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5 Topological States of Matter

5.1 Intro

Thanks to Anton Burkov, U. Waterloo, who lent me a version of these notes.

5.2 Integer Quantum Hall Effect

5.3 Graphene

Graphene is a single layer of graphite, identified as an interesting system early on by theorists, but considered unrealizable in practice until it was isolated using “scotch tape” in 2004 by Geim and Novoselov (Nobel Prize 2010). Graphene has a honeycomb lattice structure, which must be described as a Bravais lattice with a basis, hence has two primitive vectors which may be chosen, e.g. as

\[
\vec{a}_1 = \frac{a}{2}(\hat{x} + \sqrt{3}\hat{y}), \quad \vec{a}_2 = \frac{a}{2}(-\hat{x} + \sqrt{3}\hat{y}),
\]

where \(a\) is the lattice constant of the triangular Bravais lattice. The reciprocal space is spanned by

\[
\vec{b}_1 = \frac{1}{a}(\hat{x} + \frac{\hat{y}}{\sqrt{3}}), \quad \vec{b}_2 = \frac{1}{a}(-\hat{x} + \frac{\hat{y}}{\sqrt{3}}),
\]

so it is convenient to write any vector in 1st BZ as \(\vec{k} = \kappa_1 \vec{b}_1 + \kappa_2 \vec{b}_2\), \(\pi/a \leq \kappa_{1,2} \leq \pi/a\). The tight-binding Hamiltonian is

\[
H = -t \sum_{\langle i\alpha,j\beta \rangle} (c_{i\alpha}^{\dagger}c_{j\beta} + h.c.) + \sum_{i\alpha} m_{\alpha} c_{i\alpha}^{\dagger}c_{i\alpha},
\]

where \(i, j\) label different unit cells, while \(\alpha, \beta = 1, 2\) label the basis sites within each cell. For the moment I’ve suppressed the spin indices. \(m_{\alpha}\) is an on-site energy which can be different on the two sites within the cell. Let’s
consider in particular a site energy $+\,$ on A and $-\,$ on B, \( m_\alpha = (-1)\alpha m \).

Now diagonalize \( H \) by transforming to the new basis

\[
    c_{i\alpha}^\dagger = \frac{1}{\sqrt{N}} \sum_{k\alpha} c_{k\alpha}^\dagger e^{-i\mathbf{k} \cdot \mathbf{R}_i}. \tag{4}
\]

In this simplest tight-binding approximation, note \( \langle i\alpha, j\beta \rangle \) means hoppings only connect sublattices A(1) and B(2),

\[
    H = -t \sum_i \left( c_{i1}^\dagger c_{i2} + c_{i1}^\dagger c_{i-\vec{a}_1,2} + c_{i1}^\dagger c_{i-\vec{a}_2,2} + h.c. \right) + \sum_{i\alpha} m_\alpha c_{i\alpha}^\dagger c_{i\alpha} \\
    = -t \sum_k \left[ c_{k1}^\dagger c_{k2} \left( 1 + e^{-i\mathbf{k} \cdot \vec{a}_1} + e^{-i\mathbf{k} \cdot \vec{a}_2} \right) + c_{k2}^\dagger c_{k1} \left( 1 + e^{i\mathbf{k} \cdot \vec{a}_1} + e^{i\mathbf{k} \cdot \vec{a}_2} \right) \right] \\
    + \sum_{k\alpha} m_\alpha c_{k\alpha}^\dagger c_{k\alpha}. \tag{5}
\]

