NOTES ON TOPOLOGICAL INSULATORS

ALEXANDER B. WATSON

ABSTRACT. The experimental observation and subsequent theoretical investigation of the quantum Hall effect showed that a surprising connection exists between the physics of materials and topology. Specifically, it was found that under appropriate conditions part of the conductivity (roughly, the response of electrons in the material to an applied electric field) of certain two-dimensional materials is exactly proportional to an integer. This integer was later understood as the Chern number of a certain fiber bundle associated with the atomic structure of the material. These notes are an attempt to explain, starting from basic electromagnetism and quantum mechanics, how this correspondence arises.

1. MOTIVATION: DISAGREEMENT BETWEEN CLASSICAL AND QUANTUM HALL EFFECTS

In these notes we will be interested in certain phenomena arising in material science (a subfield of condensed matter physics), which is the branch of physics dedicated to understanding the properties of materials.

The fundamental laws of material science have been well-established since the early days of quantum mechanics. A material is nothing but a collection of a (huge) number of atoms, each of which typically splits into a positively-charged atomic core consisting of the atomic nucleus along with a number of tightly-bound electrons, and the left over negatively-charged valence electrons which are only weakly bound to the atomic nucleus. Each of these particles must be treated quantum mechanically, and hence the evolution of the system is governed by a (huge) coupled system of non-relativistic Schrödinger equations modeling the electromagnetic forces between each pair of particles. In principle, any property of interest (electrical and thermal conductivity, mechanical properties etc.) of any material is computable by solving this system of equations.

Unfortunately, this system is extremely difficult to solve: it is posed on a Hilbert space of extremely high dimension (the tensor product of the Hilbert spaces of every individual core and electron), and the evolution extremely complicated: in principle every particle in the system interacts with every other particle through electromagnetic forces. This is not to mention Fermionic statistics (in particular, the Pauli exclusion principle) which must also be taken into account. One is therefore generally interested in deriving and studying *reduced models* of materials which capture essential information about the system well enough to predict material properties. Such models have been successful in explaining many diverse phenomena arising in material science.

In these notes we will concentrate on simplified descriptions of *electron transport* in certain kinds of materials which generally predict the electrical conductivity of such materials well. This description is sufficient to understand the main subject of these notes, which is how the electrical conductivity of certain materials (known as "topological insulators") can be linked with topological invariants. We make the following assumptions:

(1) Each atomic core of the material becomes fixed in place by forming strong bonds with its neighbors by sharing some of its valence electrons. The resulting arrangement of atomic cores and shared electrons is perfectly periodic with respect to some lattice.

Materials satisfying this assumption are known as as crystals, and the structure they form is known as the crystal structure. Crystals are common in nature, since periodic arrangements of atomic cores generally serve to minimize total electromagnetic energy of the material.

(2) Any valence electrons which are left over, i.e. which are not used up forming bonds, are free to roam around the material.

These electrons are known as free electrons.

(3) Interactions between free electrons, other than through the Pauli exclusion principle, are weak enough to be neglected. This is known as the independent electron approximation.

In these notes we will restrict attention to *one and two dimensional* materials whose crystal structure and free electrons are confined to a line or plane, respectively, although the phenomena we discuss do not only occur in such materials.

To motivate what follows, we describe the experimental observation of the quantum Hall effect which triggered the first interest in so-called "topological phases of matter" and lead to the award of multiple Nobel prizes.

For context, we first consider what is known as the classical Hall effect. Consider electrons confined to a two-dimensional material lying in the x-y plane. We assume that opposite ends of the material are identified (as if the material were shaped like a torus: this assumption, while nonsensical, is commonly made since it is convenient to assume that the material is finite but has no edges).

We study the dynamics of electrons using what is known as the Drude model, which says that electrons in the material behave like classical point particles, except that they feel a friction because of occasionally scattering from atomic cores. If we apply an electric field $\boldsymbol{E}$ across the material, the equations of motion for the position $\boldsymbol{q}$ and momentum $\boldsymbol{p}$ of an electron in the material (in appropriate units) are simply:

$$\dot{\boldsymbol{q}} = \boldsymbol{p}, \quad \dot{\boldsymbol{p}} = -\boldsymbol{E} - \frac{\dot{\boldsymbol{q}}}{\tau} \tag{1.1}$$

Here $\tau > 0$ is the scattering time, which measures the strength of the friction felt by the electron as it moves. We are interested in the current density induced in the material by the field $\boldsymbol{E}$. The current density is related to the electron velocity by:

$$\boldsymbol{j} = -n\dot{\boldsymbol{q}} \tag{1.2}$$

where n is the density of electrons (more properly charge carriers e.g. holes, but we ignore this). At steady state, where $\dot{\boldsymbol{p}} = 0$, we find that:

$$\dot{\boldsymbol{q}} = -\tau \boldsymbol{E} \implies \boldsymbol{j} = n\tau\boldsymbol{E}. \tag{1.3}$$

Predictably, applying an electric field to the material leads to a current flowing in the same direction.

When we add a magnetic field through the material things are more interesting. The equation of motion for the momentum $\boldsymbol{p}$ of an electron in the material must be modified to:

$$\dot{\boldsymbol{p}} = -\boldsymbol{E} - \dot{\boldsymbol{q}} \times \boldsymbol{B} - \frac{\dot{\boldsymbol{q}}}{\tau} \tag{1.4}$$

where $\boldsymbol{B} = B\hat{\boldsymbol{z}}$. At steady state, we must solve the system of equations:

$$\begin{aligned} 0 &= -E_x - B\dot{q}_y - \frac{\dot{q}_x}{\tau} \\ 0 &= -E_y + B\dot{q}_x - \frac{\dot{q}_y}{\tau} \end{aligned} \tag{1.5}$$

where $\dot{q}(t) = (\dot{q}_x, \dot{q}_y)^\top$ and $\boldsymbol{E} = (E_x, E_y)^\top$ (note that we abuse notation and regard two-vectors as three-vectors and vice versa where it is convenient). In matrix form, this system becomes:

$$\begin{pmatrix} -\frac{1}{\tau} & -B \\ B & -\frac{1}{\tau} \end{pmatrix} \dot{\boldsymbol{q}} = \boldsymbol{E}. \tag{1.6}$$

In terms of the current density $\boldsymbol{j}$ we have:

$$\begin{aligned} \rho\boldsymbol{j} &= \boldsymbol{E} \\ \rho &:= \frac{1}{n}\begin{pmatrix} \frac{1}{\tau} & B \\ -B & \frac{1}{\tau} \end{pmatrix} \end{aligned} \tag{1.7}$$

Inverting the left-hand side leads to:

$$\begin{aligned} \boldsymbol{j} &= \sigma\boldsymbol{E} \\ \sigma &= \frac{n}{\frac{1}{\tau^2} + B^2}\begin{pmatrix} \frac{1}{\tau} & -B \\ B & \frac{1}{\tau} \end{pmatrix} \end{aligned} \tag{1.8}$$

which shows that the effect of the magnetic field is to *rotate* the current relative to the applied electric field. This is the classical Hall effect. The matrices σ and $\rho = \sigma^{-1}$ are known as the conductivity tensor and resistivity tensor, respectively.

Suppose now we perform the experiment on a sample which is finite in the x and y directions and apply the electric field in the x direction. The effect of the rotation (1.8) is to cause electrons to flow in the positive y direction preferentially. When these electrons reach the edge they become stuck there, leading to a potential difference between the $+y$ and $-y$ sides of the sample known as the Hall voltage. It is this voltage which was originally measured by Edwin Hall (1879).

The classical Hall effect is usually illustrated in a simple way by plotting the top left ρ_{xx} and top right ρ_{xy} entries of the resistivity tensor ρ as functions of the magnetic field strength B for fixed n and τ. As B increases, ρ_{xx} remains constant while ρ_{xy} increases linearly.

In 1980, the same experiment was performed by Von Klitzing with *very cold* electrons, and the result disagreed dramatically with the classical theory. It was found that as B is increased, the behavior of ρ_{xy} is to increase like a staircase. The behavior of ρ_{xx} is to remain very small, except for delta function-like jumps at each value of B where a new "step" of the staircase is started.

In the remainder of these notes I hope to explain how this kind of behavior can occur, and what this phenomenon has to do with topology. The quantum Hall effect itself turns out to be quite tricky to explain in detail so I will instead focus on what is known as the anomalous Hall effect and its quantum analog: the quantum anomalous Hall effect. The term anomalous in this context refers to the fact that this effect occurs *in the absence of a magnetic field.* The materials which exhibit this effect are known as "topological" or "Chern" insulators.

2. Bloch theory, the semiclassical theory of conduction, and naïve classification of materials as conductors and insulators

The classical description we discussed in the previous section is incapable of explaining the quantum anomalous Hall effect. We need quantum mechanics. Throughout this section we work in one spatial dimension to simplify calculations, and then state the general result at the end.

