

I. TOPOLOGICAL INSULATORS IN 1,2 AND 3 DIMENSIONS

A. Edge mode of the Kitaev model

Let's assume that the chain only stretches between $x = 0$ and $x \rightarrow \infty$. In the topological phase there should be a Jackiw-Rebbi state at the $x = 0$ edge. Can we guess that it is going to be at zero? Let's try to find a particle hole symmetry. Both $\mathcal{R} = \sigma^y$ and $\mathcal{C} = \hat{K}\sigma^x$ would give:

$$\mathcal{R}\hat{\mathcal{H}}\mathcal{R} = \mathcal{C}\hat{\mathcal{H}}\mathcal{C} = -\hat{\mathcal{H}} \quad (1)$$

So a single edge state would be pinned to $E = 0$. Let's find it.

If we guess an exponential decay, we can replace e^{ikn} with $e^{-\kappa n} = \zeta^n$. The solution, we guess, will have the form:

$$|\psi(x)\rangle = \zeta^n \begin{pmatrix} u \\ v \end{pmatrix} \quad (2)$$

The lattice SE of the Kitaev mode then becomes:

$$\left[(-J(\zeta + 1/\zeta)/2 - \mu)\sigma^z - i\frac{g}{2}(\zeta - 1/\zeta)\sigma^x \right] \begin{pmatrix} u \\ v \end{pmatrix} = 0 \quad (3)$$

Which can only have a solution by:

$$-\frac{J}{2}(\zeta + 1/\zeta) - \mu = \pm \frac{g}{2}(\zeta - 1/\zeta) \rightarrow \zeta^2(J \pm g) + \mu\zeta + (J \mp g) = 0 \quad (4)$$

This would give a SE of the form:

$$(\sigma^z - \mp i\sigma^x) \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1 & -\mp i \\ \pm i & -1 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0 \quad (5)$$

Which does have a solution:

$$(u, v) = (1, \mp i) \quad (6)$$

For ζ this yields

$$\zeta = \frac{\mu \pm \sqrt{\mu^2 - (J^2 - g^2)}}{J \pm g} \quad (7)$$

four solutions. Two of the solution actually belong to decaying solutions of the bound states on the right edge, with $|\zeta| > 1$. The other two must be $|\zeta| < 1$ with the same spinor.

But why two solutions? We need to satisfy boundary conditions. In first order difference equation, it is okay to require that the wave function vanishes at site $n = 0$ (the first site to the left of where the chain terminates). With a single exponent this is impossible. But if we have two solutions for ζ with the same spinor associated with them, then we can write the solution as:

$$|\psi(n)\rangle = (\zeta_1^n - \zeta_2^n) \begin{pmatrix} u \\ v \end{pmatrix}. \quad (8)$$

Choosing then the + option for the denominator of (7), we have the two solutions:

$$\zeta_{1,2} = \frac{\mu \pm \sqrt{\mu^2 - (J^2 - g^2)}}{J + g} \quad (9)$$

and $(u, v) = (1, -i)$.

Crucially, this is a σ^y eigenvalue. This is going to be very important below.

When do we stop having a solution? When ζ touches 1. Indeed, substitute $\mu = J$ and you find it:

$$\zeta_{1,2} = \frac{J \pm g}{J + g} \quad (10)$$

and the edge state penetrate the bulk.

II. 2D TOPOLOGICAL INSULATOR

The same kind of physics can be done also in 2d. there are two good examples close to our hearts. First is the BHZ model. Second, the Haldane model.

A. The BHZ hamiltonian

The easiest path to topological 2d behavior is to try to get a nontrivial Berry curvature in na 2d band structure. We already have the 1d Kitaev model as a template that gives us a winding in the z-x lane. Sitting at $p = 0$ would be good then to have another dimension introduced, p_y , that will cause a winding in the $z - y$ plane. This is not hard:

$$\hat{H} = (m - J \cos p_x)\sigma^z + v \sin p_x \sigma^x \rightarrow (m - J \cos p_x - J \cos p_y)\sigma^z + v \sin p_x \sigma^x + v \sin p_y \sigma^y \quad (11)$$

That ought to do the trick! This is the Bernevig, Hughes, and Zhang model. Or half of it at least - more on that below.

