\]

\[
= \frac{e}{2\pi \hbar} (E(R) - E(L)) = \frac{e^2 \Delta V}{2\pi \hbar} \quad \text{(535)}
\]

\[
\sigma_{xy} = \frac{I_y}{\Delta V} = \frac{e^2}{2\pi \hbar} \quad \text{(536)}
\]

C. Chern number of the LLL

We know \( C = 1 \) from \( \sigma_{xy} \). However we cannot readily compute it because we do not have wavefunctions \( u(k) \) in a BZ. In the Landau gauge \( k_y \equiv k \) is a good quantum number but there is no \( k_x \). The states are localized in \( x \) near \( x = kl^2 \).

The problem with finding \( k \) states is that the translation group acts differently here because of this fact: even if \( B \) is uniform \( A \) is not. For example \( A_y \propto x \) in the Landau gauge where

\[
H = \frac{P_x^2}{2m} + \frac{(P_y - eB_0 x)^2}{2m} \quad \text{(537)}
\]

Whereas translation of \( a \) along \( y \) implemented by

\[
T_y(a) = e^{a \partial_y} \quad \text{(538)}
\]
is a symmetry of $H$ because it has no $y$-dependence, a translation in $x$ by $a$ (in this gauge) has to be accompanied by a ($y$-dependent) gauge transformation that compensates for the change in $A_y$.

Here is a $T_x(a)$ that does the job:

$$T_x(a) = \exp[a\partial_x]\exp[-\frac{i\alpha B_0 y}{\hbar}]$$  

$$T_x(a)H(x, y)T_x^\dagger(a) = H(x, y).$$

(539)

(540)

This means that in general $[T_x, T_y] \neq 0$. Instead

$$T_y T_x T_y^{-1} T_x^{-1} = \exp\left[\frac{2\pi i}{\Phi_0} \frac{\Phi}{\Phi_0}\right]$$

(541)

where $\Phi = a^2 B_0$ is the flux enclosed in the square cell of side $a$. This flux has to be an integral multiple of $\Phi_0$ for the two translations to commute and for us to define $k$ as their simultaneous eigenvalue. In the simplest case this multiple is 1.

**Exercise X.1** Verify that $T_x(a)H(x, y)T_x^\dagger(a) = H(x, y)$. Then fill in the steps leading to Eqn. 541. (Hint: $e^A e^B = e^{A+B} e^{[A,B]}$ if the commutator is a $c$-number.)

So we take the planar sample in the continuum and divide it into unit cells, which are squares of size $a^2$ such that

$$B_0 a^2 = \Phi_0 \quad \text{or} \quad a^2 = 2\pi l^2.$$  

(542)

Consider now a rectangle of width $a$ and height $L_y = Na$ with its left edge at $x = 0$. It can be shown that it contains $L_y/a$ strip states with momenta

$$k_y = \frac{2\pi m}{L_y} \quad m = 1, \ldots N = (L_y/a)$$

(543)

**Exercise X.2** Show this.

Pick a strip state at some $k$ (or at $x = kl^2$) in the chosen rectangle and form superpositions with its counterparts at the same location in the rectangles $ja$ away with phase factor $\exp[i k_x ja]$.

**Exercise X.3** Show (ignoring normalization) the states obtained by the prescription above are

$$\psi_{k_x, k_y}(x, y) = \sum_j \exp[i y(k_y + ja/l^2)] \exp[i k_x ja] \phi_0(x - k_y l^2 - ja).$$

(544)

Confirm that they respond to $T_x(a)$ and $T_y(a)$ as they should. Remember $a^2 = 2\pi l^2$ if there is one flux quantum per unit cell.

Both $k_x$ and $k_y$ will lie within a BZ of sides $2\pi/a$. It is in this BZ that one must compute the Berry flux and from it the Chern number. The fact that $C \neq 0$ happens to imply that one cannot find Bloch functions $u(k)$ defined in all of the BZ; instead we will need at least two patches, exactly as in the monopole problem and for the same reason. At the end we will find $C = 1$.

