

PHY392T NOTES: TOPOLOGICAL PHASES OF MATTER

ARUN DEBRAY
SEPTEMBER 12, 2019

These notes were taken in UT Austin's PHY392T (Topological phases of matter) class in Fall 2019, taught by Andrew Potter. I live-TeXed them using vim, so there may be typos; please send questions, comments, complaints, and corrections to a.debray@math.utexas.edu. Any mistakes in the notes are my own.

CONTENTS

1.	: 8/29/19	1
2.	Second quantization: 9/3/19	1
3.	The Majorana chain: 9/5/19	4
4.	The Majorana chain, II: 9/10/19	7
5.	Classification of band structures: 9/12/19	10

Lecture 1.

: 8/29/19

Lecture 2.

Second quantization: 9/3/19

Today we'll describe second quantization as a convenient way to describe many-particle quantum-mechanical systems.

In "first quantization" (only named because it came first) one considers a system of N identical particles, either bosons or fermions. The wavefunction $\psi(r_1, \dots, r_N)$ is redundant: if σ is a permutation of $\{1, \dots, N\}$, then

$$(2.1) \quad \psi(r_1, \dots, r_n) = (\pm 1) \psi(r_{\sigma(1)}, \dots, r_{\sigma(N)}),$$

where the sign depends on whether we have bosons or fermions, and on the parity of σ .

For fermionic systems specifically, $\psi(r_1, \dots, r_N)$ is the determinant of an $N \times N$ matrix, which leads to an exponential amount of information in N . It would be nice to have a more efficient way of understanding many-particle systems which takes advantage of the redundancy (2.1) somehow; this is what second quantization does.

Another advantage of second quantization is that it allows for systems in which the total particle number can change, as in some relativistic systems.

The idea of second quantization is to view every degree of freedom as a quantum harmonic oscillator

$$(2.2) \quad H := \frac{1}{2} \omega^2 (p^2 + x^2).$$

We set the lowest eigenvalue to zero for convenience. If $a := (x + ip)/\sqrt{2}$ and $a^\dagger := (x - ip)/\sqrt{2}$, then $\hat{n} := a^\dagger a$ computes the eigenvalue of an eigenstate.

Now let's assume our particles are all identical bosons. Then we introduce these operators $a_\sigma(\mathbf{r})$, $a_\sigma^\dagger(\mathbf{r})$ which behave as annihilation, respectively creation operators, in that they satisfy the commutation relations

$$(2.3) \quad \begin{aligned} [a_\sigma^\dagger(\mathbf{r}), a_{\sigma'}(\mathbf{r}')] &= -\delta_{\sigma\sigma'} \delta(\mathbf{r} - \mathbf{r}') \\ [a^\dagger, a^\dagger] &= 0. \end{aligned}$$

The Hamiltonian is generally of the form

$$(2.4) \quad H := \sum_{\sigma, \sigma'} \int_{\mathbf{r}, \mathbf{r}'} a_{\sigma}^{\dagger}(\mathbf{r}) h_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') a_{\sigma'}(\mathbf{r}) + V_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta},$$

where the first term is the free part and the second term determines a two-particle interaction.

Letting $n_{\sigma}(\mathbf{r}) := a_{\sigma}^{\dagger}(\mathbf{r}) a_{\sigma}(\mathbf{r})$, which is called the *number operator* (since it counts the number of particles in state σ), there is a state $|\emptyset\rangle$ called the *vacuum* which satisfies $n_{\sigma}(\mathbf{r})|\emptyset\rangle = 0$ and $a_{\sigma}(\mathbf{r})|\emptyset\rangle = 0$. Particle creation operators commute, in that

$$(2.5) \quad a^{\dagger}(\mathbf{r}_1) a^{\dagger}(\mathbf{r}_2) |\emptyset\rangle = a^{\dagger}(\mathbf{r}_2) a^{\dagger}(\mathbf{r}_1) |\emptyset\rangle.$$

This is encoding that the particles are bosons: we exchange them and nothing changes.

The fermionic story is similar, but things should anticommute rather than commute. Letting α be an index, let f_{α} , resp. f_{α}^{\dagger} be the annihilation, resp. creation operators for a fermion in state α . There's again a vacuum $|\emptyset\rangle$, with $f_{\alpha}|\emptyset\rangle = 0$ for all α . Now we impose the relation

$$(2.6) \quad f_{\alpha}^{\dagger} f_{\beta}^{\dagger} |\emptyset\rangle = -f_{\beta}^{\dagger} f_{\alpha}^{\dagger} |\emptyset\rangle.$$

That is, define the *anticommutator* by

$$(2.7) \quad \{f_{\alpha}^{\dagger}, f_{\beta}^{\dagger}\} := f_{\alpha}^{\dagger} f_{\beta}^{\dagger} + f_{\beta}^{\dagger} f_{\alpha}^{\dagger}.$$

Then we ask that $\{f_{\alpha}^{\dagger}, f_{\beta}^{\dagger}\} = 0$, and $\{f_{\alpha}^{\dagger}, f_{\beta}\} = \delta_{\alpha\beta}$.

Again we have a number operator $n_{\alpha} := f_{\alpha}^{\dagger} f_{\alpha}$; it satisfies $n_{\alpha} f_{\alpha} = f_{\alpha} (n_{\alpha} - 1)$, and measures the number of particles in the state α . Because

$$(2.8) \quad (f_{\alpha}^{\dagger})^2 = f_{\alpha}^{\dagger} f_{\alpha}^{\dagger} = -f_{\alpha}^{\dagger} f_{\alpha}^{\dagger} = 0,$$

then n_{α} is a projector (i.e. $n_{\alpha}^2 = n_{\alpha}$), and therefore its eigenvalues can only be 0 or 1. This encodes the Pauli exclusion principle: there can be at most a single fermion in a given state.