Note that the sum \( k \) runs over the hexagonally shaped 1st Brillouin zone of the triangular lattice (Fig. 1). This can be represented in a simple way if we identify the sublattice degree of freedom 1,2 as a pseudospin $\uparrow, \downarrow$, and rewrite
\[ H = -\frac{t}{2} \sum_{k,\alpha,\beta} \left[ \sigma_{\alpha\beta}^+ c_{k\alpha}^\dagger c_{k\beta} (1 + e^{ik\cdot\vec{a}_1} + e^{ik\cdot\vec{a}_2}) + \sigma_{\alpha\beta}^- c_{k\alpha}^\dagger c_{k\beta} (1 + e^{ik\cdot\vec{a}_1} + e^{ik\cdot\vec{a}_2}) \right] + \\
+ m \sum_{k\alpha} \sigma_{\alpha\alpha}^z c_{k\alpha}^\dagger c_{k\alpha}, \tag{6} \]

where \( \sigma^{\pm} = \sigma^x \pm i\sigma^y \). To compactify even further, introduce a vector \( \mathbf{d} \) such that

\[
\begin{align*}
    d^z(k) &= m \\
    d^{\pm}(k) &= -t \left( 1 + e^{\mp ik\cdot\vec{a}_1} + e^{\mp ik\cdot\vec{a}_2} \right) \\
    d^x(k) &= \frac{1}{2}(d^+(k) + d^-(k)) = -t \left( 1 + \cos k \cdot \vec{a}_1 + \cos k \cdot \vec{a}_2 \right) \\
    d^y(k) &= \frac{1}{2i}(d^+(k) - d^-(k)) = -t \left( \sin k \cdot \vec{a}_1 + \sin k \cdot \vec{a}_2 \right) \tag{7}
\end{align*}
\]

such that the Hamiltonian takes the form

\[ H = \sum_{k,\alpha,\beta} \mathbf{d} \cdot \vec{\sigma}_{\alpha\beta} c_{k\alpha}^\dagger c_{k\beta}. \tag{8} \]

Now we can find the eigenvalues and eigenstates of \( H \) easily by using the properties of the Pauli matrices. Let \( H = \sum_{k\alpha\beta} H_{\alpha\beta}(k)c_{k\alpha}^\dagger c_{k\beta} \) with \( H(k) = \mathbf{d}(k) \cdot \vec{\sigma} \) and note that

\[
H^2(k) = (\mathbf{d}(k) \cdot \vec{\sigma})(\mathbf{d}(k) \cdot \vec{\sigma}) = d_id_j\sigma^i\sigma^j = \mathbf{d}(k) \cdot \mathbf{d}(k) + \vec{\sigma} \cdot (\mathbf{d} \times \mathbf{d}) = \mathbf{d}(k) \cdot \mathbf{d}(k). \tag{9}
\]

So eigenvalues are

\[ \epsilon_{\pm}(k) = \pm \sqrt{\mathbf{d}(k) \cdot \mathbf{d}(k)}, \tag{10} \]

i.e. two bands symmetric around zero energy. If the “mass” \( m = 0 \), all atoms are alike, \( d^z = 0 \), and both \( d^x(k) \) and \( d^y(k) \) vanish at two distinct wave vectors in the Brillouin zone:

\[ k \cdot \vec{a}_1 = \kappa_1 = \frac{2\pi}{3}, \quad k \cdot \vec{a}_2 = \kappa_2 = -\frac{2\pi}{3}, \tag{11} \]
so that \( k_x = (\kappa_1 - \kappa_2)/a \) and \( k_y = (\kappa_1 + \kappa_2)/(\sqrt{3}a) \). Recalling

\[
\mathbf{k} = \kappa_1 \mathbf{b}_1 + \kappa_2 \mathbf{b}_2 = \kappa_1 \left( \hat{x} + \frac{\hat{y}}{\sqrt{3}} \right) + \kappa_2 \left( -\hat{x} + \frac{\hat{y}}{\sqrt{3}} \right)
\]  

(12)

Now we can rewrite

\[
d^x(\mathbf{k}) = -t (1 + \cos \kappa_1 + \cos \kappa_2) = -t \left[ 1 + 2 \cos \frac{k_x a}{2} \cos \frac{\sqrt{3}k_y a}{2} \right]
\]

\[
d^y(\mathbf{k}) = -t (\sin \kappa_1 + \sin \kappa_2) = -2t \cos \frac{k_x a}{2} \sin \frac{\sqrt{3}k_y a}{2}
\]  

