PHY392T NOTES: TOPOLOGICAL PHASES OF MATTER

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Contents

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

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

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

$$H \coloneqq \frac{1}{2}\omega^2(p^2 + x^2). \tag{2.2}$$

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

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

The Hamiltonian is generally of the form

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

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

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

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

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. $f_\alpha^\dagger$ be the annihilation, resp. creation operators for a fermion in state α. There's again a vacuum $|\varnothing\rangle$, with $f_\alpha|\varnothing\rangle = 0$ for all α. Now we impose the relation

$$f_\alpha^\dagger f_\beta^\dagger|\varnothing\rangle = -f_\beta^\dagger f_\alpha^\dagger|\varnothing\rangle. \tag{2.6}$$

That is, define the *anticommutator* by

$$\{f_\alpha^\dagger, f_\beta^\dagger\} \coloneqq f_\alpha^\dagger f_\beta^\dagger + f_\beta^\dagger f_\alpha^\dagger. \tag{2.7}$$

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 $n_\alpha \coloneqq f_\alpha^\dagger f_\alpha$; it satisfies $n_\alpha f_\alpha = f_\alpha(n_\alpha - 1)$, and measures the number of particles in the state α. Because

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

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

$$H \coloneqq \sum_{\alpha,\beta} f_\alpha^+ h_{\alpha\beta} f_\beta. \tag{2.9}$$

The *number operator* $N \coloneqq \sum n_\alpha$ 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

$$u_\theta \coloneqq \exp(i\theta N). \tag{2.10}$$

Then

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

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 $vv^\dagger = \mathrm{id}$. Let $v_{n\alpha} \coloneqq v_\alpha^{(n)}$ and

$$\psi_n \coloneqq \sum_\alpha v_{n\alpha} f_\alpha. \tag{2.12}$$

Then $\psi_n^\dagger$ and ψ_n satisfy the same creation and annihilation relations as $f_\alpha^\dagger$ and f_α:

$$\{\psi_n^\dagger, \psi_m\} = \{\sum_\alpha v_{n\alpha}^* f_\alpha^\dagger, \sum_\beta v_{m\beta} f_\beta\} \tag{2.13}$$

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

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

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

$$H = \sum_n \lambda_n \psi_n^\dagger \psi_n, \tag{2.16}$$

and we can explicitly calculate its action on a state:

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

The term $(*)$ is equal to

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

Then (2.17) is equal to

$$(2.17) = \lambda_{n_1} \psi_{n_1}^\dagger \left(\psi_{n_2}^\dagger \cdots \psi_{n_N}^\dagger\right)|\varnothing\rangle, \tag{2.19}$$

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

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

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

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

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

$$\psi_k \coloneqq \frac{1}{\sqrt{L}} \sum_{j=1}^L e^{ikj} f_j, \tag{2.23}$$

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

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

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

$$= \sum_k e^{ik} \psi_k^\dagger \psi_k. \tag{2.26}$$

That is, the diagonalized Hamiltonian is

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

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:

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

If L is fixed, k only takes on L different values, but implicitly we'd like to take some sort of thermodynamic limit $L \to \infty$, 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

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

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

$$\Psi_{\alpha,\tau} \coloneqq \begin{pmatrix} f_\alpha \\ f_\alpha^\dagger \end{pmatrix}, \tag{2.31}$$

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

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

However, Ψ and $\Psi^\dagger$ have some redundancy: if σ^x denotes the Pauli matrix $\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, then $\Psi_\tau^\dagger = \sigma^x_{\tau\tau'}\Psi_{\tau'}$.

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

$$\Psi^\dagger H \Psi = \Psi^{\mathrm{T}}\sigma^x H \sigma^x (\Psi^\dagger)^{\mathrm{T}} = -\Psi^\dagger \sigma^x H^{\mathrm{T}} \sigma^x \Psi, \tag{2.33}$$

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

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

and

$$\gamma_E \coloneqq \sum_{\alpha,\tau} v_{\alpha\tau}\Psi_{\alpha\tau} \tag{2.35}$$

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 $\mathcal{H}_i \coloneqq \mathbb{C} \cdot \{|0\rangle, |1\rangle\}$, and the total Hilbert space of states is the tensor product of these over all of the states.

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

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

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

$$\tilde{c}_k \coloneqq \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ikj} c_j \tag{3.2a}$$

$$\tilde{c}_k^\dagger \coloneqq \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ikj} c_j^\dagger. \tag{3.2b}$$

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

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

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

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

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

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

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

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

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 $\mu \to -\infty$, this is adiabatically connected to a trivial phase, and thus is itself trivial: there are no particles. For $\mu \to \infty$, 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,

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

[1] To 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.