We'd like to write our second-quantized systems with quadratic Hamiltonians, largely because these are tractable. Let $(h_{\alpha\beta})$ be a self-adjoint matrix and consider the Hamiltonian

$$(2.9) \quad H := \sum_{\alpha, \beta} f_{\alpha}^{\dagger} h_{\alpha\beta} f_{\beta}.$$

The *number operator* $N := \sum n_{\alpha}$ commutes with the Hamiltonian, which therefore defines a symmetry of the system. The associated conserved quantity is the particle number. Slightly more explicitly, we have a symmetry of the group U_1 (i.e. the unit complex numbers under multiplication): for $\theta \in [0, 2\pi)$, let

$$(2.10) \quad u_{\theta} := \exp(i\theta N).$$

Then

$$(2.11) \quad u_{\theta}^{\dagger} H u_{\theta} = \sum_{\alpha, \beta} \underbrace{u_{\theta}^{\dagger} f_{\alpha}^{\dagger} u_{\theta}}_{=e^{-i\theta} f_{\alpha}^{\dagger}} h_{\alpha\beta} \underbrace{u_{\theta} f_{\beta} u_{\theta}}_{=e^{i\theta} f_{\beta}} = H.$$

When you see a Hamiltonian, you should feel a deep-seated instinct to diagonalize it: we want to find $\lambda_n, v^{(n)}$ such that $h_{\alpha\beta} v_{\beta}^{(n)} = \lambda_n v_{\alpha}^{(n)}$ and $v v^{\dagger} = \text{id}$. Let $v_{n\alpha} := v_{\alpha}^{(n)}$ and

$$(2.12) \quad \psi_n := \sum_{\alpha} v_{n\alpha} f_{\alpha}.$$

Then ψ_n^{\dagger} and ψ_n satisfy the same creation and annihilation relations as f_{α}^{\dagger} and f_{α} :

$$(2.13) \quad \{\psi_n^{\dagger}, \psi_m\} = \left\{ \sum_{\alpha} v_{n\alpha}^* f_{\alpha}^{\dagger}, \sum_{\beta} v_{m\beta} f_{\beta} \right\}$$

$$(2.14) \quad = \sum_{\alpha, \beta} v_{n\alpha}^* v_{m\beta} \underbrace{\{f_{\alpha}^{\dagger}, f_{\beta}\}}_{=\delta_{\alpha\beta}}$$

$$(2.15) \quad = \sum_{\alpha} v_{m\alpha} (v^{\dagger})_{n\alpha} = \delta_{m,n}.$$

Let $\hat{n}_n := \psi_n^\dagger \psi_n$. Now the Hamiltonian has the nice diagonal form

$$(2.16) \quad H = \sum_n \lambda_n \psi_n^\dagger \psi_n,$$

and we can explicitly calculate its action on a state:

$$(2.17) \quad H \psi_{n_1}^\dagger \psi_{n_2}^\dagger \cdots \psi_{n_N}^\dagger |\emptyset\rangle = \underbrace{\left(\sum_m \lambda_m \psi_m^\dagger \psi_m \right)}_{(*)} \psi_{n_2}^\dagger \cdots \psi_{n_N}^\dagger |\emptyset\rangle.$$

The term $(*)$ is equal to

$$(2.18) \quad \psi_m^\dagger (\delta_{mn} - \psi_{n_1}^\dagger \psi_m) = \delta_{mn_1} \psi_{n_1}^\dagger + \psi_{n_1}^\dagger \psi_m^\dagger \psi_m.$$

Then (2.17) is equal to

$$(2.19) \quad (2.17) = \lambda_{n_1} \psi_{n_1}^\dagger (\psi_{n_2}^\dagger \cdots \psi_{n_N}^\dagger) |\emptyset\rangle,$$

so we've split off a term and can induct. The final answer is

$$(2.20) \quad = \left(\sum_{i=1}^N \lambda_i \right) \psi_{n_1}^\dagger \cdots \psi_{n_N}^\dagger |\emptyset\rangle.$$

Example 2.21 (1d tight binding model). Let's consider the system on a circle with L sites (you might also call this periodic boundary conditions). We have operators which create fermions at each state and also some sort of tunneling operators. The Hamiltonian is

$$(2.22) \quad H := -t \sum_{j=1}^L (f_{j+1}^\dagger f_j + f_j^\dagger f_{j+1}) - \mu \sum_{j=1}^L f_j^\dagger f_j,$$

where $j+1$ is interpreted mod L as usual. One of t and N (TODO: which?) can be interpreted as the chemical potential. The eigenstates are the Fourier modes

$$(2.23) \quad \psi_k := \frac{1}{\sqrt{L}} \sum_{j=1}^L e^{ikj} f_j,$$

where $k = 2\pi n/L$. Hence in particular $e^{ik(L+1)} = e^{ik}$. Now we can compute

$$(2.24) \quad \sum_{j=1}^L f_{j+1}^\dagger f_j = \frac{1}{L} \sum_{j,k,k'} e^{ik'(j+1)} e^{-ikj} \psi_{k'}^\dagger \psi_k$$

$$(2.25) \quad = \frac{1}{L} \sum_{k,k'} e^{ik'} \sum_j e^{ij(k-k')} \psi_{k'}^\dagger \psi_k$$

$$(2.26) \quad = \sum_k e^{ik} \psi_k^\dagger \psi_k.$$

That is, the diagonalized Hamiltonian is

$$(2.27) \quad H = \sum_{k=1}^L (-2t \cos k - \mu) \psi_k^\dagger \psi_k.$$

You can plot λ_k as a function of k , but really k is defined on the circle $\mathbb{R}/2\pi\mathbb{Z}$, which is referred to as the *Brillouin zone*. The ground state of the system is to fill all states with negative energy:

$$(2.28) \quad |\text{G.S.}\rangle = \left(\prod_{k: \lambda_k < 0} \psi_k^\dagger \right) |\emptyset\rangle.$$

If L is fixed, k only takes on L different values, but implicitly we'd like to take some sort of thermodynamic limit $L \rightarrow \infty$, giving us the actually smooth function $\lambda_k = -2t \cos k - \mu$. ◀

We said that second quantization is useful when the particle number can change, so let's explore that now. This would involve a Hamiltonian that might look something like

$$(2.29) \quad H = f_\alpha^\dagger h_{\alpha\beta} f_\beta + \frac{1}{2} (\Delta_{\alpha\beta} f_\alpha^\dagger f_\beta^\dagger + \Delta_{\alpha\beta}^\dagger f_\alpha f_\beta).$$

These typically arise in mean-field descriptions of superconductors. This typically arises in situations where electrons are attracted to each other — this is a little bizarre, since electrons have the same charge, but you can imagine an electron moving in a crystalline solid with some positive ions. The electron attracts the ions, but they move more slowly, so the electron keeps moving and we get an accumulation of positive charge, and this can attract additional electrons.