How can we tell? There is a trick. Notice that the points $p_x, p_y = 0, \pi$ are special points. They are sometimes called time-reversal invariant momenta (TRIM's for short). Time reversal maps $\vec{p} \rightarrow -\vec{p}$. But since momentum is defined mod 2π , $p = \pi$ and $p = -\pi$ are the same point. For these points, the model has only σ^z components, since $\sin p_{x,y} = 0$. A nontrivial wrapping would result in the spin pointing in the north or south pole an odd number of points. You can easily see that this boils down to:

$$m - 2J < 0, \text{ and } m + 2J > 0. \quad (12)$$

This would give the topological phase, with an integer winding when $|m| < 2J$. To be more precise, using symmetries such as $\mathcal{R}_1 = \mathcal{K}$ (complex conjugation) or $\mathcal{R}_2 = \mathcal{K}\sigma^z$ which map:

$$\mathcal{R}_1 \hat{H}(p_x, p_y) \mathcal{R}_1 = \hat{H}(-p_x, p_y), \quad \mathcal{R}_2 \hat{H}(p_x, p_y) \mathcal{R}_2 = \hat{H}(-p_x, -p_y) \quad (13)$$

From this we can infer that on the TRIM's the Hamiltonian can only depend on σ^z :

$$\hat{H}(\vec{p}_{TRIM}) = h_z(\vec{p})\sigma^z \quad (14)$$

Using that we can write:

$$I_p = \frac{1}{2} \left(1 - \prod_{\vec{p} \in TRIM} \text{sign}(h_z(\vec{p})) \right) = I_{mod 2} \quad (15)$$

With:

$$I = \frac{1}{2\pi} \int dp_x \int dp_y \Omega(p_x, p_y) \quad (16)$$

being the wrapping of the Bloch sphere by the spinor of each of the bands. I is also called the Chern number. And the model is referred to as a Chern insulator.

In the case above, since we only expect one wrapping, the Chern number is the same as the product inde I_p of Eq. (28).

The BHZ model also has a continuum version which we can obtain by expanding in small \vec{p} :

$$\hat{H} = (m - J\vec{p}^2)\sigma^z + vp_x \sigma^x + vp_y \sigma^y \quad (17)$$

Instead of a Brillouine zone, we should think about the whole 2d momentum space. By inspecting the Hamiltonian, which has the form $\hat{H} = \vec{h} \cdot \vec{\sigma}$ we see that the vector $\vec{h}(\vec{p})$ covers the bloch sphere if $J > 0$. At $\vec{p} = 0$, \vec{h} points in the z-direction. The x and y components make sure that the \vec{h} covers all longitudes. So the only question for making sure that there is a complete wrapping has to do with what happens when $\vec{p} \rightarrow \infty$. If $J > 0$, the p^2 term will drive the z-component of \vec{h} negative at some momentum, and at $\vec{p} \rightarrow \infty$ \vec{h} would point strictly in the south pole of the bloch sphere.

B. edge states of the BHZ model

Topological behavior, at least in my mind, is synonymous with an interesting edge state behavior. The 2d Chern band has propagating chiral edge states. They move in one direction. Let's see how this works. Consider an edge along the y direction. If we set $p_y = 0$, the BHZ model has the same form as the 1d topological superconductor. Therefore it has a zero energy edge state of the form:

$$|\psi(x)\rangle = (e^{-\kappa_1 x} - e^{-\kappa_2 x}) \begin{pmatrix} 1 \\ -i \end{pmatrix} \quad (18)$$

Now turn on a small p_y , and the model becomes:

$$\hat{\mathcal{H}} \approx \hat{\mathcal{H}}_{edge} + \sigma^y v p_y \quad (19)$$

How do we solve it? No problem!

$$|\psi(x, y)\rangle = e^{-\kappa x} \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{-ik_y y} \quad (20)$$

and the energy will be:

$$\epsilon_{edge}(k_y) \approx v k_y \quad (21)$$

This is a propagating state with the spin in the direction of propagation. It is chiral - only propagates along the positive y direction. Just like the edge states of a Landau level. This is a hallmark of a Chern insulator.