(13)

which vanish when

\[
k_x = \frac{4\pi}{3a}, \quad k_y = 0 \quad \text{(14)}
\]

\[
k_x = -\frac{4\pi}{3a}, \quad k_y = 0 \quad \text{(15)}
\]

Of course these are just two of the 6 \( \mathbf{k} \) related by 60° rotations where the bands touch.

Now let’s expand the Hamiltonian around the 2 Dirac points we’ve picked. Let \( k_x = k_x^0 + \delta k_x, \ k_y = \delta k_y \), and expand the cos and sin’s.

\textsuperscript{1}Recall \( \sigma^2 = 1 \) and \( \sigma^i \sigma^j = i\epsilon_{kij} \sigma^k \) for \( i \neq j \).
Result is
\[ d^x_\pm = \pm \frac{\sqrt{3}ta}{2} \delta k_x \]  
\[ d^y_\pm = \frac{\sqrt{3}ta}{2} \delta k_x, \]  
where ± just means the two points with \( k_x = \pm \frac{4\pi}{3a} \).

Now let \( v = \sqrt{3}ta/2 \) (dimensions of velocity), and rewrite

\[ H_+(k) = v(k_x \sigma^x + k_y \sigma^y) \]  
\[ H_-(k) = v(-k_x \sigma^x + k_y \sigma^y), \]

and for fun (now; later it will be important), let’s add the mass term which distinguishes the two sublattices:

\[ H_+(k) = v(k_x \sigma^x + k_y \sigma^y) + m\sigma^z \]  
\[ H_-(k) = v(-k_x \sigma^x + k_y \sigma^y) + m\sigma^z, \]

and again the eigenvalues can be found by constructing \( H^2_\pm \), so that we have two bands

\[ \epsilon(k) = \pm \sqrt{v^2 k^2 + m^2}, \]

i.e. we have the dispersion of a massive Dirac particle. When \( m = 0 \) the Dirac fermion has a linear spectrum; this corresponds to true graphene.

### 5.4 Quantum spin Hall effect and Kane-Mele model

Reference: Kane and Mele, PRL 95, 226801 (2005).

We will start by considering the Hamiltonian (18) as a model of something, and add some new physics to make it more interesting. Before we go further, let’s discuss the effects of parity \((P : k \rightarrow -k)\) and time reversal \((T : k \rightarrow -k, \ S \rightarrow -S)\). Recall \( \sigma^i \) in (18) acts on the sublattice
degree of freedom. Let’s call the two symmetry-distinct band touching wave vectors $k_{\pm} = \pm (4\pi/(3a), 0)$, and introduce a new pseudospin variable (sometimes called “valley degeneracy”) $\vec{\tau}$ which acts on the $k_{\pm}$ degree of freedom. Then instead of writing $H_{\pm}(k)$ let’s just write $H(k)$ with

$$H(k) = v(k_x \tau^z \sigma^x + k_y \sigma^y) + m \sigma^z,$$

where I’ve reintroduced our sublattice mass modulation term. Let’s examine the effects of parity and time reversal on this $H$. First of all, parity takes sublattice 1 into 2 and vice versa, so that

$$\mathcal{P} : \sigma^z \rightarrow -\sigma^z. \quad (24)$$

(Under $\mathcal{P}$, $\sigma^x \rightarrow \sigma^x$ and $\sigma^y \rightarrow -\sigma^y$, so $d(k) \cdot \vec{\sigma}$ (graphene) is invariant [check!]). But $\mathcal{P}$ also interchanges $k_{\pm}$ so