This binds pairs of electrons together at a certain point, and this forms a *condensate*, i.e. a superposition of states with different particle numbers. (2.29) describes a superconducting condensate, in which $\Delta_{\alpha\beta}$ describes pairs of particles appearing or disappearing in the condensate. To learn more, take a solid-state physics class.

Remark 2.30. You have to have pairs of fermionic terms — if you try to include an odd number of fermions, or a single fermionic term, you'll get nonlocal interactions between the lone fermion and others. Thus, even though the particle number is not conserved, its value mod 2, which is called *fermion parity*, is conserved. ◀

If you try to directly diagonalize (2.29), some weird stuff happens, so we'll rewrite the Hamiltonian such that it looks like it's particle-conserving, and then apply our old trick. This approach is due to Nambu. Let

$$(2.31) \quad \Psi_{\alpha,\tau} := \begin{pmatrix} f_\alpha \\ f_\alpha^\dagger \end{pmatrix},$$

where τ denotes the vertical index. We can rewrite the Hamiltonian as

$$(2.32) \quad H = \frac{1}{2} \begin{pmatrix} f_\alpha^\dagger & f_\alpha \end{pmatrix} \begin{pmatrix} h_{\alpha\beta} & \Delta_{\alpha\beta} \\ \Delta_{\alpha\beta}^\dagger & -h_{\alpha\beta}^\dagger \end{pmatrix} \begin{pmatrix} f_\beta \\ f_\beta^\dagger \end{pmatrix} + (\text{constant}) = \frac{1}{2} \Psi_{\alpha\tau}^\dagger \mathcal{H}_{\alpha\beta\tau\tau'} \Psi_{\beta\tau'}.$$

However, Ψ and Ψ^\dagger have some redundancy: if σ^x denotes the Pauli matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, then $\Psi_\tau^\dagger = \sigma_{\tau\tau'}^x \Psi_{\tau'}$.

This is telling us that Ψ and Ψ^\dagger create particles with energies (say) e and $-e$, respectively. Now

$$(2.33) \quad \Psi^\dagger H \Psi = \Psi^T \sigma^x H \sigma^x (\Psi^\dagger)^T = -\Psi^\dagger \sigma^x H^T \sigma^x \Psi,$$

and therefore $\mathcal{H} = -\sigma^x \mathcal{H}^* \sigma^x$. Using this, we can determine the eigenstates: $\mathcal{H}v = Ev$ iff $\mathcal{H}\sigma^x v^* = -E\sigma^x v^*$. Then

$$(2.34) \quad \mathcal{H}\sigma^x v^* = \sigma^x (\sigma^x \mathcal{H} \sigma^x) v^* = \sigma^x (\sigma^x \mathcal{H}^* \sigma^x v)^* = \sigma^x (-\mathcal{H}v)^* = -E\sigma^x v^*$$

and

$$(2.35) \quad \gamma_E := \sum_{\alpha,\tau} v_{\alpha\tau} \Psi_{\alpha\tau}$$

satisfies $\gamma_{-E} = \gamma_E^\dagger$. **TODO:** what are we trying to show here?

This $E \leftrightarrow -E$ symmetry is an instance of what's traditionally called “particle-hole symmetry,” but it's a little weird — we can't break this symmetry by introducing additional terms to the Hamiltonian. So it might be more accurate to call it *particle-hole structure*, which conveniently has the same acronym.

TODO: some other stuff I missed. I think $\{\Psi_{\alpha\tau}, \Psi_{\beta\tau'}^\dagger\} = \delta_{\alpha\beta} \delta_{\tau\tau'}$ and $\{\gamma_E, \gamma_{E'}^\dagger\} = \delta_{EE'}$, which tells us these (I think) behave like creation and annihilation operators.

At zero energy, $\gamma_0 = \gamma_0^\dagger$, so we have a fermion which is its own antiparticle. This is called a *Majorana fermion*. It will be helpful to have a slightly different normalization here, which we'll discuss more later.

Lecture 3.

The Majorana chain: 9/5/19

Today we will discuss a one-dimensional system studied by Kitaev [Kit01]. Introduce periodic boundary conditions, so that the sites live on a circle with length L . At each site i , we have a local Hilbert space $\mathcal{H}_i := \mathbb{C} \cdot \{|0\rangle, |1\rangle\}$, and the total Hilbert space of states is the tensor product of these over all of the sites.

Let c_j and c_j^\dagger denote the annihilation, resp. creation operators at site j . Then the Hamiltonian is

$$(3.1) \quad H := - \sum_{j=1}^L t(c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}) - \mu \sum_{j=1}^L c_j^\dagger c_j - \Delta(c_{j+1}^\dagger c_j^\dagger + c_j c_{j+1}).$$

Here t , Δ , and μ are parameters; μ is called the *chemical potential*.

To solve this Hamiltonian, we will introduce a different set of creation and annihilation operators: let

$$(3.2a) \quad \tilde{c}_k := \frac{1}{\sqrt{L}} \sum_{j=1}^L e^{ikj} c_j$$

$$(3.2b) \quad \tilde{c}_k^\dagger := \frac{1}{\sqrt{L}} \sum_{j=1}^L e^{ikj} c_j^\dagger.$$

Here $k \in 2\pi n/L$, like last time, and we only consider those k in $[0, 1)$.¹ Using these, we can rewrite (3.1) as

$$(3.3) \quad H = \sum_k (-2t \cos k - \mu) \tilde{c}_k^\dagger \tilde{c}_k - \Delta \sum_k (e^{ik} \tilde{c}_k^\dagger \tilde{c}_{-k}^\dagger + e^{ik} \tilde{c}_{-k} \tilde{c}_k).$$

To get the last term, use the fact that $\tilde{c}_k^\dagger \tilde{c}_{-k}^\dagger = -\tilde{c}_{-k}^\dagger \tilde{c}_k^\dagger$, so

$$(3.4) \quad \frac{1}{2} \sum_k \tilde{c}_k^\dagger \tilde{c}_{-k}^\dagger e^{ik} + \frac{1}{2} \sum_k (-e^{-ik} \tilde{c}_k^\dagger \tilde{c}_{-k}^\dagger).$$

Again introduce the Nambu spinor $\Psi := \begin{pmatrix} \tilde{c}_k \\ \tilde{c}_k^\dagger \end{pmatrix}$; then we can rewrite (3.3) as

$$(3.5) \quad H = \frac{1}{2} \sum_k \Psi_k^\dagger \begin{pmatrix} -2t \cos k - \mu & 2i\Delta \sin k \\ -2i\Delta \sin k & 2t \cos k + \mu \end{pmatrix} \Psi_k.$$

So now all we have to do is diagonalize a 2×2 matrix, which isn't so hard. In particular, the eigenvalues (energy levels) are

$$(3.6) \quad E_k = \pm \frac{1}{2} \sqrt{(2t \cos k + \mu)^2 + (2\Delta \sin k)^2}.$$

In particular, we can plot these as k varies and see whether the system is gapped.