C. CdTe/HgTe quantum wells

The BHZ model describes a Chern band with a time reversal symmetry broken. how do we know that it is broken? Simple - the electronic edge states move in a very specific direction - in the way we set it up it was clockwise. But quantum wells do not break time reversal symmetry. Actually, the BHZ hamiltonian arose from an attempt to describe the band structure of mass-inverted quantum 2d wells. Particularly Mercury Telluride - a 2-6 semiconductor.

There is a simple way of turning the model that we wrote above to be time reversal symmetric: Double it. Let's add another degree of freedom in the form of another set of Pauli matrices, $\vec{\tau}$. When in doubt, time reversal is given by $\hat{T} = i\sigma^y \hat{K}$. And in the case of the hamiltonian in (11), we have:

$$\hat{\mathcal{H}} = (m - J \cos p_x - J \cos p_y) \sigma^z + v \sin p_x \sigma^x + v \sin p_y \sigma^y \rightarrow \hat{T} \hat{\mathcal{H}} \hat{T} = -(m - J \cos p_x - J \cos p_y) \sigma^z + v \sin p_x \sigma^x + v \sin p_y \sigma^y \quad (22)$$

We can put both sectors into a 4X4 matrix in the following way:

$$H_{BHZ} = \begin{pmatrix} \hat{\mathcal{H}} & 0 \\ 0 & \hat{T} \hat{\mathcal{H}} \hat{T} \end{pmatrix} \quad (23)$$

and with the time reversal sector occupying the $\tau^z = -1$ part of the matrix, and $\hat{\mathcal{H}}$ the $\tau^z = 1$ part, we have:

$$\hat{\mathcal{H}}_{BHZ} = \mathbf{1}_\tau + v \sin p_x \sigma^x + v \sin p_y \sigma^y + \sigma^z \tau^z (m - J \cos p_x - J \cos p_y) \quad (24)$$

This describes a 4-band model where the σ matrices could be thought of as spin, while the τ^z indicate the pseudo spin. You could think about this as a model for a total angular momentum $J = 3/2$ with 4 states. The $m = 3/2, 1/2$ form one Chern insulator, while the $m = -1/2, -3/2$ form another one.

Indeed, the edge state we found above, will now have a counter propagating counter part with:

$$|\psi+\rangle = (e^{-\kappa_1 x} - e^{-\kappa_2 x}) \begin{pmatrix} 1 \\ -i \end{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix}, |\psi-\rangle = (e^{-\kappa_1 x} - e^{-\kappa_2 x}) \begin{pmatrix} 0 \\ 1 \\ +i \end{pmatrix} \quad (25)$$

In the full 4-d space.

III. 3D TOPOLOGICAL INSULATORS

And we can get this also up to 3 dimensions. Here I will do it without a derivation. By now, however, I think you get the idea of how to construct these phases. To go from 1d to 2d, we expanded the number of anticommuting matrices to 3 from 2. Now we need to add yet another anticommuting matrix. With 4 anticommuting operators, we can have an operator for each of the $\sin p_\alpha$ for $\alpha = x, y, z$, as well for the momentum even term, $m - J \left(\sum_{\alpha=x,y,z} \cos p_\alpha \right)$. What could these matrices be? we have the three σ^α Pauly matrices. We can have more if we incorporate the τ^α for pseudo-spin. How about using the $\vec{\sigma}\tau^x$ product for the $\sin p_\alpha$, and the τ^z matrix for the $\cos p_\alpha$ parts? This results in the guess:

$$H_{3DTI} = v \sum_{\alpha=x,y,z} \tau^z \sigma^\alpha \sim p_\alpha + \tau^z (m - J \left(\sum_{\alpha=x,y,z} \cos p_\alpha \right)) \quad (26)$$

This is the standard band structure for a 3d TI. The discovery of 3dTI was a great and rare example of theory-first with Joel Moore and Leon Balents suggesting them a couple of days before Charlie Kane and Liang Fu. But these four are all credited with the discovery. Following Moore and Balents description, we need to look at the TRIM's. You can easily come up with the symmetries that convince you that only the τ^z pieces in the hamiltonian are important at $p_\alpha = 0, \pi$. To be topological, we need these 8 points to have an odd number of positive and negative values. the trims τ^z term has (number of trims to the side):

$$\begin{array}{cc} m - 3J & 1 \\ m - J & 3 \\ m + J & 3 \\ m + 3J & 1 \end{array} \quad (27)$$