$$\mathcal{P} : \tau^z \rightarrow -\tau^z. \quad (25)$$

So if we ever had a term like $\tau^z \sigma^z$ it would be invariant. However such a term would violate time reversal ($\mathcal{T}$). To see this, note that since all momenta change sign under time reversal, $\mathcal{T} : \tau^z \rightarrow -\tau^z$. However time reversal does not affect the sublattice degree of freedom, $\mathcal{T} : \sigma^z \rightarrow \sigma^z$. We can generate a term which is invariant under both $\mathcal{P}$ and $\mathcal{T}$ if we remember that until now we have suppressed the true electron spin, and bring it back in the form of an interaction

$$\sigma^z \tau^z S^z,$$

where $S^z$ is the z-component of the electron spin. Since $\mathcal{T} : S^z \rightarrow -S^z$, and $S$ doesn’t care about parity, the product of all three is invariant under $\mathcal{T}, \mathcal{P}$.

This is a simplified version of the spin-orbit interaction in these materials, which we now proceed to discuss. Let’s imagine adding a term to the nearest-neighbor tight-binding Hamiltonian we have so far involving imaginary spin-dependent hoppings on the next-nearest neighbor bonds.
Figure 3: Sense of hoppings leading to positive hopping in spin-orbit Hamiltonian.

(Haldane Phys. Rev. Lett. 61, 2015 (1988), Kane & Mele 2005 ), as shown in Fig. 3. Thus

\[ H_{SO} = -it_2 \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} (S^z)_{\alpha\beta} c^\dagger_{i\alpha} c_{j\beta} + h.c., \]  

(27)

where \( \nu_{ij} = -\nu_{ji} = \pm 1 \), depending on the orientation of the two nearest neighbor bonds \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \) the electron traverses in going from site \( j \) to \( i \). \( \nu_{ji} = +1(-1) \) if the electron makes a left (right) turn to get to the second bond (see arrows in Fig. 3). The spin dependent factor \( \nu_{ij} S^z \) can be written in a coordinate independent representation as \( \mathbf{d}_1 \times \mathbf{d}_2 \cdot \mathbf{S} \). Just as with the nearest-neighbor hopping for the tb graphene model, we can Fourier transform (27) and calculate corrections to \( \mathbf{d}(k) \), and then linearize around the Dirac points. This gives a term in our compact notation (check!!!)

\[ H_{SO}(k) = \Delta_{SO} \sigma^z \tau^z S^z, \]  

(28)

which is invariant under both \( \mathcal{T}, \mathcal{P} \) as discussed above. \( \Delta_{SO} \) turns out to be \( 3\sqrt{3}t_2^2 \).  

\(^2\)Remember the origin of spin-orbit coupling in atoms: it’s a relativistic effect which can be understood crudely
Notice that there is no term in the Hamiltonian at present which actually couples up and down real electron spin.

5.4.1 $S^z = 1$

Therefore let’s consider one spin sector at a time. For spins up, $S^z = 1$, we have

$$H(k) = v(k_x \tau^z \sigma^x + k_y \sigma^y) + \Delta_{SO} \sigma^z \tau^z,$$

or for each “valley” (Dirac point) separately:

$$H_+(k) = v(k_x \sigma^x + k_y \sigma^y) + \Delta_{SO} \sigma^z,$$

$$H_-(k) = v(-k_x \sigma^x + k_y \sigma^y) - \Delta_{SO} \sigma^z. \tag{31}$$

This is the same situation we analyzed for the sublattice mass problem, so we know

$$\epsilon(k) = \pm \sqrt{v^2 k^2 + \Delta_{SO}^2}. \tag{32}$$

Now let’s reintroduce the mass, which cared about sublattice but not about valley pseudospin. Therefore if we have both $m$ and $\Delta_{SO}$ we get

$$H_+(k) = v(k_x \sigma^x + k_y \sigma^y) + (m + \Delta_{SO}) \sigma^z \tag{33}$$

$$H_-(k) = v(-k_x \sigma^x + k_y \sigma^y) - (m - \Delta_{SO}) \sigma^z \tag{34}.$$