We start by writing down the non-relativistic single-particle Schrödinger equation satisfied by the wavefunctions of the (independent) free electrons in a *one dimensional* crystal (in appropriate units):

$$i\partial_t \psi = H\psi \quad H := -\frac{1}{2}\partial_x^2 + V(x). \tag{2.1}$$

All of the effect of the crystal structure is now bound up in the potential $V(x)$. By assumption, $V(x)$ is a periodic function:

$$V(x+a) = V(x), \tag{2.2}$$

for some $a > 0$. Just as we did in the previous section, we assume that the ends of the crystal are identified. This amounts to working in the Hilbert space $L^2_{per}([0, Na])$ for some integer $N > 0$, where the space L^2_{per} differs from the standard L^2 space only in that we assume periodicity of the wavefunction ψ:

$$\psi(0,t) = \psi(Na,t). \tag{2.3}$$

It is convenient to write the standard inner product by the bra-ket notation as follows:

$$\langle \psi_1(x) | \, \psi_2(x) \rangle_{L^2([0,Na])} := \int_0^{Na} \overline{\psi_1(x)} \psi_2(x) \, \mathrm{d}x. \tag{2.4}$$

As usual, it is natural to seek energy eigenstates, which satisfy the time-independent Schrödinger equation:

$$H\Phi = \mu\Phi \quad H = -\frac{1}{2}\partial_x^2 \Phi + V(x). \tag{2.5}$$

Since $V(x)$ is assumed periodic, we have that H commutes with the operator which shifts $x \to x + a$ and hence all solutions of (2.5) are *quasi-periodic*:

$$\Phi(x+a) = Z\Phi(x) \tag{2.6}$$

for some possibly complex Z. Condition (2.6), when combined with the periodicity assumption (2.3), is a very strong constraint. It implies that Z must satisfy:

$$Z^N = 1, \tag{2.7}$$

which implies that the possible values of Z are the roots of unity:

$$Z = e^{ika} \text{ where } k = \frac{2\pi m}{Na}, \quad m = 0, 1, ..., N-1. \tag{2.8}$$

We may therefore find all possible Φ by considering the family of boundary value problems on any single fundamental cell indexed by the parameter k:

$$\begin{aligned} -\frac{1}{2}\partial_x^2 \Phi + V(x)\Phi = \mu\Phi \\ \Phi(x+a;k) = e^{ika}\Phi(x;k). \end{aligned} \tag{2.9}$$

For fixed values of k, the eigenvalue problem (2.9) is as nice as they come: it is Sturm-Liouville. This means that there exist infinitely many values of μ for which solutions exist:

$$\mu_1(k) < \mu_2(k) < ... \tag{2.10}$$

Varying k over the values (2.8), we obtain sets of eigenvalues $\mu_j(k)$ which are known as the bands of the potential $V(x)$. The spaces between bands are known as gaps. The set of bands and gaps is known as the band structure of the crystal. The parameter k which appears here is known as the crystal momentum. The associated eigenfunctions $\Phi_n(x;k)$ of (2.9) are known as Bloch waves. When $V(x) = 0$, a little calculation shows that the Bloch functions in this case are simply plane waves $e^{\pm ikx}$.

We now pause to consider the free electrons in a crystal in the absence of any external fields. We have seen that there are precisely N energy eigenstates in the first band, one for each value of the crystal momentum k. Suppose now that for each unit cell, there is one free electron. The ground state of these electrons, after taking into account the Pauli exclusion principle and spin, is for precisely half of the band to be filled with each state occupied with one electron with spin up and one with spin down. We will see below that (at the level of approximation we will work at) such a material is a metal, or conductor. If for each unit cell there are *two* free electrons, then the ground state of the system will be to have every state in the first band filled with two electrons. Such a material will turn out to be an insulator.

To understand this classification, we need to consider in detail how electrons move around the material in response to an applied electric field. Note that it is not entirely obvious how to do this: what does it mean for an electron to travel through the crystal when the electron wavefunction (given by the solution of (2.9) extended to the whole crystal) is extended throughout the entire material?

We pause to develop some notation and derive an important identity. Note that the function (here we suppress the band index n since it is unimportant):

$$\chi(x;k) := e^{-ikx}\Phi(x;k) \tag{2.11}$$

is actually periodic with respect to x. A short calculation shows that $\chi(x;k)$ satisfies an eigenvalue problem which is equivalent to (2.9):

$$\begin{aligned} &\frac{1}{2}\left(k - i\partial_x\right)^2 \chi + V(x)\chi = \mu\chi \\ &\chi(x+a) = \chi(x). \end{aligned} \tag{2.12}$$

It is often much more convenient to work with Bloch waves in the form $e^{ikx}\chi(x;k)$ rather than in the form $\Phi(x;k)$, and we will usually do so in the remainder of these notes.

We derive an important identity by differentiating both sides of the eigenvalue problem for χ:

$$(k - i\partial_x)\chi + \frac{1}{2}(k - i\partial_x)^2 \partial_k \chi + V(x)\partial_k \chi = (\partial_k \mu)\chi + \mu \partial_k \chi. \tag{2.13}$$

and then taking the inner product in $L^2([0,a])$ with χ and using self-adjointness:

$$\langle \chi | (k - i\partial_x)\chi \rangle_{L^2([0,a])} = \partial_k \mu(k). \tag{2.14}$$

To this end, we make two adjustments to the Schrödinger equation we considered before. We add a new term, which describes the effect of an applied electric field:

$$i\partial_t \psi = -\frac{1}{2}\partial_x^2 \psi + V(x)\psi + W(\delta x)\psi \tag{2.15}$$

here $\delta > 0$ denotes a small parameter: in the limit $\delta \to 0$, the applied electric field is *weak*. We then consider wave-packet initial conditions, which correspond to an electron which is approximately, but not exactly, concentrated in a Bloch state with crystal momentum k_0:

$$\psi_0(x) = a_0(\epsilon x)e^{ik_0 x}\chi(x; k_0) \tag{2.16}$$

Here $a_0(z)$ is a function (known as the wave-packet envelope which decays as $z \to \infty$, and $\epsilon > 0$ denotes another small parameter: in the limit $\epsilon \to 0$ the initial condition reduces to a Bloch wave with crystal momentum k_0. (Note that the initial condition is not L^2-normalized: normalizing just amounts to multiplying the initial condition and solution by an overall factor of $\epsilon^{1/2}$ so we ignore this). For simplicity we now assume that $\delta = \epsilon$ which yields:

$$\begin{aligned} i\partial_t \psi &= -\frac{1}{2}\partial_x^2 \psi + V(x)\psi + W(\epsilon x)\psi \\ \psi(x,0) &= a_0(\epsilon x)e^{ik_0 x}\chi(x; k_0). \end{aligned} \tag{2.17}$$

We finally re-scale x and t:

$$X = \epsilon x, \quad T = \epsilon t \tag{2.18}$$

to obtain (we abuse notation to write X as x etc.):

$$\begin{aligned} i\epsilon\partial_t \psi &= -\frac{1}{2}\epsilon^2 \partial_x^2 \psi + V\left(\frac{x}{\epsilon}\right)\psi + W(x)\psi \\ \psi(x,0) &= a_0(x)e^{\frac{ik_0 x}{\epsilon}}\chi\left(\frac{x}{\epsilon}; k_0\right). \end{aligned} \tag{2.19}$$

This scaling is often known as "semiclassical scaling" and turns out to be particularly convenient when we consider the limit $\epsilon \to 0$. We will find that in this limit, the solution retains wave-packet form for $t > 0$, and the wave-packet center satisfies an effective *classical* system. The idea of the semiclassical theory of conductivity is to approximate the quantum mechanical evolution of electrons by this classical system. This (crude) description turns out to be powerful enough to explain many observed conductivity phenomena.

To build intuition, we first consider the case where the background potential due to atomic cores and the external field are both zero. The problem reduces to:

$$\begin{aligned} i\epsilon\partial_t \psi &= -\frac{1}{2}\epsilon^2 \partial_x^2 \psi \\ \psi(x,0) &= a_0(x)e^{\frac{ik_0 x}{\epsilon}}. \end{aligned} \tag{2.20}$$

In this case the solution is explicit via the Fourier transform, but we ignore this since that approach doesn't generalize to the general case. We instead inject the "WKB" ansatz:

$$\psi(x,t) = e^{\frac{i\phi(x,t)}{\epsilon}} A(x,t), \tag{2.21}$$

which puts the problem into an equivalent form, upon dropping the overall exponential factor, which is an equation for the functions A and ϕ:

$$\begin{aligned} &-\partial_t\phi A + i\epsilon\partial_t A = \frac{1}{2}(\partial_x\phi)^2 A - i\epsilon\frac{1}{2}\partial_x^2\phi - i\epsilon\partial_x\phi\partial_x A - \epsilon^2\frac{1}{2}\partial_x^2 A \\ &\left[\partial_t\phi + \frac{1}{2}\left(\partial_x\phi\right)^2\right] A = i\epsilon\left[\partial_t A + (\partial_x\phi)\partial_x A + \frac{1}{2}(\partial_x^2\phi)A\right] + \epsilon^2\left[\frac{1}{2}\partial_x^2 A\right]. \end{aligned} \tag{2.22}$$

