## Fermions and Topological Phases, III

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There is one topic we discussed the first time that I want to say a little more about. In the first lecture, we studied Weyl semimetals and by explicitly solving the Dirac equation, we learned that there must be surface states – Fermi arcs. We considered the Hamiltonian

$$H = -i\vec{\sigma} \cdot \frac{\partial}{\partial \vec{x}}$$

on a half-space  $x_1 \ge 0$  with the boundary condition

$$\sigma_2 \psi | = \psi.$$

We found surface localized states at zero energy

$$\psi = \exp(ikx_3 - kx_1)\psi_0, \quad \sigma_2\psi_0 = \psi_0, \quad k > 0.$$

I should have pointed out that there are analogous surface-localized states of energy  $\varepsilon$ , for any  $\varepsilon$ :

$$\psi = \exp(i\varepsilon x_2)\exp(ikx_3-kx_1)\psi_0, \quad \sigma_2\psi_0=\psi_0, \quad k>0.$$

Pictures I drew that only showed surface-localized states of  $\varepsilon = 0$  were a little misleading.

Actually, the original paper predicting these states (Wan, Turner, Vishwanath, and Savrasov, 2011) did not proceed by explicitly picking a boundary condition and solving the Dirac equation. Rather, they deduced the result from some things that we discussed yesterday. I want to explain how this goes.

First we recall the basic setup. Weyl points arise at special points in the Brillouin zone at which valence and conduction bands meet.



Near a boundary of a finite sample, only two of the three components of momentum are conserved. So it is useful to project the Brillouin zone and the bad points in it to two dimensions, "forgetting" the component of momentum that is not conserved:



It is important to remember that in a crystal, the momentum components, including the component that is being "forgotten", are periodic, and in particular the horizontal direction in the picture represents a circle  $U \cong S^1$ , though it is hard to draw this.

Now draw a little circle U' around the projection of one of the bad points:



The product  $U \times U'$  is a two-torus



We define an integer  $k^*$  as the Berry flux through  $U \times U'$ :

$$k^* = \int_{U \times U'} \mathrm{d}^2 p \, \frac{\mathrm{Tr} \, \mathcal{F}}{2\pi}.$$

It receives a contribution of 1 or -1 for each positive or negative Weyl point enclosed by  $U \times U'$ . So in the example drawn,  $k^* = 1$ , but we would get  $k^* = 0$  or  $k^* = -1$  if we take U' to encircle one of the other two special points in the projection. We have arranged so that the two-torus  $U \times U'$  does not intersect any of the Weyl points. So the restriction to  $U \times U'$  of the original 3d band Hamiltonian on the 3d Brillouin zone *B* is a gapped Hamiltonian  $H^*$  on a two-torus  $U \times U'$ . We can intepret  $H^*$  as the band Hamiltonian of some 2d lattice system that has a Hall conductivity of  $k^*$ . So as we have learned,  $H^*$  has edge modes, equal in number to  $k^*$ , that "bridge the gap" in energy between the filled and empty bands



So there have to be edge states that intersect U' (the edge states are not labeled by U since U parametrizes the component of momentum that is not relevant to edge states). Since we had a lot of freedom in the choice of U', the spectrum of edge-localized points has to consist of arcs that link the appropriate boundary projections. In our example, this means edge states as shown



The auxiliary 2d quantum Hall system that was used in this argument does not have any simple relation to the 3d Weyl sem-metal that we were studying, as far as I know.

Inspired partly by Hasan's lecture of yesterday, I want to consider a simple explicit model in which Weyl point of positive and negative chirality annihilate and disappear. A particle physicist would perhaps try to do this by starting with a 4-component Dirac fermion and adding suitable perturbations, but in condensed matter what we want can easily happen with two bands. We consider the Hamiltonian

$$H = \sigma_1 p_1 + \sigma_2 p_2 + \sigma_3 (p_3^2 - a).$$

For a > 0, there are Weyl points at

$$p_1 = p_2 = 0, \ p_3 = \pm \sqrt{a}.$$

It is not hard to see that they have opposite chirality. There is a reflection symmetry

$$(p_1, p_2, p_3) \rightarrow (p_1, p_2, -p_3)$$

that makes it natural that they are at the same energy. For a < 0, the two Weyl points annihilate and disappear.