**XI. TIME-REVERSAL SYMMETRIC (TRS) MODELS**

So far we have considered topological insulators which violate TR. A non-zero Chern number is possible only if TR is violated. Now we consider two models which respect TR and yet are topologically distinct from trivial insulators. They also have gapless modes at the edge. They involve spin in an essential way.
A. BHZ model

Consider the following Hamiltonian:

\[ H = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix} \] \hspace{1cm} (545)

where

\[ h(k) = \sigma_x \sin k_x + \sigma_y \sin k_y + \sigma_z (\Delta - \cos k_x - \cos k_y). \] \hspace{1cm} (546)

We define \( \tau \) matrices acting on the \( 2 \times 2 \) blocks

\[ \tau_y = \begin{pmatrix} 0 & -iI \\ iI & 0 \end{pmatrix} \quad \tau_z = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \] \hspace{1cm} (547)

where \( I \) is the \( 2 \times 2 \) identity in \( \sigma \) space. Let us note that

\[ h(k) = \sigma_x \sin k_x + \sigma_y \sin k_y + \sigma_z (\Delta - \cos k_x - \cos k_y) \] \hspace{1cm} (548)

and

\[ h^*(-k) = -\sigma_x \sin k_x + \sigma_y \sin k_y + \sigma_z (\Delta - \cos k_x - \cos k_y) \] \hspace{1cm} (549)

This means

\[ H = (\sigma_y \sin k_y + \sigma_z (\Delta - \cos k_x - \cos k_y) \otimes I + \sigma_x \otimes \tau_z \sin k_x. \] \hspace{1cm} (550)

This problem has charge conjugation symmetry

\[ CH(k)C^{-1} = -H(k) \] \hspace{1cm} (551)

where \( C = i\sigma_y \cdot K \) \hspace{1cm} (552)

and TR symmetry

\[ \Theta H(k)\Theta^{-1} = H(-k) \] \hspace{1cm} (553)

where \( \Theta = i\tau_y \cdot K. \) \hspace{1cm} (554)

We also have Kramers’ degeneracy because

\[ \Theta^2 = -1. \] \hspace{1cm} (555)

Exercise XI.1 Verify these two symmetries.

TRS implies that if

\[ H(k)|u_k\rangle = E(k)|u_k\rangle \] \hspace{1cm} (556)

then

\[ H(-k)|\Theta u_k\rangle = E(k)|\Theta u_k\rangle. \] \hspace{1cm} (557)

Thus every energy eigenket \( |u_k\rangle \) has a degenerate Kramers partner \( |\Theta u_k\rangle \). The situation is summarized in Figure 28.

B. Edge states of the BHZ model

We can look at edges of

\[ H = (\sigma_y \sin k_y + \sigma_z (\Delta - \cos k_x - \cos k_y) \otimes I + \sigma_x \otimes \tau_z \sin k_x \] \hspace{1cm} (558)

in the sectors with \( \tau_z = \pm 1 \). If we are to use the continuum Dirac theory we have to be near a gapless state. Let us stay near the transition at \( \Delta = 2, k = (0,0) \) and \( m = \Delta - 2 \). The system goes from a \( C = -1 \) state to the vacuum with \( C = 0 \) as we increase \( x \).

I ask you to verify that when \( \tau_z = +1 \),

\[ |u_+(k)\rangle = \exp \left[-\int_0^x m(x')dx'\right] e^{iky} \chi_+ \] \hspace{1cm} (559)

where

\[ \sigma_y \chi_+ = +\chi_+ \] \hspace{1cm} (560)

\[ E(k) = k \] \hspace{1cm} (561)
FIG. 28 The effect of charge conjugation (C) and time-reversal Θ on energy eigenstates. States of opposite energy at the same \( k \) are related by C and states at same energy and opposite \( k \) are Kramers’ pairs related by Θ.

and that when \( \tau_z = -1 \),

\[
|u_-(k)\rangle = \exp \left[ -\int_{0}^{x} m(x') dx' \right] e^{iky} \chi_- \quad \text{where}
\]

\[
\sigma_y \chi_- = -\chi_-
\]

\[
E(k) = -k.
\]

Exercise XI.2 Provide the proof of the above claims.