Expanding the amplitude function $A(x,t)$ in a perturbation series:

$$A(x,t) = \sum_{n=0}^{\infty} \epsilon^n A^n(x,t), \tag{2.23}$$

leads to an infinite sequence of equations obtained by equating terms of each order in ϵ:

$$\begin{aligned} &\left[\partial_t\phi + \frac{1}{2}\left(\partial_x\phi\right)^2\right] A^0 = 0 \\ &\left[\partial_t\phi + \frac{1}{2}\left(\partial_x\phi\right)^2\right] A^1 = i\left[\partial_t A^0 + (\partial_x\phi)\partial_x A^0 + \frac{1}{2}(\partial_x^2\phi)A^0\right] \\ &\ldots \end{aligned} \tag{2.24}$$

We now impose the initial conditions:

$$A^0(x,0) = a_0(x) \quad A^n(x,0) = 0 \ (n \neq 0) \quad \phi(x,0) = k_0 x. \tag{2.25}$$

To satisfy the first equation, we must choose ϕ to satisfy the following initial value problem:

$$\begin{aligned} &\partial_t\phi + \frac{1}{2}(\partial_x\phi)^2 = 0 \\ &\phi(x,0) = k_0 x. \end{aligned} \tag{2.26}$$

This equation is known as the eikonal, and has the exact solution:

$$\phi(x,t) = k_0 x - \frac{1}{2}k_0^2 t. \tag{2.27}$$

The relationship between frequency $\omega(k) = \frac{1}{2}k^2$ and wavenumber k is known as the dispersion relation. Substituting this expression into the next equation now yields what is known as the transport equation:

$$\begin{aligned} &\partial_t A^0 + k_0\partial_x A^0 = 0 \\ &A^0(x,0) = a_0(x), \end{aligned} \tag{2.28}$$

which has the exact solution:

$$A^0(x,t) = a_0(x - k_0 t). \tag{2.29}$$

Putting everything together we derive:

$$\psi(x,t) = e^{\frac{ik_0}{\epsilon}\left[x - \frac{1}{2}k_0 t\right]} a_0(x - k_0 t) + O(\epsilon), \tag{2.30}$$

from which two conclusions are clear: the phase of the wave-packet propagates with velocity $\frac{1}{2}k_0$ (this is known as the phase velocity: in terms of the dispersion relation $\omega(k)$ it is $\frac{\omega(k)}{k}$), and the amplitude propagates with velocity k_0 (the group velocity: in terms of the dispersion relation $\omega(k)$ it is $\partial_k \omega(k)$). Note that this description is very much approximate; we have neglected dispersive (tendency of solutions of Schrödinger equation to spread out) effects, which are important for $t \sim \frac{1}{\epsilon}$ and would show up if we kept more terms in the perturbation series.

We now consider the case where the external field is zero: $W(x) = 0$ but the field generated by the atomic cores is non-zero; indeed, it may be large! We consider:

$$\begin{aligned} i\epsilon \partial_t \psi &= -\frac{1}{2}\epsilon^2 \partial_x^2 \psi + V\left(\frac{x}{\epsilon}\right)\psi \\ \psi(x,0) &= a_0(x) e^{\frac{ik_0 x}{\epsilon}} \chi\left(\frac{x}{\epsilon}; k_0\right), \end{aligned} \tag{2.31}$$

where we assume that the associated eigenvalue $\mu(k)$ of the Bloch function $e^{\frac{ikx}{\epsilon}}\chi\left(\frac{x}{\epsilon};k\right)$ is *non-degenerate* for all $k \in \left[0, \frac{2\pi}{a}\right]$. This time we inject a slightly more general "WKB"-type ansatz:

$$\psi(x,t) = e^{\frac{i\phi(x,t)}{\epsilon}} A\left(z,x,t\right)\Big|_{z=\frac{x}{\epsilon}}, \tag{2.32}$$

where the amplitude function now depends on the "fast" scale $\frac{x}{\epsilon}$. We assume that A is actually *periodic* in this variable, with period a. We then again expand the amplitude function as a perturbation series:

$$A(z,x,t) = \sum_{n=0}^{\infty} \epsilon^n A^n(z,x,t). \tag{2.33}$$

Collecting terms proportional to 1 this time yields:

$$\left[\partial_t \phi + \frac{1}{2}\left(\partial_x \phi - i\partial_z\right)^2 + V(z)\right] A^0(z,x,t) = 0. \tag{2.34}$$

We solve this equation by taking:

$$\begin{aligned} \partial_t \phi + \mu(\partial_x \phi) &= 0 \\ \phi(x,0) &= k_0 x \end{aligned} \tag{2.35}$$

where $\mu(k)$ is a Bloch function. This equation has the exact solution:

$$\phi(x,t) = k_0 x - \mu(k_0) t. \tag{2.36}$$

This puts the leading order equation into the form:

$$\left[\frac{1}{2}\left(k_0 - i\partial_z\right)^2 + V(z) - \mu(k_0)\right] A^0(z,x,t) = 0. \tag{2.37}$$

Since we assumed $A^0(z,x,t)$ is periodic in a and that the band function $\mu(k)$ is non-degenerate, this equation has the unique solution:

$$A^0(z,x,t) = \tilde{A}^0(x,t)\chi(z;k_0). \tag{2.38}$$

The as-yet unknown function $\tilde{A}^0(x,t)$ will be specified at the next order.

Equating terms proportional to ϵ yields:

$$\left[\frac{1}{2}\left(k_0 - i\partial_z\right)^2 + V(z) - \mu(k_0)\right] A^1(z,x,t) = i\left[\partial_t \tilde{A}^0(x,t)\chi(z;k_0) + \partial_x \tilde{A}^0(x,t)\left(k_0 - i\partial_z\right)\chi(z;k_0)\right]. \tag{2.39}$$

Note that this is an equation in z: x and t are simply parameters. It has a solution if and only if the right-hand side is orthogonal (in the space $L^2([0,a])$) to $\chi(z;k_0)$ (this is the Fredholm alternative: it is easy to see this condition is necessary by simply taking the inner product of both sides with χ and using self-adjointness). After using the identity (2.14) this condition implies:

$$\begin{aligned} &\partial_t \tilde{A}^0 + (\partial_k \mu(k_0))\partial_x \tilde{A}^0 = 0 \\ &\tilde{A}^0(x,0) = a_0(x) \end{aligned} \tag{2.40}$$

which has the exact solution:

$$\tilde{A}^0(x,t) = a_0\left(x - \partial_k \mu(k_0) t\right). \tag{2.41}$$

Putting everything together, we find that:

$$\psi(x,t) = e^{\frac{ik_0}{\epsilon}\left[x - \frac{\mu(k_0)}{k_0}t\right]} a_0\left(x - \partial_k \mu(k_0) t\right) + O(\epsilon) \tag{2.42}$$

where again dispersive effects only appear at higher order in the expansion. The phase and group velocities are now $\frac{\mu(k_0)}{k_0}$ and $\partial_k \mu(k_0)$ respectively. This result can be summarized as follows: the effect of adding the periodic "background" potential $V(z)$ is to change the dispersion relation: $\frac{1}{2}k^2 \to \mu(k)$.

We now want to consider what happens when we add an external potential. Since the method is similar but more complex when $V(z) \neq 0$, we go through details only for the case where the periodic potential is zero: $V(z) = 0$. We consider the model:

$$\begin{aligned} &i\epsilon \partial_t \psi = -\frac{1}{2}\epsilon^2 \partial_x^2 \psi + W(x)\psi \\ &\psi(x,0) = a_0(x) e^{\frac{ik_0 x}{\epsilon}}. \end{aligned} \tag{2.43}$$

Injecting the "WKB"-type ansatz:

$$\psi(x,t) = e^{\frac{i\phi(x,t)}{\epsilon}} A(x,t) \tag{2.44}$$

leads to:

$$\left[\partial_t \phi + \frac{1}{2}\left(\partial_x \phi\right)^2 + W(x)\right] A = i\epsilon \left[\partial_t A + (\partial_x \phi)\partial_x A + \frac{1}{2}(\partial_x^2 \phi) A\right] + \epsilon^2 \left[\frac{1}{2}\partial_x^2 A\right]. \tag{2.45}$$

Expanding the amplitude function $A(x,t)$ in a perturbation series as usual:

$$A(x,t) = \sum_{n=0}^{\infty} \epsilon^n A^n(x,t), \tag{2.46}$$

leads to an infinite sequence of equations obtained by equating terms of each order in ϵ:

$$\begin{aligned} &\left[\partial_t \phi + \frac{1}{2}\left(\partial_x \phi\right)^2 + W(x)\right] A^0 = 0 \\ &\left[\partial_t \phi + \frac{1}{2}\left(\partial_x \phi\right)^2 + W(x)\right] A^1 = i\left[\partial_t A^0 + (\partial_x \phi)\partial_x A^0 + \frac{1}{2}(\partial_x^2 \phi) A^0\right] \\ &\dots \end{aligned} \tag{2.47}$$

We now impose the initial conditions:

$$A^0(x,0) = a_0(x) \quad A^n(x,0) = 0 \ (n \neq 0) \quad \phi(x,0) = k_0 x. \tag{2.48}$$

To satisfy the first equation, we must choose ϕ to satisfy the following initial value problem:

$$\begin{aligned} &\partial_t \phi + \frac{1}{2}(\partial_x \phi)^2 + W(x) = 0 \\ &\phi(x,0) = k_0 x. \end{aligned} \tag{2.49}$$

When $W(x) \neq 0$, the eikonal equation no longer has an explicit exact solution. Its solution can be constructed by what is known as the method of characteristics.