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

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

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

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

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

$$\tilde{\gamma} = \int \mathrm{d}x\, \phi_\alpha(x)\hat{\psi}_\alpha(x), \tag{3.10}$$

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

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

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

$$\phi_\pm(x) = \exp\left(\pm\int_0^x \frac{M(x)}{v}\,\mathrm{d}x\right)\phi_\pm(0). \tag{3.12}$$

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 $x \to \pm\infty$, $\phi_+(x) \to \exp(-|M_0||x|)$.
- 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 $\gamma_1, \ldots, \gamma_{2N}$, hence N ordinary fermion creation/annihilation operator pairs $\psi^\dagger, \psi$ as we discussed above. This system has a 2^N-dimensional

[2] This 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.

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

$$P_f \coloneqq \prod_{i=1}^{N} i\gamma_{2i-1}\gamma_{2i} \in \{\pm 1\} \tag{3.13}$$

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 $N = 2$,

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

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

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

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

$$\gamma \times \gamma = 0 + f, \tag{3.16}$$

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. Writring $\psi \coloneqq (\gamma_L + i\gamma_R)/2$, $\psi + \psi^\dagger = \gamma_L$ and $\psi - \psi^\dagger = \gamma_R$.

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

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

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 $\gamma_i, \overline{\gamma_i}$ as before, but now γ_i is coupled to $\overline{\gamma_i}$, 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 $H_i \colon \mathcal{H}_i \to \mathcal{H}_i$, the stacked phase has Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ and Hamiltonian $H_1 \otimes \mathrm{id}_{\mathcal{H}_2} + \mathrm{id}_{\mathcal{H}_1} \otimes H_2$, 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 interval[5] into a bunch of pieces, and then each piece can be adiabatically transformed into the trivial insulator.

$\sim \cdot \sim$

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

$$P_F = (-1)^{\sum_i \hat{n}_i} = \prod_j i\gamma_j \overline{\gamma_j}, \tag{4.3}$$

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.

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

[4] The 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.

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

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 $P_F \mathcal{O} P_F^\dagger$.

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

$$i\gamma_i\overline{\gamma_{i+1}} \longmapsto i\gamma_i\sigma^z_{i,i+1}\overline{\gamma_{i+1}}. \tag{4.4}$$

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

$$\sigma^z_{i,i+1} \longmapsto s_{i+1}s_i\sigma^z_{i,i+1}. \tag{4.5}$$

The generator of this symmetry is the operator

$$\prod_i \left((\sigma^x_{i-1,i}\sigma^x_{i,i+1})(\gamma_i\overline{\gamma_i})\right)^{(1+s_i)/2}. \tag{4.6}$$

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

$$A_\mu \longmapsto A_\mu + \partial_\mu\phi \tag{4.7}$$

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

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

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 $\{\pm 1\}$, $\sigma^z_{i,i+1}$ plays the role of $\exp(i\int_i^{i+1} A\cdot \mathrm{d}\ell)$, 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,

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

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

$$\prod_i \sigma^z_{i,i+1} \longmapsto \prod_i (s_i\sigma^z_{i,i+1}s_{i+1}) = \dots s_i\sigma^z_{i,i+1}s_{i+1}s_{i+1}\sigma^z_{i+1,i+2}\dots \tag{4.10}$$

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

$$H_{\text{triv}} - \mu\sum_i c_i^\dagger c_i. \tag{4.11}$$

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

$$H_{\text{top}} = -i\Delta\sum_j \gamma_j\overline{\gamma_{j+1}} \longmapsto i\Delta\sum_j \gamma_i\sigma^z_{j,j+1}\overline{\gamma_{j+1}}. \tag{4.12}$$

The total fermion parity of the ground state is

$$P_F^{GS} = \prod_j i\overline{\gamma_j}\gamma_j \tag{4.13}$$

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

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

$$FP_F F^{-1} P_F^{-1} = -1 \tag{4.15}$$

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

$$H = \sum_k \psi^\dagger_{k,\alpha} h^{(k)}_{\alpha\beta} \psi_{k,\beta}. \tag{4.18}$$

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

$$h(k) = \sum_n \varepsilon_n(k) \prod_n (k). \tag{4.19}$$

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

So in general, we're interested in maps $T^d \to \mathrm{U}_{N+M}$, 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

$$T^d \to \mathrm{U}_{N+M}/(\mathrm{U}_N \times \mathrm{U}_M). \tag{4.20}$$

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 ourself 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

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

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 $\left(\begin{smallmatrix} I_n & 0 \\ 0 & -I_m \end{smallmatrix}\right)$: 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 $\varepsilon_1(k), \dots, \varepsilon_n(k) \colon T^d \to \mathbb{R} \setminus 0$, 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:

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

In this case the Hamiltonian simplifies to

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

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 $T^d \to \mathrm{U}_{n+m}$. 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 $\mathrm{U}_{n+m}/(\mathrm{U}_n \times \mathrm{U}_m)$.
- 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 $[T^d, \mathrm{U}_{n+m}/(\mathrm{U}_n \times \mathrm{U}_m)]$.
- 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

$$T^d \longrightarrow \bigcup_{n,m} \mathrm{U}_{n+m}/(\mathrm{U}_n \times \mathrm{U}_m). \tag{5.4}$$

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

$$\bigcup_n \mathrm{O}_{2n}/\mathrm{U}_n. \tag{5.5}$$

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.