Notice that the spectrum has the features of Figure 28: at each \( k \) there are states of opposite energy and at each \( E \) there are states of opposite \( k \).

Exercise XI.3 Show by explicit computation that \( \Theta|u_k\rangle \) with \( E = k \) is the eigenstate of \( H(-k) \) with same energy.

XII. KANE-MELE MODEL

This is a celebrated example of a TI with TRS. The idea is to include spin in a TRS manner, say by using the spin-orbit interaction.

Let me first write down the model and then describe the origin of the various terms.

\[
H = t \sum_{\langle ij \rangle} c_i^\dagger c_j + i\lambda_{\text{so}} \sum_{\langle ii \rangle} c_i^\dagger \nu_{ij} c_j s_z + i\lambda_R \sum_{\langle ij \rangle} c_i^\dagger (s \times \hat{d}_{ij})_z c_j + \lambda_v \sum_{i} c_i^\dagger c_i \sigma_z
\]  

(565)

Look at the honeycomb lattice in Figure 29. The first term is the usual nearest-neighbor hopping between \( A \) and \( B \) sublattices with hopping amplitude \( t \).

The second describes spin orbit coupling with strength \( \lambda_{\text{so}} \). Here the particle goes from the central site shown by boldface \( A \) to the 6 second-neighbor \( A \) sites numbered \( A_1 \ldots A_6 \). The orbital angular momentum (along the \( z \)-axis which is normal to the plane of the lattice) has a sign depending whether the particle swings clockwise or anticlockwise. Moving with the particle we assign a + sign to a left turn and a - sign to a right turn. For example the journey \( A \rightarrow A_2 \) comes with a + sign. The physical spin \( s_z \) couples to this angular momentum \( L_z \).

The Rashba coupling \( \lambda_R \) describes the interaction of the spin with the surface electric field \( E \) normal to the plane. A particle with velocity \( v \) will see a magnetic field \( B = v \times E \) in its rest frame and couple with a Zeeman term

\[
s \cdot B = s \cdot (v \times E) = E \cdot (s \times v) \propto \hat{z} \cdot (s \times v).
\]

(566)

We represent the particle velocity \( v \) with \( \hat{d}_{ij} \) which is unit vector separating the nearest neighbors. The coupling \( \lambda_v \) is an alternating on-site potential with opposite signs on the two sub-lattices.
FIG. 29 The spin-orbit interaction couples $s_z$ to the orbital angular momentum whose sign depends whether the particle turns clockwise or anticlockwise at the neighboring site as it goes to its second neighbor. For example the journey $A \rightarrow A_2$ comes with a $+$ sign.

Here is the final answer with details left as an exercise.

$$H(k) = t(\sigma_x(1 + 2 \cos x \cos y) + 2\sigma_y \sin y \cos x) + 2\lambda_{so}(\sin 2x - 2 \sin x \cos y)\sigma_z s_z + \lambda_v \sigma_z$$

$$+ \lambda_R(\sigma_x s_x \cos x \sin y - \sqrt{3}\sigma_x s_y \sin x \cos y + \sigma_y s_x (1 - \cos x \cos y) - \sqrt{3}\sigma_y s_y \sin x \sin y).$$

(567)

In the above

$$x = \frac{1}{2}k_x \quad y = \frac{\sqrt{3}}{2}k_y.$$ 

(568)

Exerci\textcolor{red}{s}e XII.1 Derive Eqn. 567.

All these terms are invariant under TR. We expect this because spin and velocity change sign under TR and their product is invariant. You may verify that

$$\Theta = is_y K$$

(569)

does the job.