Recall that when $W(x) = 0$, $\partial_x \phi$ and $\partial_t \phi$ corresponded to the wavenumber and frequency of the solution; we therefore define $\partial_x \phi$ and $\partial_t \phi$ now to be the local wavenumber and local frequency, respectively.

The idea of the method is to find, at each x, a curve $q(t;x)$ in space (known as the characteristic) such that $q(0;x) = x$ such that the solution evaluated along those curves $\phi(q(t;x),t)$ can be computed easily. Define $k(t;x)$ to be the local wavenumber along the curve $q(t;x)$:

$$k(t;x) := \partial_x \phi(q(t;x),t). \tag{2.50}$$

From the initial condition we see that:

$$k(0;x) = k_0. \tag{2.51}$$

What makes the method work is that it turns out to be possible to choose the curves $q(t;x)$ in such a way that $q(t;x)$ and $k(t;x)$ satisfy a *closed* system of *ODEs*. To see how this can occur, consider that differentiating $k(t;x)$ with respect to t gives:

$$\dot{k}(t;x) = \dot{q}(t;x)\partial_x^2 \phi(q(t,x),t) + \partial_t \partial_x \phi(q(t;x),t). \tag{2.52}$$

On the other hand, differentiating (2.49) with respect to x yields, at each x and t:

$$\partial_t \partial_x \phi + (\partial_x \phi)(\partial_x^2 \phi) + \partial_x W = 0. \tag{2.53}$$

Evaluating this identity on the characteristic gives:

$$\partial_t \partial_x \phi(q(t;x),t) + k(t;x)\partial_x^2 \phi(q(t;x),t) + \partial_x W(q(t;x)) = 0. \tag{2.54}$$

Substituting this identity into (2.52) yields:

$$\dot{k}(t;x) = [\dot{q}(t;x) - k(t;x)]\, \partial_x^2 \phi(q(t,x),t) - \partial_x W(q(t;x)). \tag{2.55}$$

We now see that if we want the system to close, we simply take $q(t;x)$ and $k(t;x)$ to satisfy the characteristic equations:

$$\dot{q}(t;x) = k(t;x) \quad \dot{k}(t;x) = -\partial_x W(q(t;x)). \tag{2.56}$$

The idea then is the following. At each x, we solve the characteristic equations (2.56) subject to the initial conditions:

$$q(0;x) = x \quad k(0;x) = k_0. \tag{2.57}$$

This yields the value of $\partial_x \phi$ along the characteristic (it is equal to $k(t;x)$). To compute the value of ϕ along the characteristic, it is necessary to do one more integration:

$$\begin{aligned}\dot{\phi}(q(t;x),t) &= \dot{q}(t;x)k(t;x) + \partial_t\phi(q(t;x),t) \\ &= \dot{q}(t;x)k(t;x) - \frac{1}{2}\left(k(t;x)\right)^2 - W(q(t;x)) \\ &= \frac{1}{2}\left(k(t;x)\right)^2 - W(q(t;x))\end{aligned} \tag{2.58}$$

$$\implies \phi(q(t;x),t) = k_0 x + \int_0^t \frac{1}{2}(k(t';x))^2 - W(q(t';x))\,\mathrm{d}t', \tag{2.59}$$

which shows that the value of $\phi(q(t;x),t)$ is simply the classical action along the characteristic.

Note that this method is a little "backwards", though. To find the value of $\phi(x,t)$ at some point X, T in spacetime, the method requires that we find the characteristic $q(t;x)$ which passes through the point X at time T:

$$q(T;x) = X, \tag{2.60}$$

and then perform the integration (2.59). A natural question arises: can it be that no characteristic, or more than one characteristic passes through the point X, T? Unfortunately, the answer is yes. The question to be answered is:

$$\text{when is the change of variables } x \mapsto q(t;x) \text{ invertible?} \tag{2.61}$$

Invertibility of this transform is measured by the quantity (this is just a Jacobian in one dimension, in higher dimensions $J(x,t)$ is defined through a determinant):

$$J(t;x) := \frac{\partial}{\partial x} q(t;x). \tag{2.62}$$

Since $J(x,0) = \frac{\partial x}{\partial x} = 1$, this quantity is initially non-zero for every x, but may equal zero for $t > 0$. A place where this occurs is known as a caustic, and to describe the solution past the time of the first caustic is more involved than the method of characteristics and beyond the scope of these notes.

So far we have seen that the characteristic equations yield information about the phase of the solution. For example, in higher dimensions one finds that the wavefronts (sets of constant phase) of the solution must lie perpendicular to characteristics. In fact, the characteristic equations turn out to also characterize how the *wavepacket envelope* propagates.

Pushing the expansion to the next order in ϵ, we must solve the transport equation:

$$\begin{aligned}&\partial_t A^0 + (\partial_x \phi)\partial_x A^0 + \frac{1}{2}(\partial_x^2\phi)A^0 = 0 \\ &A^0(x,0) = a_0(x),\end{aligned} \tag{2.63}$$

where ϕ is the solution of the eikonal equation. We recognize the first two terms of the transport equation as expressing the derivative of A^0 along a characteristic:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}A^0(q(t;x),t) &= \partial_t A^0(q(t;x),t) + k(t;x)\partial_x A^0(q(t;x),t) \\ &= \partial_t A^0(q(t;x),t) + \partial_x\phi(q(t;x),t)\partial_x A^0(q(t;x),t)\end{aligned} \tag{2.64}$$

and hence we may re-write the transport equation as an ODE along a characteristic:

$$\frac{\mathrm{d}}{\mathrm{d}t}A^0(q(t;x),t) = -\frac{1}{2}\partial_x^2\phi(q(t;x),t)A^0(q(t;x),t). \tag{2.65}$$

The right-hand side of this equation turns out to express the fact that the magnitude of the wavepacket envelope changes with the *density of characteristics* as measured by the size of the Jacobian $J(t;x)$. To see this, we note that along a characteristic:

$$\frac{\mathrm{d}}{\mathrm{d}t}J(t;x) = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial x}q(t;x) = \frac{\partial}{\partial x}k(t;x) = \partial_x^2\phi(q(t;x),t)J(t;x). \tag{2.66}$$

It now follows that:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(J(t;x)^{1/2}A^0(q(t;x),t)\right) = 0 \implies A^0(q(t;x),t) = J(t;x)^{-1/2}a_0(x), \tag{2.67}$$

which shows that the wavepacket envelope is simply *transported along characteristics*. Where characteristics converge, the amplitude of the wave is large. Where they diverge, the amplitude is small. Putting everything together we derive the leading order behavior of the solution:

$$\psi(x,t) = e^{\frac{i\phi(x,t)}{\epsilon}}A^0(x,t) + O(\epsilon), \tag{2.68}$$

where the functions ϕ and A^0 are defined along characteristics by (2.59) and (2.67), respectively. Although the solution is no longer as explicit as when $W = 0$, the dynamics are clear. The initial conditions (both wavefronts and envelope) are transported along solutions of the characteristic equations (2.56). In particular, if the wavepacket is well localized in space then the motion of the wavepacket center may actually be reasonably described by the characteristic *through the initial wavepacket center only*. The fact that the dynamics of the Schrödinger equation (2.43) is controlled by the classical system (2.56) in the limit $\epsilon \to 0$ has lead to this limit being known as the semiclassical limit.