- Suppose $\Delta = \mu = 0$. Then there are values of k such that the spectrum isn't gapped, but as soon as you make $\Delta \neq 0$, there is a spectral gap.
- If $\mu = -2t$, we again close the gap at $\Delta = 0$ and $k = 0$, but in general there is a gap.

So the phase diagram in μ appears to have three phases and two transitions between them, and is symmetric about $\mu \mapsto -\mu$. For $\mu \rightarrow -\infty$, this is adiabatically connected to a trivial phase, and thus is itself trivial: there are no particles. For $\mu \rightarrow \infty$, it is also trivial: every site is occupied in the ground state. The third phase is a topological superconductor (though we have yet to show it).

So the two phase transitions happen at $\mu = \pm 2t$. Suppose $\mu = -2t + M$, where M is close to zero, so that we can study the phase transition. Since $-2t \cos k + 2t = O(k^2)$, we'll ignore it, and therefore replace M with $M - 2t \cos k + 2t$. Similarly,

$$(3.7) \quad 2i\Delta \sin k = 2i\Delta k + O(k^3),$$

and we will drop the higher-order terms. Under these approximations, the Hamiltonian now is

$$(3.8) \quad \begin{aligned} H &\approx \frac{1}{2} \sum_k \Psi_k^\dagger \left(\begin{pmatrix} M & 0 \\ 0 & -M \end{pmatrix} + \begin{pmatrix} 0 & 2 - \Delta \\ -2i\Delta & 0 \end{pmatrix} k \right) \Psi_k \\ &= \frac{1}{2} \sum_k \Psi_k^\dagger (M\sigma^z - 2k\Delta\sigma^y) \Psi_k. \end{aligned}$$

¹To me (Arun), this looks like k is in the Pontrjagin dual $(\mathbb{Z}/L)^\vee$, which would be appropriate if this is a Fourier transform.

Here σ^z and σ^y are the usual Pauli matrices. Now (3.8) looks like a Dirac equation with a mass term: letting $a := -2\Delta$, we get

$$(3.9) \quad H \approx \frac{1}{2} \sum_k \Psi_k^\dagger (ak\sigma^y + M\sigma^z) \Psi_k \approx \frac{1}{2} \int dx \psi^\dagger(x) (-iv\partial_x \sigma^y + M(x)\sigma^z) \psi(x).$$

Let's let M vary in space, so that we have a defect between the two phases at $x = 0$. We'll show that the defect has a bound state.

Consider the $E = 0$ solution to the continuum approximation in (3.9). Then

$$(3.10) \quad \tilde{\gamma} = \int dx \phi_\alpha(x) \hat{\psi}_\alpha(x),$$

and we end up with an ordinary differential equation for the solution:

$$(3.11) \quad (-iv\partial_x \sigma^y + M(x)\sigma^z) \phi_\alpha(x) = 0,$$

and therefore $\frac{\partial}{\partial x} \phi_\pm = \pm(M/v)\phi$ (TODO: some details here are missing). Therefore

$$(3.12) \quad \phi_\pm(x) = \exp\left(\pm \int_0^x \frac{M(x)}{v} dx\right) \phi_\pm(0).$$

One of these blows up at infinity and makes no physical sense, but there is a solution which is largest at $M = 0$ and decays to zero at infinity. This is the bound zero mode ϕ_+ . Here are a few more facts about this zero mode.

- As $x \rightarrow \pm\infty$, $\phi_+(x) \rightarrow \exp(-|M_0||x|)$.
- We didn't use much about $M(x)$, only the fact that it switches sign at $M = 0$. This is the sense in which the zero mode is topological: we can deform $M(x)$ and obtain the same behavior.²
- $\gamma = \gamma^\dagger$: in a sense, this mode is both a creation and annihilation operator. For this reason, it's called a *Majorana zero mode*.
- The side of these bound states is determined by the *correlation length* $v/M = 1/3$.

This is not a critical system — besides this zero mode, all other phases are gapped. For $M > 0$, we get a trivial insulator, and for $M < 0$, we have the topological phase, a topological superconductor. The bound state at the defect is what implies that the $M < 0$ phase isn't trivial.

How realistic are the periodic boundary conditions? Well, we can't create an infinite wire in the lab, so maybe we should work on the unit interval of length L , which is large with respect to the correlation length. Then, you maybe can convince yourself that there are two Majorana modes, one at each boundary site, and they overlap a little bit in the bulk, approximately at order $e^{-L/3}$. Call these modes γ_L and γ_R . If you let $\psi = (\gamma_M + i\gamma_R)/2$ and $\psi^\dagger = (\gamma_L - i\gamma_R)/2$, then these satisfy the anticommutation relations of creation and annihilation operators of ordinary fermions: for example, $\{\psi, \psi^\dagger\} = 1$. This is a little bit weird.

Another weird aspect of this system is that if L is large enough, you can't couple to both γ_L and γ_R at the same time. If you tried to perturb the system, say by introducing a bosonic field with an electric potential $V = \phi\gamma_L$, well, that's not allowed, because you would get an odd number of fermions. So these Majorana modes are protected by small perturbations, and in that sense might be useful if you care about quantum memory. The drawback is that you can't put a state with an even number of fermions and a state with an odd number of fermions into superposition, which is unfortunate; the solution is to consider several separate copies of this system.

So let's work with N wires, meaning we have $2N$ Majorana zero modes $\gamma_1, \dots, \gamma_{2N}$, hence N ordinary fermion creation/annihilation operator pairs ψ^\dagger, ψ as we discussed above. This system has a 2^N -dimensional space of ground states: for any subset $S \subset \{1, \dots, n\}$, we say that the fermion state ψ is occupied for $i \in S$ and unoccupied for $i \notin S$.