Exerci\textcolor{red}{s}e XII.2 Verify that

$$\Theta H(k)\Theta^{-1} = H(-k).$$

(570)

A. Dirac points of the KM model

We are going to handle this in the limited case of $\lambda_R = 0$ which is subject to analysis very similar to what we have encountered. In this case

$$H(k) = t(\sigma_x(1 + 2 \cos x \cos y) + 2\sigma_y \sin y \cos x) + 2\lambda_{so}(\sin 2x - 2 \sin x \cos y)\sigma_z s_z + \lambda_v \sigma_z$$

(571)

We are free to work with $s_z = +1$ since it is diagonal. We will also set $t = 1$.

To get $E = 0$ we need

$$0 = 1 + 2 \cos x \cos y$$

(572)

$$0 = \cos x \sin y$$

(573)

$$0 = 2\lambda_{so}(\sin 2x - 2 \sin x \cos y) + \lambda_v$$

(574)
We can kill the middle term in two ways. If we kill $\cos x$, the first condition cannot be satisfied by any $y$. So we kill the $\sin y$:

$$y = 0, \pi.$$  \hfill (575)

Here is the first option.

$$y = 0$$ \hfill (576)
$$1 + 2 \cos x = 0 \rightarrow x = \frac{2\pi}{3}$$ \hfill (577)
$$2\lambda_{so}(\sin 2x - 2 \sin x \cos y) + \lambda_v = 0 \rightarrow \frac{\lambda_v}{\lambda_{so}} = 3\sqrt{3}$$ \hfill (578)

We could also choose $(x = \frac{4\pi}{3}, y = 0)$, but the results will coincide with the option considered below.

$$y = \pi$$ \hfill (579)
$$1 - 2 \cos x = 0 \rightarrow x = \frac{\pi}{3}$$ \hfill (580)
$$2\lambda_{so}(\sin 2x - 2 \sin x \cos y) + \lambda_v = 0 \rightarrow \frac{\lambda_v}{\lambda_{so}} = -3\sqrt{3}$$ \hfill (581)

These two Dirac points $\frac{\lambda_v}{\lambda_{so}} = \pm 3\sqrt{3}$ are the boundaries of the non-trivial phase.

Remember we had chosen $s_z = +1$. If we repeat with $s_z = -1$ we will find the Dirac points get exchanged.

If we turn on $\lambda_R$, there will be a two-dimensional region of the non-trivial phase in the $\lambda_R/\lambda_{so}$ versus $\lambda_v/\lambda_{so}$ plane bounded by $\frac{\lambda_v}{\lambda_{so}} = \pm 3\sqrt{3}$ when $\lambda_R = 0$.

**B. Edge states of the KM model when $\lambda_R = 0$**

Start with

$$H = (\sigma_x(1 + 2 \cos x \cos y) + 2\sigma_y \sin y \cos x$$
$$+ 2\lambda_{so}(\sin 2x - 2 \sin x \cos y)\sigma_z s_z + \lambda_v \sigma_z)$$ \hfill (582)

and choose $s_z = +1$. Near the Dirac point

$$x = \frac{2\pi}{3} + \frac{p_x}{2}, \quad y = 0 + \frac{\sqrt{3}}{2} p_y.$$ \hfill (583)

The factors of $\frac{1}{2}$ and $\frac{\sqrt{3}}{2}$ appear in $p_x$ and $p_y$ because of the definitions in Eqn. 568:

$$x = \frac{1}{2} k_x, \quad y = \frac{\sqrt{3}}{2} k_y$$ \hfill (584)
$$\delta x = \frac{1}{2} \delta k_x = \frac{1}{2} p_x, \quad \delta y = \frac{\sqrt{3}}{2} \delta k_y = \frac{\sqrt{3}}{2} p_y$$ \hfill (585)

We have to first order in $p$,

$$H = \left[ \frac{\sqrt{3}}{2} (\sigma_x p_x + \sigma_y p_y) + \sigma_z (\lambda_v - 3\sqrt{3}\lambda_{so}) \right].$$ \hfill (586)

**Exercise XII.3** Derive the $H$ above.

Let is introduce an $x$-dependent mass term

$$m(x) = \frac{2}{\sqrt{3}} \left[ \lambda_v(x) - 3\sqrt{3}\lambda_{so} \right].$$ \hfill (587)
which goes from very negative values (nontrivial insulator) to very positive (trivial insulator) and changes sign at $x = 0$.