Now let us look at Fermi arcs connecting to the Weyl points. We take a boundary at  $x_1 = 0$  and for simplicity we take the boundary condtion to be

$$M\psi|=\psi|, \ M=\pm\sigma_2.$$

Also for simplicity we will only discuss the edge localized states at  $\varepsilon = 0$ . The condition  $\pm p_3 > 0$  that we had in the first lecture is simply replaced by

$$\pm (p_3^2 - a) > 0$$

where the sign is the sign of M.

For a > 0 where there are Weyl points, the condition  $\pm (p_3^2 - a) > 0$  gives two quite different pictures depending on the sign.



In the first case, for a < 0, there are Fermi arcs at  $\varepsilon = 0$  that no longer have Weyl points to connect to, and in the second case, for a < 0, there no longer are any Fermi arcs at  $\varepsilon = 0$ .

Yesterday Hasan described a more elaborate version of this.



There remain three topics that I want to describe:

(1) More on the fractional quantum Hall effect.

(2) Another explanation of edge modes in the integral quantum Hall effect.

(3) Haldane's model of quantum Hall physics without an applied magnetic field.

As yesterday, we describe a fractional quantum Hall system macroscopically by an effective action for the electromagnetic vector potential A and an "emergent" U(1) vector potential a that only exists inside the fractional Hall material. We can take the effective action to be the sum of the bulk Maxwell action

$$\frac{1}{2e^2}\int_{\mathbb{R}^{3,1}}\mathrm{d}^3x\mathrm{d}t\,\left(\vec{E}^2-\vec{B}^2\right)$$

plus a term that "lives" in the material:

$$I_{\text{eff}} = \frac{1}{2\pi} \int_{M_2 \times \mathbb{R}} \mathrm{d}^2 x \mathrm{d}t \, \epsilon^{ijk} A_i \partial_j a_k - \frac{r}{4\pi} \int_{M_2 \times \mathbb{R}} \mathrm{d}^3 x \, \epsilon^{ijk} a_i \partial_j a_k.$$

For a first orientation, let us consider the interpretation of a "quasiparticle" that has a charge q under a. Here q must be an integer or  $I_{\text{eff}}$  would not make sense! If such a quasiparticle is present at rest at a point  $x = x_0$  in  $M_2$ , the part of the action that involves a acquires an extra term and becomes

$$\frac{1}{2\pi}\int_{M_2\times\mathbb{R}} \mathrm{d}^2 x \mathrm{d}t \,\,\epsilon^{ijk} A_i \partial_j a_k - \frac{r}{4\pi}\int_{M_2\times\mathbb{R}} \mathrm{d}^3 x \,\,\epsilon^{ijk} a_i \partial_j a_k + q \int \mathrm{d}t \,a_0(x_0,t).$$

The field equation for  $a_0$  becomes

$$\frac{F_{12}(x)}{2\pi} - \frac{rf_{12}(x)}{2\pi} + q\delta(x-x_0) = 0.$$

To solve this equation, we obviously need a delta function in  $F_{12}$  and/or  $f_{12}$ . But which? In condensed matter, a delta function in f or F is really an idealization of a very tiny flux tube. Because a and f live only in two space dimensions, a delta function in f makes sense. It represents a little flux tube supported near  $x_0$ 



Because A lives throughout all of 3 + 1 dimensional spacetime, such a delta function does not make sense for F = dA. Of course, we can imagine a thin solenoid generating a flux tube of F, but this would extend into the third spatial dimension. If instead we assume a small current loop creating a flux tube of F in  $M_2$  (the spatial volume of the fractional quantum Hall sample), this will create a magnetic dipole with no net flux of F integrated over  $M_2$ :



After coarse-graining, this will give 0, not a delta function in F.