$\sim \cdot \sim$

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

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 naïvely, 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 diractions 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*

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

Adding this kind of term to the usual Hamiltonian

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

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

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

to the Hamiltonian, where

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

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:

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

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

$$\Psi_0 = \int_{x<0} e^{ik_F x}\psi(x) + ue^{-ik_F x}\psi(x) + ve^{ik_F x}\psi^\dagger(x). \tag{5.11}$$

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

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

Additionally,

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

where v_F is the *Fermi velocity* and

$$n = \int \frac{\mathrm{d}k}{2\pi}\Theta(-\varepsilon_k + \mu). \tag{5.14}$$

Differentiating gives us

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

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, $\frac{\mathrm{d}I}{\mathrm{d}V}$ 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).

Lecture 6.

Review of symmetries in quantum mechanics: 9/17/19

Andrew Potter isn't here today, so (TODO: didn't get his name since I was late) gave today's lecture. On Thursday, we'll begin discussing symmetry-protected topological phases, so today we'll review how symmetries manifest in quantum mechanics.

Suppose we have a phase diagram of some gapped physical system with two parameters, and suppose the system has some symmetry which is preserved by the first parameter λ_1 and is broken by the second parameter λ_2. Moving along λ_1 does not change the physical behavior of the system under any observations you can make which respect the symmetry — but for paths which vary λ_2, this is not true. But maybe the things you care about don't see that symmetry anyways, in which case this whole system is in the same phase. That is, the classification of phases of a system depends on what parameters and what symmetries you allow; more symmetries means "being in the same phase" is a stricter equivalence relation, which often means more phases. Studying this has led to a great deal of interesting research.

Definition 6.1. A *symmetry* of a quantum system is a set G of operations on quantum states that leave physical measurements unchanged. We can combine any two operations g_1 and g_2 by first doing g_2, then g_1; call this new operation g_1g_2. We ask for G to be a *group*, meaning it satisfies the following axioms.

(1) For any $g_1, g_2 \in G$, the product $g_1g_2 \in G$.
(2) There is an element $e \in G$, called the *identity* or *unity*, such that $eg = ge = g$ for all $g \in G$. Physically, this is the operation that doesn't do anything.
(3) Every operation can be undone: for each $g \in G$ there's a $g^{-1} \in G$ such that $gg^{-1} = g^{-1}g = e$.

When one studies groups abstractly in mathematics, one must impose another axiom, called *associativity*, on triples of elements, but if your groups arise as sets of transformations on some system, this is already true.

Remark 6.2. It is *not* true that $g_1g_2 = g_2g_1$ in general! If that holds for all $g_1, g_2 \in G$, G is called *abelian*. ◂

Example 6.3. Let N be a positive integer. The group of *integers mod* N, denoted $\mathbb{Z}/N\mathbb{Z}$, $\mathbb{Z}/N$, or $\mathbb{Z}_N$,[7] is $\{0, 1, 2, \ldots, n-1\}$, where the group operation is defined to be addition mod n, i.e. given $p, q \in \mathbb{Z}/N$, take the remainder of dividing $p + q$ by N. For example, the hours of a clock form a $\mathbb{Z}/12$, unless you have a 24-hour clock, in which case it's $\mathbb{Z}/24$.

These groups are all abelian. ◂

[7]The names $\mathbb{Z}/N\mathbb{Z}$ and $\mathbb{Z}/N$ are more common in mathematics and $\mathbb{Z}_N$ is more common in physics. This is because there's a different object called $\mathbb{Z}_N$ in number theory.

Example 6.4. The *circle group* $\mathrm{U}(1)$[8] describes phases. Concretely, the underlying set is $[0,1)$, and the group operation is addition mod 1, i.e. add two elements, then take the non-integer part. This group is also abelian. ◂

Example 6.5. The *unitary group* $\mathrm{U}(N)$ (also U_N) is the group of unitary $N \times N$ matrices, and the group operation is matrix multiplication. Similarly, the *special unitary group* $\mathrm{SU}(N)$ (or SU_N, etc.) is the subset of $\mathrm{U}(N)$ of matrices with determinant 1 — since this is preserved under matrix multiplication, this is indeed a group.

Similarly, the *orthogonal group* $\mathrm{O}(N)$ denotes the group of $N \times N$ orthogonal matrices (with real coefficients), and $\mathrm{SO}(N)$, the *special orthogonal group*, denotes the subgroup with determinant equal to 1. ◂

We now have two different things called U_1; they had better be the same. And indeed, a 1×1 unitary matrix is a unit complex number, and these all can be described as $\exp(2\pi i\theta)$ for exactly one $\theta \in [0,1)$; furthermore, the identity, multiplication, and inverses match. So this is not a problem.