Now we can consider two extreme possibilities. First, imagine $m \gg \Delta_{SO}$. As discussed above, this opens up a gap $m$ at the Dirac points, so we have an insulator simply because we put a different potential on the 1 and 2 sublattices. This is called an “atomic” or “trivial” insulator. Now increase $\Delta_{SO}$ relative to $m$. Nothing happens in the $H_+$ block, but in the $H_-$ block the gap closes and reopens again when $\Delta_{SO} > m$. The $\Delta_{SO} > m$ insulator is separated from the atomic insulator by a gap-closing phase transition. Therefore (see below) the distinction between the two is topological.

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*by boosting to a moving electron’s frame, and saying there is a magnetic field $B$ due to the moving charged nucleus (or here, the ionic lattice), equal to $B = (v \times E)/c = (p \times E)/(mc)$. $B$ acts on the electron spin, thus coupling spin and momentum.*
Let’s investigate what this really means by looking at the response of the system to an applied field. We are really interested in the $T$ invariant case without field, but it will help us to classify the states and then we will take the field strength to zero. To include the field we will replace $k$ everywhere by $-i\nabla + \frac{e}{c}A$, and choose gauge $A = xB\hat{y}$ for a field $B\hat{z}$. This gives for valleys $\pm$:

\begin{align*}
H_+ &= -iv\frac{\partial}{\partial x}\sigma^x + \left(-i\frac{\partial}{\partial y} + \frac{x}{\ell_B^2}\right)\sigma^y + (m + \Delta_{SO})\sigma^z \tag{35} \\
H_- &= iv\frac{\partial}{\partial x}\sigma^x + \left(-i\frac{\partial}{\partial y} + \frac{x}{\ell_B^2}\right)\sigma^y + (m - \Delta_{SO})\sigma^z, \tag{36}
\end{align*}

where $\ell_B = \sqrt{c/eB}$ is magnetic length. Again we will use the trick of squaring $H_\pm$ in order to find the eigenvalues. For example

\begin{align*}
H_+^2 &= \left[-iv\frac{\partial}{\partial x}\sigma^x + \left(-i\frac{\partial}{\partial y} + \frac{x}{\ell_B^2}\right)\sigma^y + (m + \Delta_{SO})\sigma^z \right] \\
&\quad \cdot \left[-iv\frac{\partial}{\partial x}\sigma^x + \left(-i\frac{\partial}{\partial y} + \frac{x}{\ell_B^2}\right)\sigma^y + (m + \Delta_{SO})\sigma^z \right] \\
&= -v^2\frac{\partial^2}{\partial x^2} + v^2 \left(i\frac{\partial}{\partial y} + \frac{x}{\ell_B} \right)^2 + (m + \Delta_{SO})^2 + \text{cross-terms},
\end{align*}

and for the cross-terms we use the anticommutation of the Pauli matrices $\sigma_i\sigma_j = \sigma_j\sigma_i$ for $i \neq j$. Check then that these just reduce to $-iv^2i\sigma^z(1/\ell_B^2)[(\partial/\partial x),x] = (v^2/\ell_B^2)\sigma^z$, so

\begin{equation}
H_+^2 = -v^2\frac{\partial^2}{\partial x^2} + v^2 \left(i\frac{\partial}{\partial y} + \frac{x}{\ell_B} \right)^2 + (m + \Delta_{SO})^2 + \omega_B^2\sigma^z, \tag{37}
\end{equation}

where $\omega_B = v/\ell_B$ is the Dirac cyclotron frequency. Note the first two terms have the form of $H$ (not $H^2$) for a regular 2DEG with “mass”
1/(2v^2). The corresponding “cyclotron frequency” is

$$\omega_{c}^{\text{eff}} = \frac{eB}{mc} \equiv \frac{2v^2}{l_B^2} = 2\omega_B^2.$$  \hfill (38)