The fermion parity

$$(3.13) \quad P_f := \prod_{i=1}^N i\gamma_{2i-1}\gamma_{2i} \in \{\pm 1\}$$

²This is an instance of a very general theorem in mathematics called the Atiyah-Singer index theorem, which can be used to produce zero modes in fermionic systems.

is a conserved quantum number of this system (intuitively, it tells us whether there are an even or odd number of fermions present). Therefore we have 2^{N-1} states available as quantum memory.

These give us different ways to label the ground states, but different labelings interact in complicated ways. For example, if $N = 2$,

$$(3.14) \quad |P_{14} = 1, P_{23} = 1\rangle = \frac{1}{\sqrt{2}}(|P_{12} = 1, P_{34} = 1\rangle - |P_{12} = -1, P_{34} = -1\rangle).$$

You can imagine this as follows: we begin with no particles, and create two fermions on each copy of the chain. This doesn't change the parity, because we created them from nothing. Now, we smush together sites 2 and 3 and measure there, and get zero. Then, this is telling us that the remaining states are maximally uncertain. This was an operator

$$(3.15) \quad |++\rangle \mapsto \frac{1}{\sqrt{2}}(|++\rangle - |--\rangle).$$

This is a topologically protected operation, which is exciting if you want to make quantum computers. But it's proven to not be universal, i.e. we can't get (or even well-approximate) all quantum gates in the Majorana chain. In fact, what we get can be efficiently approximated by a classical computer, and this isn't even universal for classical computer! But there are other examples of phases which are universal for quantum computing, and Microsoft is researching how these might be actually implemented.

These states can have (quasi)particle modes akin to the Majorana modes here. In general these are called *nonabelian anyons* or *nonabelian defects*. The defining property of these is that there is a topologically protected ground state degeneracy associated to the zero modes, and it grows exponentially in the number of particles present. The process of turning two particles into something else will be called *fusion*; for the Majorana chain we have the relation

$$(3.16) \quad \gamma \times \gamma = 0 + f,$$

as we either get nothing or a fermion. This is akin to the fact that if we collide two spin-1/2 particles, they could annihilate each other or produce a spin-1 particle. The fact that the Hilbert space grows exponentially is reminiscent of the fact that for a spin- s particle, the Hilbert space of states has dimension $2s + 1$ to the number of particles: the local dimension is the number of objects. Here, though, we will encounter examples of nonabelian anyons whose quantum dimensions are irrational.

Next time, we'll argue that the Majorana chain is the only nontrivial topological phase that can occur among 1D superconductors (unless we add additional symmetries to the Hamiltonian). We'll also discuss how to see that the phase is nontrivial in the bulk; after that, we'll discuss some possible physical realizations in real system, such a spin-orbit coupled semiconductor wire, put in contact with a normal superconductor.

Lecture 4.

The Majorana chain, II: 9/10/19

Today, we'll continue to discuss the Kitaev chain from last time. Recall that the phase diagram in μ has two trivial phases for $\mu \gg 0$ and $\mu \ll 0$, and the phase in between them is topological, specifically some kind of topological superconductor. The trivial phase corresponds to $\mu \neq 0$ and $t, \Delta = 0$, and the topological phase to $\mu = 0$ and $t = \Delta$.

In the topological phase formulated on an interval, there are protected zero modes at the boundary, corresponding to operators γ_L and γ_R (for the left-hand and right-hand sides of the interval, respectively). These are both self-adjoint. Writing $\psi := (\gamma_L + i\gamma_R)/2$, $\psi + \psi^\dagger = \gamma_L$ and $\psi - \psi^\dagger = \gamma_R$.

In the topological phase, we can simplify the Hamiltonian slightly:

$$(4.1) \quad H = \Delta \sum_i (c_{i=1}^\dagger - c_{i+1})(c_i^\dagger + c_i) = i\Delta_j \overline{\gamma_{j+1}} \gamma_j,$$

where $\gamma_i = c_i + c_{i+1}^\dagger$ and $\overline{\gamma_i} = -i(c_i - c_{i+1}^\dagger)$. These look like particle creation and annihilation operators for a pair of Majorana fermions. These commute with the Hamiltonian.

This system admits the following interpretation. At each site i , we have two places where there can be a Majorana fermion, γ_i and $\overline{\gamma_i}$. However, the Majorana corresponding to γ_i and the one corresponding to $\overline{\gamma_{i+1}}$ are coupled. This explains what we see on the interval: at each boundary site, one of the two terms can't be

paired up, and we obtain the boundary zero modes. With periodic boundary conditions, all Majoranas can be paired up, and we obtain a single ground state.

We can also consider anti-periodic boundary conditions, where we say that traversing once around the circle picks up a minus sign: specifically, throw a minus sign onto the interaction term between sites 1 and N .³ This means that we again obtain a single ground state, but the number of fermions differs by 1 from the ground state of the periodic boundary conditions.⁴ This was a little handwavy, but we'll go into more detail in a bit; in general, the difference in fermion parity in different boundary conditions is a useful invariant of these systems.

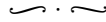
Remark 4.2. The trivial phase of the Kitaev chain admits a similar description: we have $\gamma_i, \bar{\gamma}_i$ as before, but now γ_i is coupled to $\bar{\gamma}_i$, and there are no interactions between different sites. Therefore on an interval or circle, we always pair up the Majorana fermions, and don't obtain any boundary zero modes. ◀

Another thing we can do is combine phases: formulate two copies of the Kitaev chain on the interval, but such that they interact very weakly, certainly not enough to close the gap. This operation, called *stacking*, is an algebraic operation on phases. In particular, given two Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 with Hamiltonians $H_i: \mathcal{H}_i \rightarrow \mathcal{H}_i$, the stacked phase has Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ and Hamiltonian $H_1 \otimes \text{id}_{\mathcal{H}_2} + \text{id}_{\mathcal{H}_1} \otimes H_2$, maybe plus some small interaction term. By commutativity of tensor product, stacking is an associative and commutative operation; moreover, the trivial insulator is an identity for this operation. All of the one-dimensional phases P we encounter will be *invertible*, i.e. there's some other phase P' such that $P \otimes P'$ is trivial. We consider two phases the same if they can be connected by a deformation which is local and never closes the gap.