We finally turn to the original model where both V and W are non-zero:

$$\begin{aligned} i\epsilon\partial_t\psi &= -\frac{1}{2}\epsilon^2\partial_x^2\psi + V\left(\frac{x}{\epsilon}\right)\psi + W(x)\psi \\ \psi(x,0) &= a_0(x)e^{\frac{ik_0x}{\epsilon}}\chi\left(\frac{x}{\epsilon};k_0\right). \end{aligned} \tag{2.69}$$

We again assume that the associated eigenvalue $\mu(k)$ of the Bloch function $e^{\frac{ikx}{\epsilon}}\chi\left(\frac{x}{\epsilon};k\right)$ is non-degenerate for all $k \in \left[0, \frac{2\pi}{a}\right]$. Injecting the multi-scale "WKB"-type ansatz:

$$\psi(x,t) = e^{\frac{i\phi(x,t)}{\epsilon}} \left. A(z,x,t)\right|_{z=\frac{x}{\epsilon}}, \tag{2.70}$$

where we again assume that A is periodic with respect to z, with period a. This leads to:

$$\left[\partial_t\phi + \frac{1}{2}\left(\partial_x\phi - i\partial_z\right)^2 + V(z) + W(x)\right]A = i\epsilon\left[\partial_tA + (\partial_x\phi - i\partial_z)\partial_xA + \frac{1}{2}(\partial_x^2\phi)A\right] + \epsilon^2\left[\frac{1}{2}\partial_x^2A\right]. \tag{2.71}$$

We then again expand the amplitude function as a perturbation series:

$$A(z,x,t) = \sum_{n=0}^{\infty}\epsilon^nA^n(z,x,t). \tag{2.72}$$

Collecting terms proportional to 1 this time yields:

$$\left[\partial_t \phi + \frac{1}{2}\left(\partial_x \phi - i\partial_z\right)^2 + V(z) + W(x)\right] A^0(z,x,t) = 0. \tag{2.73}$$

We solve this equation by first taking:

$$\begin{aligned} &\partial_t \phi + \mu(\partial_x \phi) + W(x) = 0 \\ &\phi(x,0) = k_0 x \end{aligned} \tag{2.74}$$

where $\mu(k)$ is a Bloch function. This equation can be solved (until the time of the first caustic) by the method of characteristics, where now the characteristic equations take the form:

$$\begin{aligned} &\dot{q}(t;x) = \partial_k \mu(k(t;x)) && \dot{k}(t;x) = -\partial_q W(q(t;x)) \\ &q(0;x) = x && k(0;x) = k_0. \end{aligned} \tag{2.75}$$

We again recover the phase function $\phi(q(t;x),t)$ along each characteristic by integrating the corresponding classical Lagrangian in this case:

$$\phi(q(t;x),t) = k_0 x + \int_0^t k(t';x)\partial_k \mu(k(t';x)) - \mu(k(t';x)) - W(q(t';x))\,\mathrm{d}t'. \tag{2.76}$$

This puts the leading order equation into the form:

$$\left[\frac{1}{2}\left(\partial_x \phi - i\partial_z\right)^2 + V(z) - \mu(\partial_x \phi)\right] A^0(z,x,t) = 0. \tag{2.77}$$

This equation now has the unique solution (taking into account non-degeneracy of the band):

$$A^0(z,x,t) = \tilde{A}^0(x,t)\chi(z;\partial_x \phi(x,t)). \tag{2.78}$$

Since we assumed $A^0(z,x,t)$ is periodic in a and that the band function $\mu(k)$ is non-degenerate, this equation has the unique solution:

$$A^0(z,x,t) = \tilde{A}^0(x,t)\chi(z;k_0). \tag{2.79}$$

The as-yet unknown function $\tilde{A}^0(x,t)$ will be specified at the next order.

Equating terms proportional to ϵ yields:

$$\begin{aligned} &\left[\frac{1}{2}\left(\partial_x \phi - i\partial_z\right)^2 + V(z) - \mu(\partial_x \phi)\right] A^1(z,x,t) \\ &= i\left[\partial_t \tilde{A}^0(x,t)\chi(z;\partial_x\phi) + \partial_x \tilde{A}^0(x,t)\left(\partial_x\phi - i\partial_z\right)\chi(z;\partial_x\phi) + \frac{1}{2}(\partial_x^2\phi)\tilde{A}^0(x,t)\chi(z;\partial_x\phi)\right. \\ &\qquad \left. + \tilde{A}^0(x,t)(\partial_t\partial_x\phi)\partial_k\chi(z;\partial_x\phi) + \tilde{A}^0(x,t)(\partial_x^2\phi)(\partial_x\phi - i\partial_z)\partial_k\chi(z;\partial_x\phi)\right]. \end{aligned} \tag{2.80}$$

Note that this is an equation in z: x and t are simply parameters. It has a solution if and only if the right-hand side is orthogonal (in the space $L^2([0,a])$) to $\chi(z;k_0)$ (this is the Fredholm alternative: it is easy to see this condition is necessary by simply taking the inner product of both sides with χ and using self-adjointness).

Via a series of manipulations of the Bloch eigenvalue problem, this condition can be shown to imply:

$$\begin{aligned}
&\partial_t \tilde{A}^0 + (\partial_k \mu(\partial_x \phi))\partial_x \tilde{A}^0 + \frac{1}{2}(\partial_x^2 \phi)(\partial_k^2 \mu(\partial_x \phi))\tilde{A}^0 \\
&\quad + \partial_t \partial_x \phi \left\langle \chi \right| \left. \partial_k \chi \right\rangle \tilde{A}^0 + (\partial_k \mu(\partial_x \phi))(\partial_x^2 \phi) \left\langle \chi \right| \left. \partial_k \chi \right\rangle \tilde{A}^0 = 0 \\
&\tilde{A}^0(x,0) = a_0(x),
\end{aligned} \tag{2.81}$$

where $\langle | \rangle$ denotes the $L^2([0,a])$ inner product. Differentiating the eikonal equation (2.74) with respect to x yields the identity:

$$\partial_t \partial_x \phi + (\partial_x^2 \phi)\partial_k \mu(\partial_x \phi) = -\partial_x W(x), \tag{2.82}$$

which allows us to put the transport equation into the form:

$$\begin{aligned}
&\partial_t \tilde{A}^0 + (\partial_k \mu(\partial_x \phi))\partial_x \tilde{A}^0 + \frac{1}{2}(\partial_x^2 \phi)(\partial_k^2 \mu(\partial_x \phi))\tilde{A}^0 - \partial_x W \left\langle \chi \right| \left. \partial_k \chi \right\rangle \tilde{A}^0 = 0 \\
&\tilde{A}^0(x,0) = a_0(x).
\end{aligned} \tag{2.83}$$

Each of the terms in (2.83) has a similar origin and interpretation to terms which appeared in the $V = 0$ transport equation. The final term has no analog, however. This term turns out to contribute a *phase shift*. After some re-arranging, the solution of (2.83) along a characteristic $q(t;x)$ is:

$$\tilde{A}^0(q(t;x),t) = J(t;x)^{-1/2} e^{i\phi_B(t;x)} a_0(x), \tag{2.84}$$

where:

$$\phi_B(t;x) := \int_0^t \left\langle \chi(\cdot; k(t';x)) \right| \left. i \frac{\mathrm{d}}{\mathrm{d}t'} \chi(\cdot; k(t';x)) \right\rangle \mathrm{d}t'. \tag{2.85}$$

That $\phi_B(t;x)$ is real and hence that this term genuinely constitutes a phase shift follows immediately from normalization of χ:

$$\begin{aligned}
&\left\langle \chi \right| \left. \chi \right\rangle = 1 \implies \frac{\mathrm{d}}{\mathrm{d}t} \left\langle \chi \right| \left. \chi \right\rangle = 0 \implies \left\langle \frac{\mathrm{d}}{\mathrm{d}t}\chi \right| \left. \chi \right\rangle + \left\langle \chi \right| \left. \frac{\mathrm{d}}{\mathrm{d}t}\chi \right\rangle = 0 \\
&\implies \overline{\left\langle \chi \right| \left. \frac{\mathrm{d}}{\mathrm{d}t}\chi \right\rangle} = -\left\langle \chi \right| \left. \frac{\mathrm{d}}{\mathrm{d}t}\chi \right\rangle \implies \overline{\left\langle \chi \right| \left. i\frac{\mathrm{d}}{\mathrm{d}t}\chi \right\rangle} = \left\langle \chi \right| \left. i\frac{\mathrm{d}}{\mathrm{d}t}\chi \right\rangle
\end{aligned} \tag{2.86}$$

This phase shift is known as the Berry phase associated with the path $k(t;x)$ through the Brillouin zone. Remarkably, it is a *purely geometric* quantity. Changing variables in the integral reveals this:

$$\phi_B(t;x) := \int_{k_0}^{k(t;x)} \left\langle \chi(\cdot;k) \right| \left. i\partial_k \chi(\cdot;k) \right\rangle \mathrm{d}k. \tag{2.87}$$

The idea of the semiclassical theory of conduction is to model free electrons in a material as *classical* point particles moving according to the characteristic equations (2.75). In three dimensions, this means that to model free electrons in a material we should replace the usual classical equations of motion of an electron in free space:

$$\dot{\boldsymbol{q}} = \boldsymbol{p}, \quad \dot{\boldsymbol{p}} = -\boldsymbol{E} - \dot{\boldsymbol{q}} \times \boldsymbol{B} \tag{2.88}$$

by:

$$\dot{\boldsymbol{q}} = \nabla \mu(\boldsymbol{k}), \quad \dot{\boldsymbol{k}} = -\boldsymbol{E} - \dot{\boldsymbol{q}} \times \boldsymbol{B}, \tag{2.89}$$

where $\boldsymbol{k}$ now represents the crystal momentum of the free electron, and $\mu(\boldsymbol{k})$ represents the band function of the band the electron occupies.