So we have to solve the equation

$$\frac{F_{12}(x)}{2\pi} - \frac{rf_{12}(x)}{2\pi} + q\delta(x - x_0) = 0$$

with a delta function in  $f_{12}$  and not in  $F_{12}$ , and hence near  $x = x_0$ ,

$$\frac{f_{12}(x)}{2\pi}=\frac{q}{r}\delta(x-x_0).$$

Now if we go back to the action

$$I_{\rm eff} = \frac{1}{2\pi} \int_{M_2 \times \mathbb{R}} \mathrm{d}^2 x \mathrm{d}t \, \epsilon^{ijk} A_i \partial_j a_k - \frac{r}{4\pi} \int_{M_2 \times \mathbb{R}} \mathrm{d}^3 x \, \epsilon^{ijk} a_i \partial_j a_k,$$

we see that the charge density  $J_0 = \delta I_{\rm eff}/\delta A_0$  of A is

$$J_0=\frac{q}{r}\delta(x-x_0).$$

Thus a quasiparticle with charge q for a has ordinary electric charge q/r (in units of the charge of the electron).

It is actually not necessary to go into so much detail to see that a fractional quantum Hall system must have fractionally charged quasiparticles. Return for a moment to an integer quantum Hall system:

$$I_{\text{eff}} = rac{k}{4\pi} \int \mathrm{d}^2 x \mathrm{d}t \, \epsilon^{ijk} A_i \partial_j A_k, \quad k \in \mathbb{Z}.$$

The corresponding electric charge density is

$$J_0 = \frac{\delta I_{\text{eff}}}{\delta A_0} = \frac{kF_{12}}{2\pi}$$

If we place a magnetic monopole with one Dirac quantum

$$\int \frac{F_{12}}{2\pi} = 1$$

inside a spherical sample



this induces in the material a charge

$$Q = \int_{M_2} J_0 = \int_{M_2} \frac{kF_{12}}{2\pi} = k$$

and all is well if k is an integer.

But if the effective value of k is a fraction, as in the case of the fractional quantum Hall effect, then there must be fractionally charged quasiparticles somewhere on the surface of the material



since a compact fractional quantum Hall sample is ultimately made from finitely many electrons, protons, and neutrons, and the electric charge of any state of such a system must be an integer. A full understanding of the fractional quantum Hall system requires treating *a* quantum mechanically. You will likely hear about that next week from Robbert Dijkgraaf. I will not attempt a full explanation today but there are a few points that I will explain. First of all, part of the reason that we have gotten as far as we have without treating *a* quantum mechanically is that so far we considered a fractional quantum Hall system on an infinite or semi-infinite cylinder

in which case a full quantum treatment is not necessary for many questions. For example, we treated  $\hat{\alpha} = \oint_{\gamma} a$  as an arbitrary constant, rather than a quantum variable. This is OK on the *infinite* cylinder but in the case of a compact sample we do need to treat a quantum mechanically.

In discussing the quantum mechanics of a, we will ignore A and just study the purely 2 + 1-dimensional problem:

$$I_{\mathrm{eff}} = -rac{r}{4\pi}\int_{M_2 imes\mathbb{R}}\mathrm{d}^3x\;\epsilon^{ijk}a_i\partial_ja_k.$$

A noteworthy fact is that *there is no metric tensor in sight*, and therefore what we are trying to describe is a "topological quantum field theory." It won't describe particle excitations, but only the "dynamics of the ground state(s)." At long distances, many or most gapped quantum systems simply become trivial, but more generally a gapped quantum system can lead at long distances to a nontrivial topological quantum field theory, and that is what happens in the case of the fractional quantum Hall effect. A compact sample of nontrivial topology is particularly interesting:



We want to find the quantum states of the field *a* quantized on such a manifold.

The quantum states are supposed to make up a Hilbert space  $\mathfrak{H}$ .  $\mathfrak{H}$  is supposed to provide a representation of an algebra of quantum operators that is obtained, in some sense, by quantizing the space of classical observables. In a gauge theory, we consider only the gauge-invariant classical observables. So we should ask, "What are the gauge-invariant classical observables that we can make from *a*?" As soon as we ask this question, we run into the following fact. A gauge-invariant local operator would have to be a polynomial in f = da and its derivatives. But the classical field equation of *a* is

## f = 0

and therefore there are no local, gauge-invariant classical observables.