We care about groups because they do stuff. Wigner's theorem states that a symmetry operation on a quantum system can be represented by linear operations that are unitary or antiunitary. See Weinberg's book for a proof. Unitary means $U^\dagger U = 1$, and linear means that

$$U(\alpha\psi_1 + \beta\psi_2) = \alpha \cdot U(\psi_1) + \beta \cdot U(\psi_2). \tag{6.6}$$

So $\langle \phi \mid \psi \rangle = \langle U\phi \mid U\psi \rangle$. An *antiunitary* operator A satisfies $\langle \phi \mid \psi \rangle^* = \langle A\phi \mid A\psi \rangle$ and *antilinearity*:

$$A(\alpha\psi_1 + \beta\psi_2) = \alpha^* \cdot A(\psi_1) + \beta^* \cdot A(\psi_2). \tag{6.7}$$

Time-reversal symmetries are examples of antiunitary symmetries.

If your Hilbert space is N-dimensional, U_N therefore is important, since it contains the unitary symmetry operations for the system.

Definition 6.8. A *unitary representation* of a group G is a map $\rho\colon G \to \mathrm{U}_N$ such that $\rho(g_1 g_2) = \rho(g_1)\rho(g_2)$. In particular, $\rho(e) = e$.

We will also need a more general notion.

Definition 6.9. A *projective unitary representation* of a group G is data of two maps, $\rho\colon G \to \mathrm{U}_N$ and $\phi\colon G \times G \to \mathrm{U}_1$ such that $\rho(g_1)\rho(g_2) = \phi(g_1, g_2)\rho(g_1 g_2)$.[9]

The study of group representations is a huge subject of mathematics; in particular, for the groups we care about in physics, the classifications of their representations are all known.

One interesting example is that there are interesting projective representations of SO_N which do not come from actual representations. These correspond to the notion of "half-integer spin" in physics. TODO: didn't follow the notation. In any case, there's a group structure on the set of isomorphism classes of projective representations that aren't actual representations; for $N = 3$ that group is $\mathbb{Z}/2$.

Lecture 7.

Symmetry-protected topological phases: 9/19/19

There are some situations in condensed-matter physics where we have a two-parameter system, where varying one of the parameters preserves some symmetry and varying the other breaks it. For example, we could have a time-reversal-symmetric system where we're able to introduce a magnetic field, which breaks the symmetry.

Here something curious can happen: as long as we only make deformations which preserve the symmetry, we can find phases which are different from the trivial phase, in that if you deform it to the trivial phase, there's necessarily a phase transition closing the gap; but if you allow the symmetry to be broken, there is a gap-preserving deformation. Such phases are called *symmetry-protected topological (SPT)* phases.

Here are some examples of commonly-considered symmetries in the study of SPTs.

- Time-reversal symmetry is an antiunitary symmetry squaring to 1, and is customarily denoted $\mathbb{Z}_2^T$. Often this will act on the system by complex conjugation. The generator of this symmetry is denoted $\mathcal{T}$.

[8] This group goes by several other names, including U_1, $\mathbb{T}$, and S^1, in different fields in mathematics.

[9] TODO: we may need to impose a condition on ϕ; I don't remember it offhand and missed it during the lecture.

- Some systems preserve particle number. This is a U_1 symmetry, and the generator is $\exp(-i\theta\widehat{N})$.
- Some systems have a rotation symmetry acting on the spins. This is SO_3 for integer spins, but SO_3 only acts projectively for half-integer phases, so we have to pass to the double cover $\mathrm{Spin}_3 = \mathrm{SU}_2$. The

Example 7.1 (The AKLT phase)**.** Affleck-Kennedy-Lieb-Tasaki [AKLT88] wrote down the first example of an SPT, before the idea of an SPT was ever coined, for the symmetries $\mathbb{Z}_2^T$ and SO_3. Consider a wire with L vertices as we did for the Majorana chain, and suppose that at each site, there are three options for the spins. That is, the local Hilbert space is $\mathbb{C}^3$, and the total Hilbert space is the tensor product of the local Hilbert spaces over all sites. Introduce the Pauli-like operators

$$S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad S^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad S^y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{7.2}$$

and let $\mathbf{S} = (S^z, S^y, S^x)$. Haldane [Hal83a, Hal83b, Hal85] famously studied the Hamiltonian

$$H = J\sum_{i=1}^{L} \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \tag{7.3}$$

and conjectured this is gapless for integer spins and gapped for half-integer spins. Affleck-Kennedy-Lieb-Tasaki perturbed this Hamiltonian to

$$H = J\sum_{i=1}^{L} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + K\sum_{i=1}^{L} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2. \tag{7.4}$$

The first term is generally called a *Heisenberg interaction*, and the second is called a *biquadratic interaction*. This system has an SO_3 rotation symmetry (if the spin is an integer) and a $\mathbb{Z}_2^T$ time-reversal symmetry, which is complex conjugation. The terms in (7.4) don't commute, but because this Hamiltonian satisfies a weaker condition of being *frustration-free*, we can write down a nice ground state, which for judiciously chosen J and K is an SPT.

Let's suppose $J = \cos\theta$ and $K = \sin\theta$; then we can plot the phase diagram in θ.