Thus the eigenvalues of $H_+^2$ can be read off

$$2\omega_B^2(n + 1/2) + (m + \Delta_{SO})^2 + \omega_B^2\sigma^z ; \quad n = 0, 1, 2, \ldots,$$  \hfill (39)

and the spectrum of $H_+$ itself is

$$\epsilon_{n+} = \pm \sqrt{2\omega_B^2 n + (m + \Delta_{SO})^2} ; \quad n = 1, 2, \ldots.$$  \hfill (40)

$$\epsilon_{0+} = -(m + \Delta_{SO}).$$  \hfill (41)

Now one can go back and do the same thing for $H_-$ (still for real spin up!), and find

$$H_-^2 = 2\omega_B^2(n + 1/2) + (m - \Delta_{SO})^2 - \omega_B^2\sigma^z$$  \hfill (42)

$$\epsilon_{n-} = \pm \sqrt{2\omega_B^2 n + (m - \Delta_{SO})^2} ; \quad n = 1, 2, \ldots.$$  \hfill (43)

$$\epsilon_{0-} = m - \Delta_{SO}.$$  \hfill (44)

Now when $m > \Delta_{SO}$, we have the same number of Landau levels above and below zero energy. The Hall conductivity with $\epsilon_F = 0$ is therefore $\sigma_{xy} = 0$. However, once $\Delta_{SO} > m$, both $\epsilon_{0+}$ and $\epsilon_{0-}$ are below $\epsilon = 0$, so there is one extra filled Landau level in this case so that the Hall conductivity becomes $\sigma_{xy} = e^2/h$.\textsuperscript{3} Now notice that the ordering of levels or the sign of their energies did not depend on the strength of the applied field $B$. Thus we can take $B \to 0$ and will be left with an insulator (quantum Hall insulator) which displays $\sigma_{xy} = +e^2/h$ for $S^z = 1$, i.e. spins ↑.

5.4.2 $S^z = -1$

Now follow exactly the same steps for $S^z = -1$. For completeness I’ll write it out explicitly, but basically only signs of $\Delta_{SO}$ terms change:

\textsuperscript{3}In the integer quantum Hall effect we expect $\sigma_{xy} = ne^2/h$ for a filled Landau level. For graphene $\epsilon_F$ at the Dirac point, $\sigma_{xy} = 0$, due to two doubly degenerate levels corresponding to $n = 0$. 
\[ H(k) = v(k_x \tau^z \sigma^x + k_y \sigma^y) + m \sigma^z - \Delta_{SO} \sigma^z \tau^z, \]  

(45)

\[ H_+(k) = v(k_x \sigma^x + k_y \sigma^y) + (m - \Delta_{SO}) \sigma^z \]  

(46)

\[ H_-(k) = v(-k_x \sigma^x + k_y \sigma^y) + (m + \Delta_{SO}) \sigma^z. \]  

(47)

so the Landau level structure is

\[ \epsilon_{n+} = \pm \sqrt{2 \omega_B^2 n + (m - \Delta_{SO})^2}; n = 1, 2, \ldots \]  

(48)

\[ \epsilon_{0+} = -(m - \Delta_{SO}) \]  

(49)

\[ \epsilon_{n-} = \pm \sqrt{2 \omega_B^2 n + (m + \Delta_{SO})^2}; n = 1, 2, \ldots \]  

(50)

\[ \epsilon_{0-} = m + \Delta_{SO}. \]  

(51)

so when \( \Delta_{SO} > m \), there is one more Landau level\(^4\) above \( \epsilon = 0 \), so by the same argument the Hall conductivity should become \( \sigma_{xy} = -e^2/h \), again even for \( B \to 0 \). Thus the picture which emerges is that of an insulator which differs from the trivial one in that spins have finite, but opposite Hall conductivities even in zero field, due to the spin-orbit interaction. Thus spins up and down will accumulate on opposite sides of a Hall bar carrying a longitudinal electric current due to an applied electric field. This is not unique to topological insulators, of course, but is a property of semiconductors with spin-orbit coupling.