However, there are gauge-invariant "Wilson loop" operators. We pick a closed curve  $\ell \subset M$  and define the "Wilson loop operator"

$$W_s(\ell) = \exp\left(is\oint_\ell a\right), \quad s\in\mathbb{Z}.$$

This operator is invariant under continuous deformations of  $\ell$  for two related reasons: (a) This is true because f = 0 so  $W_s(\ell)$  can only see global information like Aharonov-Bohm phases; (b) More generally, in any topological quantum field theory, any loop  $\ell$  is equivalent to any nearby loop  $\ell'$  to which  $\ell$  can be deformed. The physical meaning of the Wilson loop operator  $W_s(\ell)$  is that the amplitude for a process in which a quasiparticle of charge spropagates around a loop  $\ell$  is proportional to a factor of  $W_s(\ell)$ . If the loop  $\ell$  can be continuously shrunk to a point without any singularity, then the operator  $W_s(\ell)$  is trivial since the quasiparticle is not going anywhere. "Trivial" means that in this case  $W_s(\ell)$  is equal to 1 as an operator. We are only interested in the case that this is not so. There are two possible sources of Aharonov-Bohm-like phases that a Wilson loop operator  $W_s(\ell)$  might see. There may be another similar operator  $W_{s'}(\ell')$ , where  $\ell$  and  $\ell'$  are "linked" and cannot be disentangled:



(There will be a singularity if we try to pass  $\ell$  through  $\ell'$ .) This effect is associated to fractional statistics of the quasiparticles: It means that the presence of one quasiparticle propagating around  $\ell'$  modifies the amplitude for a second quasiparticle to propagate around  $\ell$  even if they are very far apart.

Alternatively, and more like the classical Aharonov-Bohm idea, the loop  $\ell$  might be "noncontractible" for topological reasons unrelated to the existence of other quasiparticles.



If two such loops  $\ell$  and  $\ell'$  have a nonzero intersection number on the torus



then – as one can learn with the help of the classical Poisson brackets or quantum canonical commutators – the corresponding Wilson operators do not commute. They obey

$$W_{s}(\ell)W_{s'}(\ell') = \exp(2\pi i s s'/r)W_{s'}(\ell')W_{s}(\ell).$$

We may as well just set s = s' = 1 since  $W_s(\ell)$  is just the  $\ell^{th}$  power of  $W_1(\ell)$  and similarly for  $W_{s'}(\ell')$ . If we set  $A = W_1(\ell)$ ,  $B = W_1(\ell')$ , then the algebra obeyed by A and B is

$$AB = \exp(2\pi i/r)BA$$
.

An irreducible representation of this algebra has dimension r, because

$$B \rightarrow ABA^{-1} = \exp(2\pi i/r)B$$

multiplies any eigenvalue of *B* by  $\exp(2\pi i/r)$ . So *r* states are needed to represent this algebra and actually *r* states are enough. These are the *r* "ground states of Chern-Simons theory on a torus," for the case of the gauge group U(1) at "level" *r*.

So this is the basis for the claim that *in the limit of a very large system*, a quantum Hall system on a topologically non-trivial manifold has a nontrivial vacuum degeneracy. The condition "in the limit of a very large system" is necessary, because the vacuum degeneracy is actually slightly lifted by exponentially small effects that result from quasiparticle tunneling:



This is as much as we will be able to say today about fractional quantum Hall systems. The next topi is to fulfill a promise from yesterday of another explanation of why there are edge states in the *integer* quantum Hall effect. Then we will end up by reconsidering the Haldane model.

Actually, these two topics are linked. My main goal is really to reconsider the Haldane model (it was already introduced in Kane's second lecture), but this will be easier if we first reconsider the edge states of the integer quantum Hall effect. The main goal in reconsidering the edge states is to give a(nother) completely conceptual, non computational proof of something that I asserted yesterday: A 2 + 1-dimensional system with a Chern-Simons coupling in bulk

$$I_{
m eff} = rac{k}{4\pi}\int {
m d}^3x\,\epsilon^{ijk}A_i\partial_jA_k$$

and  $n_+ - n_- = k$  chiral edge states on the boundary is completely consistent and anomaly-free. To do this, we will simply describe a physical realization. First we do this in a continuum language and then we do it via the Haldane model.