We now return to our earlier classification of conductors and insulators as materials such that Bloch bands remain partly filled or fully filled with electrons, respectively. The reason for this classification can now be explained. In a conductor, in response to an applied electric field, the crystal momenta of electrons changes through the second of the semiclassical equations (2.89). The result is an asymmetry within the band: now more electrons occupy states where $\nabla\mu$ points in the direction of the applied field as occupy states where $\nabla\mu$ points in the opposite direction. The result is a *net flow* of charge in the direction $\nabla\mu$. In an insulator, such an asymmetry cannot occur: the motion of any electrons moving to occupy states where $\nabla\mu$ points in the direction of the applied field are immediately cancelled by electrons which must, by the Pauli exclusion principle, occupy states where $\nabla\mu$ points in the opposite direction. To see this in more detail, consider that we may integrate $\dot{\boldsymbol{q}}$ over the Brillouin zone to obtain:

$$\int\!\!\int\!\!\int \dot{\boldsymbol{q}}(t)\,\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}k_3 = \int\!\!\int\!\!\int \nabla\mu(\boldsymbol{k})\,\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}k_3. \tag{2.90}$$

Closer inspection shows that every component of this vector is zero because μ must take the same value at opposite side of the Brillouin zone.

In the term topological insulator, the term insulator refers to the fact that such materials, via the predictions of a naïve semiclassical theory of conduction, ought to be insulators. In reality, charge *can* flow in such materials in a quite subtle way.

3. CORRECTION TO SEMICLASSICAL THEORY OF CONDUCTION DUE TO BERRY'S PHASE AND APPEARANCE OF CHERN NUMBER AS "ANOMALOUS" CONDUCTIVITY OF A FILLED BAND

As it turns out, the analysis given in the previous section is subtly wrong. It is wrong because we have neglected a *dynamical* effect of the Berry phase (2.85), which can shift the wave fronts of a wave-packet in a non-trivial way in more than one spatial dimension. Specifically (deriving this is a little involved, so we omit this), the semiclassical equations of motion (2.89) should be corrected by an additional velocity term (leading to so-called corrected semiclassical equations of motion for free electrons in a material):

$$\dot{\boldsymbol{q}} = \nabla\mu(\boldsymbol{k}) + \dot{\boldsymbol{k}} \times \boldsymbol{\mathcal{F}}(\boldsymbol{k}), \quad \dot{\boldsymbol{k}} = -\boldsymbol{E} - \dot{\boldsymbol{q}} \times \boldsymbol{B}, \tag{3.1}$$

where $\boldsymbol{\mathcal{F}}(\boldsymbol{k})$ is the Berry curvature:

$$\boldsymbol{\mathcal{F}}(\boldsymbol{k}) := \nabla \times \boldsymbol{\mathcal{A}}(\boldsymbol{k}) \tag{3.2}$$

and $\boldsymbol{\mathcal{A}}(\boldsymbol{k})$ is the Berry connection associated with the band $\mu(\boldsymbol{k})$:

$$\boldsymbol{\mathcal{A}}(\boldsymbol{k}) := \langle \chi(\cdot;\boldsymbol{k}) |\, i\nabla\chi(\cdot;\boldsymbol{k})\rangle\,. \tag{3.3}$$

Crucially, with the additional term, it is no longer the case that a filled band cannot carry any net current.

For example, suppose we have a two-dimensional material confined to the x-y plane. The Berry curvature now only has a single non-zero component, which points "out" of the material:

$$\boldsymbol{\mathcal{F}}(\boldsymbol{p}) = \left(\frac{\partial\mathcal{A}_{k_2}}{\partial k_1} - \frac{\partial\mathcal{A}_{k_1}}{\partial k_2}\right)\hat{\boldsymbol{k}}. \tag{3.4}$$

Suppose we now turn on an electric field pointing in the x direction, so that:

$$\boldsymbol{E} = E_x \hat{\boldsymbol{\imath}} \implies \dot{\boldsymbol{p}} = -E_x \hat{\boldsymbol{\imath}}. \tag{3.5}$$

Substituting these expressions and integrating over the Brillouin zone gives:

$$E_x \int\int_{\mathrm{BZ}} \left(\frac{\partial \mathcal{A}_{k_2}}{\partial k_1} - \frac{\partial \mathcal{A}_{k_1}}{\partial k_2} \right) \mathrm{d}k_1 \, \mathrm{d}k_2 \hat{\boldsymbol{\jmath}}. \tag{3.6}$$

If the integral is non-zero, we see that just like in the classical Hall effect the material may exhibit a *transverse conductivity* in response to an applied electric field. This effect is known as the quantum anomalous Hall effect. Via Stokes' theorem, we see that:

$$\int\int_{\mathrm{BZ}} \left(\frac{\partial \mathcal{A}_{k_2}}{\partial k_1} - \frac{\partial \mathcal{A}_{k_1}}{\partial k_2} \right) \mathrm{d}k_1 \, \mathrm{d}k_2 = \int_{\partial \mathrm{BZ}} \boldsymbol{\mathcal{A}}(\boldsymbol{k}) \cdot \mathrm{d}\boldsymbol{k} \tag{3.7}$$

which is nothing but the Berry phase of a particle transported along the boundary of the Brillouin zone. Naïvely, we would expect this to be zero: by identifying edges of the Brillouin zone we this loop is equivalent to a point. On reflection, we see that it is possible for the integral over the Brillouin zone to be non-zero without contradiction (i.e. giving the same result for the Berry phase associated to the closed loop) if and only if:

$$\int\int_{\mathrm{BZ}} \left(\frac{\partial \mathcal{A}_{k_2}}{\partial k_1} - \frac{\partial \mathcal{A}_{k_1}}{\partial k_2} \right) \mathrm{d}k_1 \, \mathrm{d}k_2 = 2\pi m \quad m \in \mathbb{Z}. \tag{3.8}$$

The integer appearing on the right-hand side of this equation is known as the Chern number. This result would not be interesting if it was always the case that $m = 0$. This is not the case but materials which exhibit a quantum anomalous Hall effect are quite special: they must break time-reversal symmetry.

We say that a material respects time-reversal symmetry if:

$$\overline{\chi(\boldsymbol{x}; -\boldsymbol{k})} = \chi(\boldsymbol{x}; \boldsymbol{k}) \tag{3.9}$$

for all $k \in \mathrm{BZ}$. A short calculation shows that if time-reversal symmetry holds, then:

$$\left[\frac{\partial \mathcal{A}_{k_2}}{\partial k_1}(-\boldsymbol{k}) - \frac{\partial \mathcal{A}_{k_1}}{\partial k_2}(-\boldsymbol{k}) \right] = - \left[\frac{\partial \mathcal{A}_{k_2}}{\partial k_1}(\boldsymbol{k}) - \frac{\partial \mathcal{A}_{k_1}}{\partial k_2}(\boldsymbol{k}) \right] \tag{3.10}$$

for all $k \in \mathrm{BZ}$. It follows from this identity (after perhaps translating by reciprocal lattice vectors) that the Chern number is zero for such materials. In the remaining talks we will discuss the Haldane model, which describes a hypothetical material whose lowest band can exhibit a non-zero Chern number and thus the quantum anomalous Hall effect.

4. The Haldane model

The Haldane model is a model of a hypothetical two-dimensional material. Before talking about the Haldane model it is necessary to introduce what is meant by a tight-binding model. Suppose we want to solve the time-independent Schrödinger equation satisfied by free electrons in a two-dimensional crystalline material:

$$H\psi = \mu\psi \quad H = -\frac{1}{2}\Delta + V(\boldsymbol{x}) \tag{4.1}$$

where $V(\boldsymbol{x})$ is assumed periodic with respect to some lattice Λ:

$$\forall \boldsymbol{v} \in \Lambda, V(\boldsymbol{x} + \boldsymbol{v}) = V(\boldsymbol{x}). \tag{4.2}$$

We assume that Λ is generated by vectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ so that:

$$\boldsymbol{v} \in \Lambda \iff \boldsymbol{v} = n_1 \boldsymbol{v}_1 + n_2 \boldsymbol{v}_2 \quad (n_1, n_2) \in \mathbb{Z}^2. \tag{4.3}$$

Let $V_a(\boldsymbol{x})$ denote the potential generated by any single atom, so that:

$$V(\boldsymbol{x}) = \sum_{\boldsymbol{v} \in \Lambda} V_a(\boldsymbol{x} - \boldsymbol{v}) = \sum_{(n_1,n_2)\in\mathbb{Z}^2} V_a(\boldsymbol{x} - n_1\boldsymbol{v}_1 - n_2\boldsymbol{v}_2). \tag{4.4}$$

One way to go about solving (4.1) is as follows. We start by solving for the atomic orbitals, which are the eigenfunctions of the one-atom Schrödinger equation:

$$H_a \phi_a = E_a \phi_a \quad H_a = -\frac{1}{2}\Delta + V_a(\boldsymbol{x}), \tag{4.5}$$

labelled $\phi_{a,1}(\boldsymbol{x}), \phi_{a,2}(\boldsymbol{x}), ...,$ with associated energies $E_{a,1}, E_{a,2}, ...$ We can then attempt to solve (4.1) approximately by making the ansatz:

$$\psi(\boldsymbol{x}) = \sum_{(n_1,n_2)\in\mathbb{Z}^2} \sum_{j=1}^{N} \psi_{j,n_1,n_2} \phi_{a,j}(\boldsymbol{x} - n_1\boldsymbol{v}_1 - n_2\boldsymbol{v}_2), \tag{4.6}$$

where ψ_{j,n_1,n_2} are complex numbers to be found, and N is the number of orbitals we are chosing to include. Obviously if we require a more accurate approximation we can take N larger. Substituting this expression into (4.1) and projecting onto each orbital gives a system of equations for the numbers ψ_{j,n_1,n_2}. Finally, assuming that each atomic orbital is well-localized at its atomic site (this is justified whenever the atomic wells are *deep*), we can approximately solve this system by dropping terms which describe interactions between far away sites. In this way we obtain a significant simplification of the original model (4.1), which often contains enough of the features of (4.1) as to be useful. This is the idea of the tight-binding approximation and of a tight-binding model.