So for $J < |m| < 3J$ we have a topological phase. Indeed, as in the 2d case, we can write the product of the sign of the hamiltonian on the TRIM's:

$$I_p = \frac{1}{2} \left(1 - \prod_{\vec{p} \in TRIM} \text{sign}(h_z(\vec{p})) \right) = I \text{ mod } 2. \quad (28)$$

And now that we understand, kind of, the topological index, we need to look for edge states. Let's look at a terminating surface that is normal to the z -axis. Again, we can construct the symmetries that would convince us that at $p_x = p_y = 0$ we expect a zero energy state. The Hamiltonian becomes:

$$H_{surface}(p_x, p_y = 0) |psi\rangle = ((m - 2J - J \cos p_z) \tau^z + v \sin p_z \sigma^z \tau^x) |\psi\rangle = 0 \quad (29)$$

Wait - this looks exactly the same as the hamiltonian for a 1d TI edge state! except $\sigma^z \rightarrow \tau^z$ and $\sigma^x \rightarrow \sigma^z \tau^x$ relative to Eq. (??). The solution of the 1d TI edge state was an eigenstate of $\sigma^y = i\sigma^x \sigma^z$. So we expect by analogy (or direct mapping, if you wish) that the solution here will be an eigenstate of $i\tau^x \sigma^z \cdot \tau^z = \sigma^z \tau^y$. So:

$$\sigma^z \tau^y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} \quad (30)$$

And the edge state would be:

$$|\psi\rangle = f(z) \begin{pmatrix} q \\ u \\ v \\ w \end{pmatrix}, \quad (31)$$

Since there are two solutions for each eigenvalue of $\sigma^z \tau^y$ we find two zero energy solutions. E.g. for:

$$\sigma^z \tau^y \begin{pmatrix} q \\ u \\ v \\ w \end{pmatrix} = 1 \rightarrow |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \\ i \\ 0 \end{pmatrix}, \text{ and, } |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -i \end{pmatrix} \quad (32)$$

What happens when we turn on the parallel momenta p_x and p_y ? We have:

$$\hat{\mathcal{H}} \approx \hat{\mathcal{H}}_{surface}(p_x, p_y = 0) + \tau^x \sigma^x v p_x + \tau^x \sigma^y v p_y \quad (33)$$

Now note that $[\tau^x \sigma^y, \tau^y \sigma^z] = [\tau^x \sigma^x, \tau^y \sigma^z] = 0!$ So the surface zero state has a spinor structure that already diagonalizes the remaining pieces of the surface hamiltonian. So a linear combination of the $|\uparrow\rangle, |\downarrow\rangle$ should diagonalize the $\tau^x \sigma^{x,y}$ matrices. Since we are working in the subspace where $\sigma^z \tau^y = 1$, we can also write, within this subspace:

$$\tau^x \sigma^y = \tau^x \sigma^y \cdot \tau^y \sigma^z = -\tau^z \sigma^x, \quad \tau^x \sigma^x = \tau^x \sigma^x \cdot \tau^y \sigma^z = \tau^z \sigma^y. \quad (34)$$

Furthermore, in the basis of $|\uparrow\rangle, |\downarrow\rangle$, these operators just operate as the σ matrix components. So we get that the surface hamiltonian is:

$$\hat{\mathcal{H}}_{Surface} = v (p_x \sigma^y - p_y \sigma^x) \quad (35)$$

A totally spin-orbit locked Dirac cone! Furthermore, a single Dirac cone! This seems to contradict Fermion doubling theorem. The resolution of that is that there is another Dirac cone with the opposite chirality on the opposite surface.

Now, adding a magnetic field (Zeeman term) perpendicular to the surface adds a term $b\sigma^z$. This will gap the surface into a hall state with half the conductance quantum with $\sigma_{xy} = e^2/2h$. Proximatizing the surface to superconductor would give a single-flavor superconducting state - a topological p-wave state! And vortices in such a superconductor would carry majorana modes.

For the high-energy aficionados amongst you, when the surface is gapped by a magnetic field, the bulk of the TI supports an Axion term in the action:

$$\mathcal{L}_{axion} = \pi \vec{E} \cdot \vec{B}. \quad (36)$$

which implies that a charge e inserted to the bulk will produce a magnetic field around it corresponding to a magnetic monopole. Many things that will be explored in 223ab!