We first couple the field A to a massive 3d Dirac fermion  $\psi$  of charge 1:

$$I_{\psi} = \int \mathrm{d}^3 x \, \bar{\psi} \left( i \not \! D - m 
ight) \psi.$$

Since  $\psi$  is gapped, we can try to "integrate it out" and get a local effective action for A only. The dominant term at low energies turns out to be

$$\frac{\mathrm{sign} m}{2} \mathrm{CS}(A) = \frac{\mathrm{sign} m}{2} \frac{1}{4\pi} \int \mathrm{d}^3 x \epsilon^{ijk} A_i \partial_j A_k.$$

The factor of 1/2 is worrisome as it contradicts gauge invariance. However, we will always consider combinations in which it is absent. The factor sign*m* follows from reflection symmetry (under which *m* and CS(A) are both odd) and dimensional analysis. The effective action (sign m/2)CS(A) was first found from Feynman diagrams, and this is not a difficult calculation:



However, in the spirit of the present school, it is more natural to get this result from the Berry flux (as Kane and also Ong essentially explained).

We know that when any gapped system of charged fermions is "integrated out," the resulting coefficient of CS(A) equals the winding number of the momentum space Hamiltonian. The massive Dirac Hamiltonian in 2 + 1 dimensions is

$$H = \sigma_x p_x + \sigma_y p_y + m \sigma_z.$$

For large |p|, the mapping is

$$(p_x, p_y) \rightarrow \left( rac{p_x}{\sqrt{p_x^2 + p_y^2}}, rac{p_y}{\sqrt{p_x^2 + p_y^2}}, 0 
ight),$$

which winds around the equator



And the full mapping

$$(p_x, p_y) \rightarrow \left( \frac{p_x}{\sqrt{p_x^2 + p_y^2 + m^2}}, \frac{p_y}{\sqrt{p_x^2 + p_y^2 + m^2}}, \frac{m}{\sqrt{p_x^2 + p_y^2 + m^2}} \right)$$

has for its image the upper hemisphere or the lower hemisphere, depending on the sign of m.



So the winding number is sign m/2, and that is the Chern-Simons coefficient that we get by integrating out  $\psi$ .

For the moment, we want to consider a trivial theory, so along with  $\psi$ , we add a second field  $\psi'$  of mass -m. The total Chern-Simons coefficient obtained by integrating out  $\psi$  and  $\psi'$  is

$$\frac{1}{2}(\operatorname{sign} m + \operatorname{sign} (-m)) = 0.$$

On a sample with boundary, we want a boundary condition such that the system remains trivial even along the boundary – no edge excitations at all. This will certainly be consistent and physically sensible! On a half-space  $x_1 \ge 0$ ,



what boundary condition will ensure that nothing happens along the boundary?

Somewhat like something we said in the first lecture, a boundary condition that does the trick is

$$\psi'\big|_{x_1=0} = i\gamma_1 \psi|_{x_1=0}.$$

Recall that  $\psi$  and  $\psi'$  have equal and opposite masses

$$(i\partial - m)\psi = 0 = (i\partial + m)\psi'$$

and in 2+1 dimensions, the fermion mass is odd under reflection. So if we combine  $\psi$  and  $\psi'$  to a single fermion  $\widehat{\psi}$  defined on all of  $\mathbb{R}^3$  by

$$\widehat{\psi}(x_1, x_2; t) = egin{cases} \psi(x_1, x_2; t) & ext{if } x_1 \ge 0 \ i \gamma_1 \psi'(-x_1, x_2; t) & ext{if } x_1 \le 0 \end{cases}$$

then  $\widehat{\psi}$  just obeys

$$(i\partial - m)\,\widehat{\psi} = 0$$

and certainly there is no gapless mode.

Now, while keeping the fermion kinetic energy and the boundary conditions fixed, we change the sign of the mass of  $\psi'$  and move to the region where both  $\psi$  and  $\psi'$  have the same mass m > 0. This cannot affect the consistency of the theory since the mass is a "soft" perturbation. Of course, when the mass of  $\psi'$  passes through zero, the theory becomes ungapped and passes through a phase transition. What is there on the other side of this transition? The Hall conductivity – that is the coefficient of CS(A) in the effective action – is now

$$\frac{1}{2}(1+1) = 1.$$

By itself this would be anomalous. But the Dirac equation for  $\widehat{\psi}$  is now

$$(i\partial - m\operatorname{sign}(x_1))\widehat{\psi} = 0,$$

thus the mass of  $\hat{\psi}$  changes sign in passing through  $x_1 = 0$ . As Kane explained (and we have discussed some similar examples in my lectures), this results in the existence of a chiral edge mode supported near  $x_1 = 0$ .