- For θ near $-\pi$, the system is a dimer: nearby neighbors pair up.
- For θ in the second quadrant and part of the third quadrant, the system is a ferromagnet: nearby spins tend to point in the same direction.
- For θ a bit less than π, the system is critical.
- For the remaining θ, in particular at the *AKLT point* $K = J/3$, the system is an SPT!

We restrict to the AKLT point because it's easier to analyze.

TODO: I missed something here.

In order to analyze the SO_3-symmetry, let's assume the system has spin 1, so that the $\mathbb{C}^3$ at each site is the defining representation $\mathbf{1}$ of SO_3. Therefore the interactions between sites i and $i+1$ are in the representation

$$\mathbf{1} \otimes \mathbf{1} \cong \mathbf{0} \oplus \mathbf{1} \oplus \mathbf{2}. \tag{7.5}$$

Let $\Pi^{(i)}_{j,j+1}$ denote the orthogonal projection $\mathbf{1} \otimes \mathbf{1} \twoheadrightarrow \mathbf{i}$, for $i \in \{0,1,2\}$; this map is SO_3-equivariant.

At the AKLT point, $K = J/3$, which means that in $\mathbf{0}$, the total energy is $-2J/3$, in $\mathbf{1}$, we get $-2J/3$, and in $\mathbf{2}$, we get $4J/3$. Therefore

$$(7.4) = 2J\sum_j \Pi^{(2)}_{j,j+1} + (\text{constants}). \tag{7.6}$$

There is a projection P_1 which sends a spin-1/2 state to a spin-1 state. (TODO: I don't understand this.) The ground state at the AKLT point is P_1 applied to the *singlet state*

$$|\psi_{\text{sing}}\rangle = \bigotimes_i \frac{1}{\sqrt{2}}(\uparrow_{B,i}\downarrow_{A,i+1} - \downarrow_{B,i}\uparrow_{A,i+1}). \tag{7.7}$$

The singlet state pairs up neighbors, and therefore there are unpaired edge states, though they're not as exotic as the ones we found in the Majorana chain.

We should check that $P_1|\psi_{\text{sing}}\rangle$ is actually a ground state. One can check that the eigenvalues of the Hamiltonian are nonnegative. Then, each term in (7.4), reformulated as in (7.6), kills $P_1|\psi_{\text{sing}}\rangle$:

$$\Pi^{(2)}_{j,j+1} P_1|\psi_{\text{sing}}\rangle = P_1 \widetilde{\Pi}^{(2)}_{j,j+1}|\psi_{\text{sing}}\rangle = 0. \tag{7.8}$$

If you introduce a magnetic field term $-\mathbf{B}\cdot\sum \mathbf{S}_i$ to the Hamiltonian, you can kill these edge states, but this breaks both the SO_3 and the $\mathbb{Z}_2^T$ symmetries. Thus this system is an SPT for either SO_3 or $\mathbb{Z}_2^T$ separately; in fact, we can pick smaller subgroups of SO_3, including anything for which $-\mathbf{B}\cdot\boldsymbol{\sigma}$ isn't symmetric. For example, we could pick the $\mathbb{Z}/2\times\mathbb{Z}/2$ subgroup of rotations by π around two different axes.

If we consider the system on an interval, we have four ground states, corresponding to what the two spins on the edges are doing: each can be up or down. We therefore get spin projector operators on the edges, e.g. S^z_L, which is the identity in the bulk and on the right-hand side, but which acts by σ^x on the left-hand side; we can analogously see the other Pauli matrices and the operators on the right-hand side.

Here another strange thing happens — the macroscopic degrees of freedom in the bulk are all spin-1, but these edge operators obey the rules of a spin-1/2 system! This is an example of fractionalization. Symmetry is crucial: we can only see spin using the SO_3 (or SU_2) symmetry. ◂

In the rest of today's lecture, we'll discuss another system in the same phase whose analysis doesn't require introducing fictitious degrees of freedom. Next time, we'll discuss the entanglement properties of the AKLT phase: what happens if you cut the system somewhere? This will allow us to conclude that the system is in an SPT phase by just looking at the bulk, leading eventually to the matrix product state representation of SPTs and a general 1D classification.

Example 7.9 (Cluster state)**.** This state is easier to analyze than the AKLT system, though as $\mathbb{Z}/2\times\mathbb{Z}/2$-symmetry protected phases, they're in the same phase. It also appears in quantum information, where certain properties make it easier to reason about qubits.

The Hilbert space is again a tensor product of local Hilbert spaces, each of which is four-dimensional, with basis $|0\rangle,\dots,|3\rangle$. Let g_A generate the first $\mathbb{Z}/2$ and g_B generate the second $\mathbb{Z}/2$. We ask for $\mathbb{Z}/2\times\mathbb{Z}/2$ to act on the system as follows:

- g_A fixes $|0\rangle$ and $|1\rangle$ and flips the signs of $|2\rangle$ and $|3\rangle$.
- g_B fixes $|0\rangle$ and $|2\rangle$ and flips the signs of $|1\rangle$ and $|3\rangle$.[10]

Write $X_{a,i}$ for g_A acting at site i, and $X_{B,i}$ for g_B acting at site i. Let $Z_{A,i}$ and $Z_{B,i}$ switch the basis vectors at site i (TODO: I didn't get which ones specifically).[11] Then the Hamiltonian is

$$H = -J\sum_i (Z_{A,i}X_{B,i}Z_{A,i+1} + Z_{B,i}X_{A,i+1}Z_{B,i+1}). \tag{7.10}$$

So this looks like a ZXZ chain, though we've formulated it somewhat differently (e.g. this isn't exactly a spin system).