Free electrons in graphene are often modeled by the following tight-binding Hamiltonian:

$$(H\psi)_{m,n} = \begin{pmatrix} \psi^B_{m-1,n} + \psi^B_{m,n-1} + \psi^B_{m,n} \\ \psi^A_{m+1,n} + \psi^A_{m,n+1} + \psi^A_{m,n} \end{pmatrix}. \tag{4.7}$$

Here:

$$\psi_{m,n} = \begin{pmatrix} \psi^A_{m,n} \\ \psi^B_{m,n} \end{pmatrix} \tag{4.8}$$

denotes the wavefunction restricted to the m,nth cell which hosts two atoms. We assume for simplicity that the sample has no edges and hence $(m,n) \in \mathbb{Z}^2$. Since the Hamiltonian is invariant under translations $m \to m+1$ and $n \to n+1$ we can assume without loss of generality that all eigenfunctions of H are k-periodic:

$$\psi_{m+1,n} = e^{ik_1}\psi_{m,n} \quad \psi_{m,n+1} = e^{ik_2}\psi_{m,n} \quad \text{for all } (m,n) \in \mathbb{Z}^2. \tag{4.9}$$

Substituting this into the eigenvalue equation $H\Phi = E\Phi$ yields a 2×2 matrix problem for $\Phi_{0,0}$ which we denote by $\chi(k_1,k_2)$:

$$\begin{aligned} &H(k_1,k_2)\chi(k_1,k_2) = E(k_1,k_2)\chi(k_1,k_2) \\ &H(k_1,k_2) := \begin{pmatrix} 0 & 1 + e^{-ik_1} + e^{-ik_2} \\ 1 + e^{ik_1} + e^{ik_2} & 0 \end{pmatrix} \end{aligned}$$

where $k_1, k_2 \in [-\pi, \pi]$. Solving this problem as k_1 and k_2 vary over the Brillouin zone yields two Bloch band functions:

$$E^{\pm}(k_1, k_2) = \pm |f(k_1, k_2)| \quad f(k_1, k_2) = 1 + e^{-ik_1} + e^{-ik_2}, \tag{4.10}$$

Since:

$$\cos\left(\frac{2\pi}{3}\right) = \cos\left(-\frac{2\pi}{3}\right) = -\frac{1}{2}$$
$$\sin\left(\frac{2\pi}{3}\right) = -\sin\left(-\frac{2\pi}{3}\right) = \frac{\sqrt{3}}{2},$$

the bands touch at two points:

$$K = \left(\frac{2\pi}{3}, -\frac{2\pi}{3}\right), \quad K' = -K = \left(-\frac{2\pi}{3}, \frac{2\pi}{3}\right).$$

At these points the Hamiltonian reduces to a 2×2 matrix operator whose entries are all 0, hence the degenerate eigenspace is spanned by:

$$\chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{4.11}$$

The fact that the bands are degenerate at these points is not accidental; the Hamiltonian has a lot of symmetry.

First note that:

$$\sigma_1 H(k_1, k_2) = H(-k_1, -k_2)\sigma_1 \tag{4.12}$$

where:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.13}$$

Now let $\Phi(k_1, k_2)$ denote an eigenfunction of $H(k_1, k_2)$:

$$H(k_1, k_2)\Phi(k_1, k_2) = E(k_1, k_2)\Phi(k_1, k_2). \tag{4.14}$$

Multiplying on the left by σ_1 and then using (4.12) gives:

$$H(-k_1, -k_2)\sigma_1\Phi(k_1, k_2) = E(k_1, k_2)\sigma_1\Phi(k_1, k_2) \tag{4.15}$$

which shows that:

$$E(-k_1, -k_2) = E(k_1, k_2) \quad \Phi(-k_1, -k_2) = \sigma_1\Phi(k_1, k_2). \tag{4.16}$$

This symmetry is known as parity symmetry.

The other symmetry is as follows. Note that:

$$\overline{H(k_1, k_2)} = H(-k_1, -k_2). \tag{4.17}$$

Acting by this symmetry on (4.14) gives:

$$H(-k_1, -k_2)\overline{\Phi(k_1, k_2)} = E(k_1, k_2)\overline{\Phi(k_1, k_2)} \tag{4.18}$$

which shows that:

$$E(-k_1, -k_2) = E(k_1, k_2) \quad \Phi(-k_1, -k_2) = \overline{\Phi(k_1, k_2)}. \tag{4.19}$$

This symmetry is known as time-reversal symmetry.

Combining both symmetries shows that whenever $\Phi(k_1, k_2)$ is an eigenvector with eigenvalue $E(k_1, k_2)$,

$$H(k_1, k_2)\sigma_1\overline{\Phi(k_1, k_2)} = E(k_1, k_2)\sigma_1\overline{\Phi(k_1, k_2)}, \tag{4.20}$$

and hence so is $\sigma_1 \overline{\Phi(k_1, k_2)}$. This is known as parity-time symmetry. Notice that when we multiply χ_1 (in (4.11)) by σ_1 and take the complex conjugate we are left with χ_2. We can therefore view the degenerate modes as being "linked" by parity-time symmetry: as long as χ_1 is an eigenstate at K, so is χ_2, as long as parity-time symmetry is unbroken.

To study the local behavior of the Bloch bands, we linearize in k. Doing this about any point κ in the Brillouin zone yields:

$$H(\kappa+\tilde{k}) \approx \begin{pmatrix} 0 & 1 + e^{-i\kappa_1} - i\tilde{k}_1 e^{-i\kappa_1} + e^{-i\kappa_2} - i\tilde{k}_2 e^{-i\kappa_2} \\ 1 + e^{i\kappa_1} + i\tilde{k}_1 e^{i\kappa_1} + e^{i\kappa_2} + i\tilde{k}_2 e^{i\kappa_2} & 0 \end{pmatrix}. \tag{4.21}$$

Evaluating at $\kappa = K$ gives:

$$\begin{aligned} H(K + \tilde{k}) &\approx \begin{pmatrix} 0 & -i\tilde{k}_1 e^{-i\frac{2\pi}{3}} - i\tilde{k}_2 e^{i\frac{2\pi}{3}} \\ i\tilde{k}_1 e^{i\frac{2\pi}{3}} + i\tilde{k}_2 e^{-i\frac{2\pi}{3}} & 0 \end{pmatrix} \\ &= \tilde{k}_1 \begin{pmatrix} 0 & -ie^{-i\frac{2\pi}{3}} \\ ie^{i\frac{2\pi}{3}} & 0 \end{pmatrix} + \tilde{k}_2 \begin{pmatrix} 0 & -ie^{i\frac{2\pi}{3}} \\ ie^{-i\frac{2\pi}{3}} & 0 \end{pmatrix} \\ &= \tilde{k}_1 \begin{pmatrix} 0 & -\frac{\sqrt{3}}{2} + \frac{1}{2}i \\ -\frac{\sqrt{3}}{2} - \frac{1}{2}i & 0 \end{pmatrix} + \tilde{k}_2 \begin{pmatrix} 0 & \frac{\sqrt{3}}{2} + \frac{1}{2}i \\ \frac{\sqrt{3}}{2} - \frac{1}{2}i & 0 \end{pmatrix} \\ &= \frac{\sqrt{3}}{2} \left(\tilde{k}_2 - \tilde{k}_1\right) \sigma_1 + \frac{1}{2} \left(\tilde{k}_1 + \tilde{k}_2\right) \sigma_2. \end{aligned} \tag{4.22}$$

Hence in the new variables:

$$k_1' = \frac{\sqrt{3}}{2} \left(\tilde{k}_2 - \tilde{k}_1\right), \quad k_2' = \frac{1}{2} \left(\tilde{k}_1 + \tilde{k}_2\right) \tag{4.23}$$

the Hamiltonian near to the Dirac point is:

$$k_1' \sigma_1 + k_2' \sigma_2, \tag{4.24}$$

where:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}. \tag{4.25}$$

The Bloch bands are locally conical:

$$E^{\pm}(k_1', k_2') = \pm\sqrt{(k_1')^2 + (k_2')^2}. \tag{4.26}$$

In graphene the Fermi level lies at 0, leading to graphene being known as a semimetal: the Fermi level does not lie in a gap (so it is not an insulator) very few electrons are available to participate in conduction: only those precisely with energy 0 (hence it does not behave as a metal). The effective dynamics of an electron with energy at the Fermi level are given by an effective massless Dirac equation (compare with what we derived in Section 2):

$$i\partial_t \begin{pmatrix} \alpha_+(x, y, t) \\ \alpha_-(x, y, t) \end{pmatrix} = \begin{pmatrix} 0 & (-i\partial_x) + i(-i\partial_y) \\ (-i\partial_x) - i(-i\partial_y) & 0 \end{pmatrix} \begin{pmatrix} \alpha_+(x, y, t) \\ \alpha_-(x, y, t) \end{pmatrix}. \tag{4.27}$$

It is this remarkable fact which gives rise to many of graphene's properties as a material.