So given a dimension, we obtain an abelian group, called the group of invertible phases in that dimension. This is not always finite, e.g. the phases delineated by the integer quantum Hall effect produce a countable subgroup in dimension 2. The group itself is expected to be finitely generated.

Determining these groups is an interesting theoretical question in condensed-matter physics. Let's see what it is in dimension 1. Stack together two copies of the Kitaev chain in its topological phase, and add a small interaction term between the two copies of γ_L , and between the two copies of γ_R . Then they can be paired up, and in the end there are no edge states, suggesting that this tensor product is trivial. There's additional evidence that it's trivial, e.g. switching from periodic to antiperiodic boundary conditions doesn't change fermion parity on this system, because the two changes cancel out. Hence we obtain a $\mathbb{Z}/2$ subgroup of the group of phases in dimension 1. This may seem very abstract, but similar considerations apply to more general fermionic systems, and this has guided researchers on where to look for such systems in real materials.

In general, if ground states have even fermion parity on all closed boundary systems, and there are no edge modes, then the phase is trivial. The argument is that we can divide the interval⁵ into a bunch of pieces, and then each piece can be adiabatically transformed into the trivial insulator.



Now let's make this story into something more concrete. The *fermion parity* is defined to be

$$(4.3) \quad P_F = (-1)^{\sum_i \hat{n}_i} = \prod_j i\gamma_j \bar{\gamma}_j,$$

so 1 if there is an even number of fermions and -1 if there's an odd number. This commutes with the Hamiltonian, and in fact commutes with any local Hamiltonian, because local Hamiltonians must have an even number of fermions in each term, as we saw before.

Fermionic parity looks like a discrete symmetry, but it's a bizarre one, in that we can't break it or couple it to a local background field. Otherwise it behaves mostly like any other discrete symmetry.

The change in boundary conditions between periodic and anti-periodic correspond to a symmetry flux for fermion parity: given a local operator \mathcal{O} , we can act on it (thought of, I think, as moving it past the antiperiodic boundary condition) and obtain $P_F \mathcal{O} P_F^\dagger$.

³In the continuum perspective, this corresponds to choosing the nonbounding spin structure on S^1 , rather than the bounding spin structure.

⁴The actual fermion parity of the ground state can be changed by a local potential: flip some signs in the Hamiltonian. But the difference between the two boundary conditions is an invariant.

⁵This argument applies in dimension 1, but the result is true more generally

We will later discuss how to promote a global symmetry, such as fermion parity, to a local one, and then gauge it. This will be a powerful nonperturbative way to study phases. In the Kitaev chain, this concretely looks like considering fermions at different sites with bonds between sites i and $i+1$ with a σ^z on the bond. Then we rewrite the Hamiltonian by

$$(4.4) \quad i\gamma_i\overline{\gamma_{i+1}} \mapsto i\gamma_i\sigma_{i,i+1}^z\overline{\gamma_{i+1}}.$$

Therefore given $s_i \in \mathbb{Z}/2$ for each i , we can act by fermion parity at site i , which sends $\gamma_i \mapsto s_i\gamma_i$, $\overline{\gamma_i} \mapsto s_i\overline{\gamma_i}$, and

$$(4.5) \quad \sigma_{i,i+1}^z \mapsto s_{i+1}s_i\sigma_{i,i+1}^z.$$

The generator of this symmetry is the operator

$$(4.6) \quad \prod_i ((\sigma_{i-1,i}^x \sigma_{i,i+1}^x)(\gamma_i\overline{\gamma_i}))^{(1+s_i)/2}.$$

This may look a little bizarre, but is reminiscent of something more familiar in electromagnetism: given a function ϕ on spacetime, we act on the gauge field by

$$(4.7) \quad A_\mu \mapsto A_\mu + \partial_\mu \phi$$

and $\psi(\mathbf{r}, t) \mapsto \exp(i\phi(\mathbf{r}, t))\psi(\mathbf{r}, t)$. The generator of this symmetry is

$$(4.8) \quad \exp\left(i \int \phi(\mathbf{r})(n(\mathbf{r}) - \nabla \cdot \mathbf{E})\right).$$

This has promoted a global number symmetry to a gauge symmetry for the gauge group U_1 . In our example, U_1 is replaced with $\{\pm 1\}$, $\sigma_{i,i+1}^z$ plays the role of $\exp(i \int_i^{i+1} A \cdot d\ell)$, and s_i plays the role of $\exp(i\phi_r)$ restricted to site i — if this doesn't make perfect sense, that's OK, because this is an approximate analogy.

The physical states are obtained by projecting onto the gauge-invariant states, which you can think of as averaging over the elements of a larger group, the product of copies of $\{\pm 1\}$ indexed over the sites. Explicitly, if you call this group G ,

$$(4.9) \quad |\psi_{\text{physical}}\rangle = \frac{1}{|G|} \sum_{g \in G} |\psi_{\text{gauge-dependent}}\rangle.$$

The flux $\prod_i \sigma_{i,i+1}^z$ is gauge-invariant, in that a gauge transformation $(s_i) \in G$ acts by

$$(4.10) \quad \prod_i \sigma_{i,i+1}^z \mapsto \prod_i (s_i \sigma_{i,i+1}^z s_{i+1}) = \dots s_i \sigma_{i,i+1}^z s_{i+1} s_{i+1} \sigma_{i+1,i+2}^z \dots$$

and these two copies of s_{i+1} cancel. The flux squares to 1, so has eigenvalues $\{\pm 1\}$; the states with eigenvalue 1 are said to have no flux, and those with eigenvalue -1 are said to have flux. This will be our way of formalizing that we're in the antiperiodic boundary condition.