This is a *stabilizer Hamiltonian*, which means

- each ZXZ term in the Hamiltonian squares to 1, so its eigenvalues are in $\{\pm1\}$;
- all pairs of these terms commute; and
- no term is a product of other terms.

We can call each such term S a *stabilizer*. If you specify an eigenvalue for each stabilizer separately, you've determined a unique state, and therefore we can analyze the Hamiltonian and its ground states without writing down the entire wavefunction.

Often people write down the projectors $\Pi_S \coloneqq (1+S)/2$, which projects into the subspace where S has eigenvalue 1.

By inspection, we can write down some operators which commute with the Hamiltonian.

- Let $\Sigma^1 \coloneqq X_{A,1}Z_{A,1}$; this clearly commutes with distant terms, and you can check that it commutes with the nearby ZXZ terms.
- In the same way, you can define $\Sigma^2 \coloneqq Y_{A,1}Z_{B,1}$ and $\Sigma^3 \coloneqq Z_{A,1}$ and observe that they commute with the Hamiltonian.

[10] If σ denotes the sign representation of $\mathbb{Z}/2$, this tells us our local Hilbert space is $(\mathbf{1}\oplus\sigma_A)\otimes(\mathbf{1}\oplus\sigma_B)$.

[11] I think under the description of the local Hilbert space as a tensor product, X_A and Z_A are the usual Pauli matrices acting on the first tensor factor, and X_B and Z_B act on the second tensor factor.

So, just like in the AKLT chain, these generate a spin-1/2 at the boundary: $[\Sigma^i, \Sigma^j] = 2i\epsilon^{ij}_k \Sigma^k$.

We should next check how the $\mathbb{Z}/2 \times \mathbb{Z}/2$ symmetry acts on $\mathbf{\Sigma}$.

$$g_A \mathbf{\Sigma} g_A = X_{A,1} \begin{pmatrix} X_A Z_B \\ Y_A Z_B \\ Z_A \end{pmatrix} X_{A,1} = \begin{pmatrix} \Sigma^1 \\ -\Sigma^2 \\ -\Sigma^3 \end{pmatrix} = \Sigma^1 \mathbf{\Sigma} \Sigma^1. \tag{7.11a}$$

Similarly,

$$g_B \mathbf{\Sigma} g_B = \begin{pmatrix} -\Sigma^1 \\ -\Sigma^2 \\ \Sigma^3 \end{pmatrix} = \Sigma^3 \mathbf{\Sigma} \Sigma^3. \tag{7.11b}$$

TODO: g_A and g_B commute, but Σ^1 and Σ^3 anticommute. What happened?

TODO: also there was some other stuff which I didn't follow. ◂

Lecture 8.

Entanglement: 9/24/19

Let's say we're studying some quantum system on a wire. We can imagine cutting the wire into two pieces A and A^c, as in Figure 1.

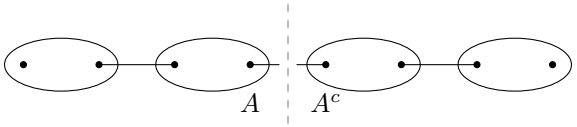


FIGURE 1. Splitting a spin chain into two subsystems which might be entangled.

Since the Hilbert space is a tensor product of local Hilbert spaces, it factorizes:[12]

$$\mathcal{H} = \bigotimes_{i=1}^{L} \mathcal{H}_i = \underbrace{\left(\bigotimes_{i \in A} \mathcal{H}_i \right)}_{=:\mathcal{H}_A} \otimes \underbrace{\left(\bigotimes_{i \in A^c} \mathcal{H}_i \right)}_{=:\mathcal{H}_{A^c}}. \tag{8.1}$$

Hence, if the system is in a state $|\psi\rangle$, we can ask whether $|\psi\rangle$ factors as a product state

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_{A^c}\rangle. \tag{8.2}$$

If so, we call $|\psi\rangle$ *entangled*; if not, it's *unentangled*.

If you choose bases $\{|i_A\rangle\}$ for $\mathcal{H}_A$ and $\{|j_{A^c}\rangle\}$ for $\mathcal{H}_{A^c}$, then you can check whether

$$|\psi\rangle = \sum_{i,j} \lambda_{ij} |i_A\rangle \otimes |j_{A^c}\rangle, \tag{8.3}$$

in which case $|\psi\rangle$ is entangled, but whether you can do this is basis-dependent, which is annoying; there's a luck component of choosing a good basis. Let's try something smarter.