To obtain an insulator, we have to force a gap between the Bloch bands. We can do this by breaking either parity or time-reversal symmetry by adding terms to the Hamiltonian. It is simplest to break parity symmetry by adding differing "onsite" potentials V^A and V^B on every A site and every B site. For simplicity, we add potentials on either site whose sign is opposite so that $V^B = -V^A$. The Hamiltonian of such a structure (rather than graphene, this Hamiltonian models another 2d material known as Hexagonal Boron Nitride) is then:

$$(H\psi)_{m,n} = \begin{pmatrix} V^A \psi^A_{m,n} + \psi^B_{m-1,n} + \psi^B_{m,n-1} + \psi^B_{m,n} \\ -V^A \psi^B_{m,n} + \psi^A_{m+1,n} + \psi^A_{m,n+1} + \psi^A_{m,n} \end{pmatrix}, \tag{4.28}$$

which leads to the Bloch Hamiltonian:

$$H(k_1,k_2) := \begin{pmatrix} V^A & 1 + e^{-ik_1} + e^{-ik_2} \\ 1 + e^{ik_1} + e^{ik_2} & -V^A \end{pmatrix}. \tag{4.29}$$

We assume that to detect a gap it is enough to check that a gap opens at the Dirac points. The linearized Hamiltonian at K is now:

$$\begin{pmatrix} m & k_1' + ik_2' \\ k_1' - ik_2' & -m \end{pmatrix}, \tag{4.30}$$

with $m = V^A$ known as the effective mass and the local behavior of the Bloch bands indeed shows a gap:

$$E^\pm(k_1',k_2') = \pm\sqrt{(k_1')^2 + (k_2')^2 + m^2}. \tag{4.31}$$

The effective dynamics of the Bloch electrons at the Dirac point is now a Dirac equation with mass $m = V^A$. Note that this insulator cannot exhibit a non-zero Chern number (and hence quantized transverse conductivity) because it retains time-reversal symmetry. It is interesting to verify this by direct calculation. A somewhat involved calculation working from (4.30) shows that the Berry curvature associated to the lower band is locally a monopole at the Dirac point in k-space:

$$\frac{\partial \mathcal{A}_{k_2}}{\partial k_1} - \frac{\partial \mathcal{A}_{k_1}}{\partial k_2} = \frac{m}{2((k_1')^2 + (k_2')^2 + m^2)^{3/2}}. \tag{4.32}$$

Integrating this over a ball in k-space using polar co-ordinates shows that the "local" contribution of the Dirac point to the Chern number is $\frac{1}{2}\text{sign}(m)$. To get an integer, we sum the contributions from the two Dirac points.

At the other Dirac point the local Hamiltonian turns out to be, using the same local co-ordinates as before:

$$H(k_1',k_2') = \begin{pmatrix} m & -k_1' + ik_2' \\ -k_1' - ik_2' & -m \end{pmatrix}. \tag{4.33}$$

Because of the change in sign of k_1', the same calculation as before yields that the local contribution to the Chern number is actually $-\frac{1}{2}\text{sign}(m)$, and hence the Chern number is zero in this case as expected.

We have already seen that to produce a non-zero Chern number it is necessary to break time-reversal symmetry. We now have a more precise necessary condition: we must produce a Hamiltonian such that the effective mass at each Dirac point has opposite sign. The Haldane Hamiltonian achieves this for certain parameter ranges by adding complex hopping terms between next-nearest neighbor hopping to the Hamiltonian as follows:

(4.34)

$$(H\psi)_{m,n} = \begin{pmatrix} \psi^B_{m-1,n} + \psi^B_{m,n-1} + \psi^B_{m,n} \\ \psi^A_{m+1,n} + \psi^A_{m,n+1} + \psi^A_{m,n} \end{pmatrix} + \begin{pmatrix} V^A \psi^A_{m,n} \\ -V^A \psi^B_{m,n} \end{pmatrix}$$
$$+ t' \begin{pmatrix} e^{i\phi}(\psi^A_{m,n+1} + \psi^A_{m-1,n} + \psi^A_{m+1,n-1}) + e^{-i\phi}(\psi^A_{m,n-1} + \psi^A_{m+1,n} + \psi^A_{m-1,n+1}) \\ e^{i\phi}(\psi^B_{m,n-1} + \psi^B_{m+1,n} + \psi^B_{m-1,n+1}) + e^{-i\phi}(\psi^B_{m,n+1} + \psi^B_{m-1,n} + \psi^A_{m+1,n-1}) \end{pmatrix}.$$

Here t' is a real number which determines the amplitude of the complex hopping. Linearizing around K gives, after changing variables just as before:

(4.35)

$$\begin{aligned} H(k_1', k_2') &= \begin{pmatrix} V^A + t' e^{i\phi} \left[3 \left(-\frac{1}{2} + i \frac{\sqrt{3}}{2} \right) \right] + \text{c.c.} & k_1' + i k_2' \\ k_1' - i k_2' & -V^A + t' e^{i\phi} \left[3 \left(-\frac{1}{2} - i \frac{\sqrt{3}}{2} \right) \right] + \text{c.c.} \end{pmatrix} \\ &= \begin{pmatrix} V^A - 3t'(\sqrt{3} \sin\phi + \cos\phi) & k_1' + i k_2' \\ k_1' - i k_2' & -V^A + 3t' \left(\sqrt{3} \sin\phi - \cos\phi \right) \end{pmatrix} \\ &= (-3t' \cos\phi) I + \begin{pmatrix} V^A - 3\sqrt{3} t' \sin\phi & k_1' + i k_2' \\ k_1' - i k_2' & -\left(V^A - 3\sqrt{3} t' \sin\phi \right) \end{pmatrix} \end{aligned}$$

so that the effective mass at K is $V^A - 3\sqrt{3} t' \sin\phi$. Linearizing around K' gives:

(4.36)

$$\begin{aligned} H(k_1', k_2') &= \begin{pmatrix} V^A + t' e^{i\phi} \left[3 \left(-\frac{1}{2} - i \frac{\sqrt{3}}{2} \right) \right] + \text{c.c.} & -k_1' + i k_2' \\ -k_1' - i k_2' & -V^A + t' e^{i\phi} \left[3 \left(-\frac{1}{2} + i \frac{\sqrt{3}}{2} \right) \right] + \text{c.c.} \end{pmatrix} \\ &= \begin{pmatrix} V^A + 3t'(\sqrt{3} \sin\phi - \cos\phi) & -k_1' + i k_2' \\ -k_1' + i k_2' & -V^A - 3t' \left(\sqrt{3} \sin\phi + \cos\phi \right) \end{pmatrix} \\ &= (-3t' \cos\phi) I + \begin{pmatrix} V^A + 3\sqrt{3} t' \sin\phi & -k_1' + i k_2' \\ -k_1' + i k_2' & -\left(V^A + 3\sqrt{3} t' \sin\phi \right) \end{pmatrix} \end{aligned}$$

so that the effective mass at K' is $V^A + 3\sqrt{3} t' \sin\phi$. We see that the effective mass flips sign at each Dirac point (and hence both bands acquire non-zero Chern numbers) if and only if $V^A + 3\sqrt{3} \sin\phi$ and $V^A - 3\sqrt{3} \sin\phi$ have opposite signs, i.e. as long as:

$$3\sqrt{3} |t'| |\sin\phi| \geq |V^A|. \tag{4.37}$$

This inequality can be understood intuitively as follows. A non-zero V^A leads to breaking of "parity" symmetry. Non-zero t' and $\phi \neq 0$ or π lead to breaking of "time-reversal" symmetry. The bands acquire a non-zero Chern number as long as the magnitude of the time-reversal symmetry-breaking perturbation is sufficiently large relative to the magnitude of the parity symmetry-breaking perturbation. The fact that the model can be tuned in such a way that bands can acquire both zero (non-topological phase) and non-zero (topological phase) Chern numbers is one feature which has caused the Haldane model to be widely studied as a toy model of a topological insulator.