Recall that the Hamiltonian for the trivial phase is

$$(4.11) \quad H_{\text{triv}} = \mu \sum_i c_i^\dagger c_i.$$

If you add σ^z bonds, this Hamiltonian does not change (**TODO**: I think). For the topological phase, we had

$$(4.12) \quad H_{\text{top}} = -i\Delta \sum_j \gamma_j \overline{\gamma_{j+1}} \mapsto i\Delta \sum_j \gamma_i \sigma_{j,j+1}^z \overline{\gamma_{j+1}}.$$

The total fermion parity of the ground state is

$$(4.13) \quad P_F^{GS} = \prod_j i\overline{\gamma_j}\gamma_j$$

$$(4.14) \quad = \pm \prod_j i\gamma_j \overline{\gamma_{j+1}}.$$

The sign is equal to $\prod_j \sigma_{j,j+1}^z$, which is -1 to the number of fluxes. Let F denote the operator that measures fluxes (**TODO**: didn't quite understand the definition), then

$$(4.15) \quad F P_F F^{-1} P_F^{-1} = -1$$

in the topological phase, but not in the trivial phase, so (4.15) is the topological invariant of phases in this dimension.

Remark 4.16. A fact (which we won't prove) is that in general fermionic systems, one can use fluxes to remove fermions unless an unusual commutation relation such as (4.15) holds. ◀

Searching for a condition such as (4.15) is a powerful way to classify invertible fermionic phases: since it didn't make reference to band structures, it also applies to interacting systems. It can be souped up a bit and made even more powerful.

Remark 4.17. Sometimes this phase is called a symmetry-protected phase (SPT), where the symmetry is fermion parity, but as mentioned above this behaves differently than other symmetries, so calling this an SPT seems a little strange. In any case, much of what we've just discussed generalizes to other symmetry groups and hence to SPTs. ◀

Now let's turn to the classification question mentioned above. Band structures are our first tool. Consider a (Fourier-transformed) Hamiltonian

$$(4.18) \quad H = \sum_k \psi_{k,\alpha}^\dagger h_{\alpha\beta}^{(k)} \psi_{k,\beta}.$$

So if there are L lattice sites, $k \in (\mathbb{Z}/L)^\vee$, or, in physical language, k is a momentum. As k varies, the spectrum is a bunch of curves, called *bands*; suppose that N are above zero and M are below zero. We can use local terms to flatten the bands, preserving the gap to be at least Δ for all bands. Concretely, suppose

$$(4.19) \quad h(k) = \sum_n \varepsilon_n(k) \prod_n (k).$$

Here $\varepsilon_n(k)$ is the n^{th} eigenvalue when the momentum is k . Thus we want to diagonalize (TODO: was erased before I could write it down), and we're interested in the topology of such basis transformations: gap-preserving deformations of the Hamiltonian produce a homotopy of these unitary operators.

As we saw, taking $L \rightarrow \infty$ means we think of k as living on the circle $S^1 = \mathbb{R}/2\pi\mathbb{Z}$ (the Brillouin zone); in general dimension d , it lives on the torus $T^d = (S^1)^{\times d}$.

So in general, we're interested in maps $T^d \rightarrow U_{N+M}$, which following what we did above we call a *band structure*. However, unitary operators in U_N or U_M give us trivially systems, in that they shuffle the indices of the bands around, so what we really want to compute is the set of homotopy classes of maps

$$(4.20) \quad T^d \rightarrow U_{N+M}/(U_N \times U_M).$$

We will delve more into this next time.

Lecture 5.

Classification of band structures: 9/12/19

As we mentioned last time, it's possible to *stack* two topological phases: put them both on the same medium, with very weak interactions between them. This defines an associative, commutative operation on phases, and the trivial phase is a unit; hence those phases which are invertible under this operation form an abelian group, and we're interested in studying this group.

For interacting systems in arbitrary dimensions, this is still a bit of an open question; certainly people know what the expected answer is, but we haven't figured out all the details.

Today, we'll restrict ourselves to something less ambitious: translation-invariant, noninteracting fermion systems in dimension d .⁶ In this setting the mathematical formalism is understood.

We impose translation-invariance so that we can work in momentum space (i.e. take the Fourier transform of the Hamiltonian); specifically, translation invariance imposes periodic boundary conditions, so momentum space, which we also call the Brillouin zone, is a d -dimensional torus. The Fourier-transformed Hamiltonian has the general form

$$(5.1) \quad H = \sum_{k \in T^d} \psi_{k,\alpha}^\dagger h_{\alpha,\beta}(k) \psi_{k,\beta}.$$

⁶Noninteracting bosons are also simple: they just form a superfluid, which cannot form a gapped phase.

Since we work on a lattice and let the number of sites go to infinity, really k also lives on a lattice inside T^d , where we also refine this lattice. We want $\sigma^x h^*(-k) \tau^x = -h(k)$, where σ^x is $\begin{pmatrix} I_n & 0 \\ 0 & -I_m \end{pmatrix}$: replacing ± 1 with identity matrices.

Hence h is self-conjugate. We also want the gap in the spectrum of H to be preserved for all k . Therefore the eigenvalues $\varepsilon_1(k), \dots, \varepsilon_n(k): T^d \rightarrow \mathbb{R} \setminus 0$, called *bands*, are continuous functions that do not cross the origin, so we obtain two invariants: let n denote the number of positive bands and m the number of negative bands.

We can diagonalize h by unitary matrices $U(k)$ that also vary continuously in k :

$$(5.2) \quad h = U(k)^\dagger \begin{pmatrix} \varepsilon_1(k) & & \\ & \ddots & \\ & & \varepsilon_n(k) \end{pmatrix} U(k).$$

In this case the Hamiltonian simplifies to

$$(5.3) \quad H = \Delta U(k)^\dagger \begin{pmatrix} I_n & 0 \\ 0 & -I_m \end{pmatrix} U(k),$$

where I_ℓ is the identity matrix of size $\ell \times \ell$.

Let U_ℓ denote the Lie group of $\ell \times \ell$ unitary matrices. By the above discussion, a gapped phase defines a map $T^d \rightarrow U_{n+m}$. However, this overdetermines the classification:

- You can permute the indices of the positive bands, and of the negative bands, so really the target space should be $U_{n+m}/(U_n \times U_m)$.
- A smooth deformation of the Hamiltonian by local terms induces a homotopy between the maps, so the classification should deal with homotopy classes of maps, denoted $[T^d, U_{n+m}/(U_n \times U_m)]$.
- Finally, one can add extra degrees of freedom, so the classification stabilizes in n and m . Therefore what we really need to consider is homotopy classes of maps

$$(5.4) \quad T^d \longrightarrow \bigcup_{n,m} U_{n+m}/(U_n \times U_m).$$

This is a mathematical question, and while the tools used to solve it are slightly beyond the scope of this class, they're well-understood; this is the part of mathematics called *K-theory*. Specifically, one can compute that in $d = 1$, the group is trivial. For $d = 2$, there's a \mathbb{Z} , corresponding to some quantized quantity. In general, the group is 0 for d odd and \mathbb{Z} for d even; there's always a periodicity in this classification.