### 5.5 Edge states

In fact we haven’t yet shown that the spin current is carried by edge states, as in Fig. 4. This can be done by a gauge argument analogous to that

\(^4\)Note that states are labelled by \( n \) and \( \sigma^z \), and that (almost) all eigenvalues are doubly degenerate, namely the eigenvalues corresponding to \( n = m - 1 \) and \( \sigma^z = 1 \) is equal to the eigenvalue with \( n = m \) and \( \sigma^z = -1 \). This is true for all eigenvalues except one: with \( n = 0 \) and \( \sigma^z = -1 \). This one is “unpaired” and its eigenvalue (for \( H^2_+ \)) is equal to \( (m + \Delta_{SO})^2 \). Since the total number of states is unchanged when you square the Hamiltonian, this state must remain a single state when we take the square root, i.e. we must pick only one sign of the eigenvalue. To find the correct sign, we simply take the \( (m + \Delta_{SO}) \sigma^z \) term in \( H_+ \) and use the fact that the zero-mode state corresponds to \( \sigma^z = -1 \). The remaining part of \( H_+ \) gives zero when acting on the zero-mode state.
given by Laughlin for the integer QHE, or by explicit solution for a given geometry. The Schrödinger equation can be solved numerically in finite geometry by imposing open transverse boundary conditions. In this case Kane and Mele showed the solution (Fig. 5), which exhibits the bulk gapped Dirac like states and two characteristic states which cross at the Dirac point and carry the current; direct examination of the eigenfunctions shows that they are indeed edge states.

We can show without involved numerics that such edge states exist if we put in the "edge" by a bit of sleight of hand. Consider for example the $H_+$ block for spin up $S^z = 1$. Assume the sample has an edge at $y = 0$, and the sample exists for $y < 0$, and $y > 0$ is vacuum. There will be some
spatial variation along the $y$ direction giving the edge state wave function, but we can assume translational invariance along $x$ and take $k_x = 0$. Then the Hamiltonian is

$$H_{-}(y) = -iv \frac{\partial}{\partial y} \sigma^y + (m - \Delta_{SO}) \sigma^z \equiv -iv \frac{\partial}{\partial y} \sigma^y + \tilde{m}(y) \sigma^z, \quad (52)$$

where I’m now considering a $y$-dependent potential given by $\tilde{m}(y)$, which I will insist change sign at the edge, such that $\tilde{m}$ is $< 0$ for $y < 0$, i.e. in the sample, $\tilde{m} > 0$ for $y > 0$. We’re looking for a zero-energy edge state wave function. Make the ansatz for the solution to the Schrödinger equation

$$\psi(y) = i \sigma^y e^{f(y)} \phi, \quad (53)$$

where $\phi$ is a 2-component spinor field. Plugging in, we get

$$\left( i v \frac{df}{dy} + \tilde{m}(y) \sigma^x \right) \phi = 0, \quad (54)$$

which has the formal solution

$$f(y) = -\frac{1}{v} \int_{0}^{y} dy' \tilde{m}(y') \quad ; \quad \sigma^x \phi = \phi, \quad (55)$$

i.e. $\phi$ is an eigenstate of $\sigma^x$ with e-value 1. Note that the effect of $i \sigma^y = \exp \frac{i \pi}{2} \sigma^y$ is to rotate by $\pi$ around the $y$-axis. So the total solution is

$$\psi(y) = \exp - \left( \frac{1}{v} \int_{0}^{y} dy' \tilde{m}(y') \right) |\sigma^x = -1). \quad (56)$$

One can be more explicit by assuming an “edge” like $\tilde{m}(y) = \tilde{m}_0 \tanh(y/y_0)$, in which case one finds $\psi \propto \exp - (y_0 \tilde{m}_0 / v) \log \cosh(y/y_0)$, which is a state of width $v/\tilde{m}_0$.