If we let $p_y = 0$ in $\psi(x) = e^{iky}u(x)$, we find by quadrature

$$u(x) = u(0) \exp \left[ - \int_0^x m(x')dx' \right] |+\rangle \quad \text{where } \sigma_y|+\rangle = |+\rangle. \quad (588)$$

This solution is normalizable because we chose $\sigma_y u = u$. Putting back the $\sigma_y p_y$ term we find,

$$E = \frac{\sqrt{3}}{2} p_y \quad v = \frac{\sqrt{3}}{2} \quad (589)$$

Thus this edge has $s_z = +1$ and runs up the interface at $x = 0$.

The solution with $s_z = -1$ leads to

$$H = \left[ \frac{\sqrt{3}}{2} (-\sigma_x p_x + \sigma_y p_y) + \sigma_z (\lambda v - 3\sqrt{3}\lambda_{so}) \right]. \quad (590)$$

and the edge state which runs down the interface is the time-reversed partner of the $s_z = +1$ state.

**Exercise XII.4** Verify both solutions at $s_z = \pm 1$.

### C. $Z_2$ nature of edge states

Let the edge run long $y$ so that $k_y = k$ is a good quantum number. Let us consider a hybrid version in which $x$ remains $x$ and $y$ gets Fourier transformed to $k_y = k$. Since $x$ is invariant under time-reversal, we have

$$\Theta H(x,k)\Theta^{-1} = H(x,-k). \quad (591)$$

Consider the points $k_y = 0, \pi$. Since these are their own negatives,

$$\Theta H(k)\Theta^{-1} = H(k). \quad (592)$$

So $\Theta$ is a symmetry and we must have Kramers’ pairs. Consider the edge states as a function of $k$ as we go from $-\pi$ to $\pi$ as shown in Figure 30. Each of these TRS points must have a doublet that splits up as we move away. How do these lines join with their TR counterparts?

I show in Figure 30 two simple cases that illustrate the choices.

In the option on the left we encounter just one Kramers pair ($A_1$ and $A_2$) and they cannot mix due to TRS and they will remain gapless. Think of a $2 \times 2$ matrix with equal diagonal matrix element to which we add an off-diagonal term from scattering. This opens up a gap unless symmetry forbids this element, which is the case here. We cannot find an energy where there is no edge states. This is the non-trivial insulator.

Why can’t $A_1 = |u_1\rangle$ scatter off its Kramers partner $A_2 = |u_2\rangle$? Let $V = \Theta^{-1}V\Theta$ be the TRS scattering amplitude. Then

$$\langle u|V|\Theta u \rangle = \langle V u|\Theta u \rangle = \langle \Theta^2 u|\Theta V u \rangle \quad \text{using } \langle \phi|\psi \rangle = \langle \Theta \psi|\Theta \phi \rangle = (-1)\langle u|\Theta V u \rangle = (-1)\langle u|V|\Theta u \rangle. \quad (593)$$

In other option option, on the right half, a slice at some energy encounters no mid-gap states or two Kramers pairs. Suppose there are two pairs. State $A_1$ can scatter off $B_2$ from the other pair and a gap can open up. So again there can be energies at which we encounter no states. This is in the same family as the trivial insulator which has no states in the gap.

The number of Kramers states modulo 2 is the topological invariant. The sector with even numbers is the trivial one since a band insulator, which has no states in the gap is trivial.
FIG. 30 At $k = 0, \pi$, we have $H(-k) = H(k)$, so that the levels must come in degenerate pairs. The trivial (right) and non-trivial (left) cases are differentiated by how the lines join up as they connect the TRS points. In the non-trivial case one cannot make a slice at any energy without encountering an odd number (= 1 in the figure) of Kramers pairs in the band gap. These are protected by TRS from gapping out upon scattering from any TRS impurity. In the trivial case a slice will meet an even number (= 0 or 2) of Kramers pairs which could pair with the oppositely moving member from the other pair and gap out.

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