So we have a manifestly consistent construction of a 2 + 1-dimensional system that in bulk has an effective action CS(A) (plus terms of higher dimension) and along the boundary has a chiral edge mode. Had we started with k pairs  $\psi, \psi'$ , we would have arrived in the same way at a bulk action kCS(A) and k chiral edge modes. So we have confirmed the consistency of this combined system without having to investigate the "anomalies" of the chiral edge modes.

It remains to describe how Haldane realized this system in a condensed matter model – a small perturbation of the standard band Hamiltonian of graphene. Graphene is an atomic monolayer of carbon atoms arranged in a hexagonal (or honeycomb) lattice



A carbon atom has 6 electrons; 2 of them are in 1s states and 3 more go into forming covalent bonds with the 3 nearest neighbors of any given atom. (One can think of the electrons in these bonds as hybridized 2s,  $2p_x$ , and  $2p_y$  electrons.) We are left with 1 electron per atom, which is going to go into the  $2p_z$  orbital – with spin up or down. Thus the two  $2p_z$  orbitals will be "half-filled."

The honeycomb lattice has two atoms per unit cell:



Each unit cell has an A atom and a B atom. So the  $2p_z$  orbitals form two bands (not counting spin) and we want to "half-fill" these bands.

What happens is dictated by symmetry up to a certain point, but the easiest way to understand it is to first solve a simple model in which the Hamiltonian describes "nearest neighbor hopping" with amplitude t from the A-lattice to the B-lattice and vice-versa. A shortcut to write the momentum space Hamiltonian is as follows.



Pick a point in the *B* lattice as shown, and let the momentum be such that the amplitudes at the three neighboring *A* points are  $1, e^{i\alpha}$ , and  $e^{i\beta}$ . Here  $\alpha$  and  $\beta$  are a convenient parametrization of the Brillouin zone, so they are arbitrary angles.

The total hopping amplitude to the indicated *B* site is then  $1 + e^{i\alpha} + e^{i\beta}$  (times the hopping constant *t*). The Hamiltonian is hermitian, so the  $B \to A$  hopping is the complex conjugate of this and the momentum space Hamiltonian is in the *A*, *B* basis

$$H=tegin{pmatrix} 0&1+e^{-ilpha}+e^{-ieta}\ 1+e^{ilpha}+e^{ieta}&0 \end{pmatrix}$$

H is traceless, so a band crossing is the same as a zero-mode of H. To find such a zero-mode, we have to solve

$$1 + e^{i\alpha} + e^{i\beta} = 0$$

with real  $\alpha, \beta$ . The equation implies that  $e^{i\alpha}$  and  $e^{i\beta}$  are complex conjugates, and there are precisely two solutions

$$e^{ilpha}=rac{1}{2}\left(-1\pm\sqrt{-3}
ight)=e^{-ieta}.$$

Expanding around either of these solutions, one finds a Dirac-like Hamiltonian, so we have found two "Dirac points" in the Brillouin zone.

This was a crude model, but the graphene lattice has a lot of symmetries.



Apart from translation symmetries, the symmetries are as follows. As shown, let p be the center of one of the hexagons. Then one can rotate around p by any multiple of  $2\pi/6$ , and one can also reflect along various axes through p.

For example, one can find a reflection that maps a given Dirac point to itself – and therefore ensures that the gapless Dirac modes that we found in the model remain gapless after any perturbation that preserves the reflection in question. One can also see that a  $2\pi/6$  rotation exchanges the two Dirac points, ensuring that they are at the same energy.

So (ignoring spin) all the conditions that we discussed in the first lecture are obeyed to ensure that the fermi level precisely passes through the two Dirac points:



Suitable perturbations involving symmetry breaking and/or spin-dependent forces can give a variety of gapped models. Haldane chose a perturbation that broke some symmetry and gave masses of the same sign to all Dirac modes. Allowing for spin, this gives a quantum Hall coefficient of  $2 \times (1/2 + 1/2) = 2$ . Kane and Mele, as Kane described in his second lecture, analyzed the effects of spin-dependent forces and arrived at the spin quantum Hall effect, the germ of a 2d topological insulator.