Now we haven't used all of the structure yet (which I think means topological superconductors rather than topological insulators? **TODO**). The self-conjugacy condition on h means we can diagonalize the system using orthogonal matrices rather than just unitary ones, and forces $m = n$. Therefore the target space is instead

$$(5.5) \quad \bigcup_n O_{2n}/U_n.$$

The classification in $d = 1$ is now $\mathbb{Z}/2$, corresponding to the $\mathbb{Z}/2$ generated by the Kitaev chain that we studied before. In general, the group is always 0, $\mathbb{Z}/2$, or \mathbb{Z} , and has periodicity of order 8.

~ ~ ~

Whether or not you like this level of mathematical formalism, you can use it to guide your considerations in experiments. For example, in a dimension where the classification is a $\mathbb{Z}/2$, you might guess it has something to do with unpaired fermions like in the Majorana chain.

If you try to do this naively, you end up asking for same-spin coupling, which is very unusual, and would be difficult to engineer. This led to a different, more relativistic answer invoking *spin-orbit coupling*. Specifically, if you have a one-dimensional wire with an inversion-breaking crystal structure (we can tell apart the directions along the wire and in the wire, e.g. if there's more charge at the bottom than the top), there's an effect called *Rashba spin-orbit coupling*

$$(5.6) \quad H_R := \alpha \mathbf{E} \cdot (\mathbf{P} \times \mathbf{S}) = \alpha p \sigma^y.$$

Adding this kind of term to the usual Hamiltonian

$$(5.7) \quad H = \left(\frac{p^2}{2m} - \mu \right) - B \sigma^z - \alpha p \sigma^y$$

shifts the bands: previously the bands were two upward-facing parabolas, one intersecting the x -axis and one above it. Now, both parabolas cross the x -axis, and there's a degenerate point where they intersect. Then, one adds a magnetic field, which pushes the bands away from that degenerate point, and it looks better.

So take your favorite semiconductor with spin-orbit coupling and put it on top of a superconductor, close enough that electrons (and specifically Cooper pairs) can tunnel through, causing a *proximity effect*. This adds a term

$$(5.8) \quad \Delta_{\text{eff}}(c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger} + \text{h.c.})$$

to the Hamiltonian, where

$$(5.9) \quad \Delta_{\text{eff}} \approx \begin{cases} t^2/\Delta, & t \ll \Delta \\ \Delta, & t \gtrsim \Delta. \end{cases}$$

Then, all you have to do is turn on an external magnetic field.

Suppose you actually do this in the lab. How would you detect whether there are Majorana fermions at the end of the wire? One approach is that the presence of a Majorana fermion affects the qualitative properties of electron tunneling near the end of the wire. However, there are other ways to cause similar-looking effects: any real material has impurities, and this together with the external magnetic field can degrade the superconductor enough to produce low-energy states. These are bound pairs of Majoranas, and in particular they aren't topologically protected and are not what we're looking for. This approach has been investigated in experiments, e.g. Zhang et al (*Nature*, 2018) and Mourik et al (*Science*, 2012).

These experiments gave nice signatures of topological behavior, which is typical of topological phases. Then one has to argue further as to why these signatures don't come from impurities; for example, Majorana fermions produce signatures at very specific values.

In more detail, suppose we have a metallic lead and a tunneling link Γ to a wire hosting a Majorana zero mode. The experiment sends in an electron at very low energy from the lead to the wire. It will either bounce off the interface or transmit as a Cooper pair and emit backscattering. The Schrödinger equation allows us to compute the conductance:

$$(5.10) \quad H = \int_{-\infty}^0 dx \psi^{\dagger}(x) \left(\frac{p^2}{2m} - \mu \right) \psi(x) + i\Gamma \gamma (\psi(0) + \psi^{\dagger}(0)).$$

We're at energies too low for the electron to propagate into the superconductor, so what we have to compute is

$$(5.11) \quad \Psi_0 = \int_{x<0} e^{ik_F x} \psi(x) + u e^{-ik_F x} \psi(x) + v e^{ik_F x} \psi^{\dagger}(x).$$

The last term comes from a particle-hole symmetry consideration. We can simplify with $[H_{x<0}, \psi_0^{\dagger}] = 0$ and

$$(5.12) \quad i\Gamma \gamma \{(\psi(0) + \psi^{\dagger}(0)), \Psi_0\} = 0.$$

Additionally,

$$(5.13) \quad 2eI = v_F \cdot \left(eV \frac{\partial n}{\partial \mu} \right) (2e),$$

where v_F is the *Fermi velocity* and

$$(5.14) \quad n = \int \frac{dk}{2\pi} \Theta(-\varepsilon_k + \mu).$$

Differentiating gives us

$$(5.15) \quad \frac{\partial n}{\partial \mu} = \int \frac{dk}{2\pi} \delta(\mu - \varepsilon_k) = \frac{1}{2\pi} \left(\left| \frac{\partial \varepsilon_k}{\partial k} \right| \right)^{-1} = \frac{1}{2\pi v_F}.$$

Hence the conductivity is $I = (2e^2/2\pi)(V)$ (if you pay attention to factors of \hbar , there's one in the denominator). One then can check that there are only two possible options, which correspond to the trivial and topological phases.

The first experiments didn't match this more detailed analysis, but by 2017 or so newer devices produced much better-looking curves.

One can see from these experiments that in the topological phase, $\frac{dI}{dV}$ does not depend very strongly on the strength of the tunneling barrier (there are a few wiggles, but not nearly as many as in the trivial phase). So while there's still a little bit of uncertainty, these figures look pretty good. The wiggles in the graph may have something to do with the fact that the Majoranas are actually fairly large relative to the length of the wire used in the experiment. There is still plenty of work before getting qubits out of this, and some more things to rule out (though, see <https://arxiv.org/abs/1908.05549> for some progress).

References

- [Kit01] A. Yu. Kitaev. Unpaired Majorana fermions in quantum wires. *Physics-Uspekhi*, 44(10S):131, 2001. <https://arxiv.org/abs/cond-mat/0010440>. 4