Remark 8.4. TODO: Be especially aware of mistakes in the following, coming from my confusion over the notation: at each site, $\dim(\mathcal{H}_i)$ isn't always 1, so straightening out what exactly we're indexing over confused me thoroughly during class. It shouldn't be too hard, but I wasn't able to figure it out in time. Sorry about that.

I also missed some stuff (e.g. some stuff about the entanglement entropy). ◂

[12] Well, this is true for bosonic systems. For fermions, this must be modified slightly to take the nonlocal effects of particle statistics into account, which amounts to using the $\mathbb{Z}/2$-graded tensor product.

Let's choose a basis s_i for each site i in the chain. Then we can write $|\psi\rangle$ as

$$|\psi\rangle = \sum_{s_1,\dots,s_L} \psi^{s_1,\dots,s_L} \tag{8.5a}$$

$$= \sum_{\substack{s_i : i\in A \\ s_j : j\in A^c}} \psi^{(s_i)_{i\in A},(s_j)_{j\in A^c}} |(s_i)_{i\in A}\rangle \otimes |(s_j)_{j\in A^c}\rangle. \tag{8.5b}$$

Think of $\psi^{(s_i)_{i\in A},(s_j)_{j\in A^c}}$ as an $|A| \times |A^c|$ matrix; if $|A| = |A^c|$, we could diagonalize and use that to check whether $|\psi\rangle$ is a product state. But in general, this is not a square matrix, so we can't diagonalize it, but there is a "next best thing," called the *singular value decomposition*. In general, an $m \times n$ matrix M factors as $M = U\Lambda V$, where

- U is an $n \times n$ unitary matrix; specifically, it's the change-of-basis matrix which diagonalizes the $n \times n$ matrix $MM^\dagger$.
- Similarly, V is an $m \times M$ unitary matrix, which is the change-of-basis matrix diagonalizing the $m \times m$ matrix $M^\dagger M$.
- Λ is a "diagonal" $m \times n$ matrix, in that its only nonzero values are the diagonal entries $\lambda_1, \dots, \lambda_n$. These are called the *singular values* of M.

This is unique in the same way as diagonalization is, and in particular the set of singular values is an invariant of M. Applying this to (8.5b),

$$|\lambda\rangle = (8.5b) = \sum \lambda_\gamma U^{\alpha\gamma} |(s_i)_{i\in A}\rangle V^{\gamma\beta} |(s_j)_{j\in A^c}\rangle. \tag{8.6}$$

Here α indexes the basis elements $|(s_i)_{i\in A}\rangle$ and β indexes the analogue for A^c.

Example 8.7. Let's consider a chain of length 2, with a qubit (i.e. a two-dimensional Hilbert space) at each site, and we'll split in the only nontrivial way. Let

$$\psi := \frac{|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{2}, \tag{8.8}$$

which is a product state. For $\beta, \alpha \in \{\uparrow, \downarrow\}$, we have

$$(\psi^{\alpha,\beta}) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \tag{8.9}$$

so computing the SVD is the same thing as diagonalizing $(\psi^{\alpha,\beta})$:

$$(\psi^{\alpha,\beta}) = \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}_{U} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}_{\Lambda} \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}_{V}. \tag{8.10}$$

In general, we order the singular values by $|\lambda_1| \geq |\lambda_2| \geq \dots$, so $\lambda_1 = 1$ and $\lambda_2 = 0$. ◂

In general, $|\psi\rangle$ is in a product state iff $|\lambda_1| = 1$ and $|\lambda_i| = 0$ for $i > 1$. Taking the SVD in this context is called the *Schmidt decomposition*; the two states are called *Schmidt states* and the singular values are called *Schmidt weights*.

There's something (TODOnot sure what) probabilistic going on here, and when you have a random variable, it's often useful to study its entropy.

Definition 8.11. The *entanglement entropy* of $|\psi\rangle$, A, and A^c is

$$S_A(|\psi\rangle) = -\sum_i |\lambda_i|^2 \log|\lambda_i|^2 = -\operatorname{tr}(\rho_A \log \rho_A), \tag{8.12}$$

where ρ_A is the partial trace.

Hence, $S_A(|\psi\rangle) = 0$ iff ψ is unentangled. The entanglement entropy satisfies

$$S_A(|\psi_1\rangle \otimes |\psi_2\rangle) = S_A(|\psi_1\rangle) + S_A(|\psi_2\rangle) \tag{8.13a}$$

and is *subadditive*, in that

$$S_{A\cup B} \leq S_A + S_B \tag{8.13b}$$

for any choice of $|\psi\rangle$.

Entanglement entropy tells you a lot about your system. For example, the "typical state" (i.e. an expectation value under some sort of Haar random measure) has entanglement entropy

$$S_A(|\psi_{\text{typical}}\rangle) = |A|\log|\mathcal{H}_i| - (\text{constant}) + \dots, \tag{8.14}$$

where the unwritten terms tend to 0 as $|A| \to \infty$. However, the ground states of a gapped Hamiltonian behave differently:

$$S_A(|\psi_{\text{GS}}\rangle) = (\text{constant}) + \dots. \tag{8.15}$$

In higher dimensions, it's conjectured that this constant is proportional to $|\partial A|$.