Remarks:

1. The fact that the state is an eigenstate of $\sigma^x$ apparently reflects the fact that it mixes the two sublattices by hopping along the boundary.
2. At finite $k_x$, the same state has energy $\epsilon(k_x) = -vk_x$, so that $v(k_x) = \partial \epsilon(k_x) / \partial k_x = -v$.

3. For $S^z = -1$ we would take $\tilde{m} \rightarrow -\tilde{m}$ in the large $\Delta_{SO}$ limit find an edge state with velocity in the opposite direction.

4. I chose arbitrarily one Dirac point $H_-$. Could have chosen $H_+$ as well. There should be two edge state solutions there as well, one for each spin.

5.6 Topological character of new insulating phase

We’ve been dancing around the obvious question, what’s actually topological about topological insulators? This question is important because to qualify as a new state of matter they need to have something fundamentally different, and the claim is that such new insulating states do NOT (necessarily) break any symmetry, as do magnets, superconductors, crystals, and other phases we regard as distinct. The claim is that there is a topological invariant which characterizes such a phase, reflecting a finite energy gap towards deformation of the state into a new phase of trivial topological invariant, i.e. the state is robust against small perturbations.

To see this explicitly, let’s again take $S^z = 1$ and consider $H_{\pm}(k)$

\[
H_{+}(k) = v(k_x \sigma^x + k_y \sigma^y) + (m + \Delta_{SO}) \sigma^z
\]

\[
H_{-}(k) = v(-k_x \sigma^x + k_y \sigma^y) + (m - \Delta_{SO}) \sigma^z,
\]

recalling that we can write the Hamiltonian in terms of a $d$-vector, $H_{\pm}(k) = d_{\pm}(k) \cdot \vec{\sigma}$,

\[
d_{\pm}(k) = (\pm vk_x, vk_y, m \pm \Delta_{SO}),
\]

and define $\hat{d}_{\pm} = d_{\pm} / |d_{\pm}|$. $\hat{d}(k)$ defines a mapping of 2D momentum space $k_x, k_y$ to a unit sphere, for given $v, m, \Delta_{SO}$. This mapping can be assigned a topological index (Berry phase) which represents the number
of times that $\hat{d}$ wraps around the sphere as a function of $k$,

$$n = \frac{1}{4\pi} \sum_{\alpha} \int d\kappa \left( \partial_{kx} \hat{d}_\alpha \times \partial_{ky} \hat{d}_{alpha} \right) \cdot \hat{d}_\alpha,$$

(60)

and for smooth $\hat{d}$ it may be shown that $n$ is always an integer. In Fig. 6 I sketch $\hat{d}_\pm$ for the simple example given above. For $m > \Delta_{SO}$ the $k_z$ component is the same, e.g. in the upper hemisphere $k_z > 0$, so we can just examine the winding in the $xy$ plane in the upper hemisphere, which is given by $+1$ for $\hat{d}_+$ and $-1$ for $\hat{d}_-$, so the sum is $\frac{1}{2} - \frac{1}{2} = 0$. For the case $m < \Delta_{SO}$, however, the $k_z$ component is reversed for $\hat{d}_-$, so one should compare/add the winding from the upper hemisphere $k_z > 0$ for $\hat{d}_+$ and from the lower hemisphere $k_z < 0$ for $\hat{d}_-$, which means the windings add, $\frac{1}{2} + (-(-\frac{1}{2})) = 1$. This index therefore distinguishes a trivial insulator from a topological one.
Figure 6: Winding of $\hat{d}_\pm$ over unit sphere. a) Case $m > \Delta_{SO}$. b) Case $\Delta_{SO} > m$. 