Example 8.16. In a 1D conformal field theory, $S_A = (c/3)\log|A| + \dots$, where c is the central charge. For CFTs in higher dimensions, we have terms $S_A = c_1|\partial A| + c_2\log|A| + \dots$.

In a Fermi liquid, $S_A = (k_F L_A)^{d-1}\log(L_A)$. ◂

As is so often true in physics, it's helpful to think of this as a statistical-mechanics system: the term $p_i \coloneqq |\lambda_i|^2$ can be valued in $[0,1]$, or alternatively we can look at $\varepsilon_i \coloneqq -\log p_i$. The *entanglement spectrum* is the plot of ε_i against i; one of the hallmarks of an SPT, which we will discover using the matrix product states formalism, is a highly nontrivial entanglement spectrum.

That means it's about time to discuss matrix product states. First, let's cut just the first site from the remaining $L-1$ sites, giving a matrix Λ_1 of singular values. Then iterate with the next site, giving another matrix Λ_2, and so on, leading to a factorization

$$\psi^{s_1\cdots s_N} = \sum \lambda_{1,\alpha}\psi^{s_1}_{A,\alpha}\left(\psi^{s_2\cdots s_N}_{A^c,\alpha}\right) \tag{8.17}$$

$$= \sum_{\alpha_1}\lambda_{1\alpha_1}\psi^{s_1}_{A\alpha_1}\sum_{\alpha_2}\lambda_{2\alpha_2}\psi^{s_2}_{A\alpha_1\alpha_2}\psi^{s_3\cdots s_N}_{\alpha_1,\alpha_2}. \tag{8.18}$$

If we iterate and let $M^{s_i}_{\alpha_{i-1}\alpha_i} \coloneqq \lambda_{i\alpha_i}\psi^{s_i}_{A\alpha_{i-1}\alpha_i}$, then this rewrites $|\psi\rangle$ as a product of these matrices:

$$= M^{s_1}_{\alpha_1}M^{s_2}_{\alpha_1\alpha_2}M^{s_3}_{\alpha_2\alpha_3}\cdots M^{s_{L-1}}_{\alpha_{L-2},L-1}M^{s_L}_{\alpha_{L_1}}. \tag{8.19}$$

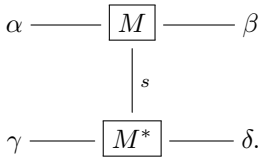
Hence the name "matrix product state."

Remark 8.20. If you want to actually simulate quantum systems, this looks computationally too big to really work with, but it's actually tractable, and much more efficient than *a priori* descriptions of ground states of gapped Hamiltonian systems, and nothing like it works for arbitrary states. ◂

You can think of this as a system of contractions across a trivalent tensor network. There are multiple ways to do this, and they're all necessarily equivalent.

For example, let's consider a simple contraction... TODO

(8.21)



This corresponds to $\sum_s M^s_{\alpha\beta}M^{*s}_{\gamma\delta} = \dots$

Lecture 9.

Matrix product states: 10/1/19

At the end of the last lecture, we described the ground state of a topological phase by cutting at every junction and describing the state as a bunch of contractions of matrices. This admits a diagrammatic representation as a *tensor network*, a graph where the vertices are tensors and the edges, labeled by indices, represent contracting the specified index. Thus a tensor network represents a computation of a number. You can contract the indices in different orders, and the answer doesn't change, but the computational complexity can change drastically. In fact, for networks representing d-dimensional systems for $d \geq 2$, it's NP-hard to determine the optimum order for evaluation!

In dimension 1, things are a little easier. In almost all experiments, what we compute is a correlation function $\langle\psi \mid \mathcal{O}_1\mathcal{O}_2 \mid \psi\rangle$, and we can represent this as a "ladder," an $N \times 2$ tensor network with $\mathcal{O}_1$ and $\mathcal{O}_2$ inserted somewhere in the middle. Here, we know what the optimum evaluation order is: first contract each leg of the ladder, then go along the line. This is polynomial in the size of the indices and linear in N.

The key operation is the transfer matrix (8.21), representing

$$T_{\alpha\gamma,\beta\delta} = \sum_s M^s_{\alpha\beta} M^*_{\gamma\delta}. \tag{9.1}$$

Diagonalizing the transfer matrix tells us that

$$T^M = \sum_{j=1}^{\chi^2} \tau_j^M V_j^\dagger V_j, \tag{9.2}$$

where $\tau_1 = 1 > \tau_2 \geq \tau_3 \geq \dots$. The fact that there is a unique largest eigenvalue is a linear-algebraic consequence of the fact that there's a unique ground state.

Suppose the insertions of $\mathcal{O}_1$ and $\mathcal{O}_2$ are separated by R steps in the ladder, where R is large. Then most of the terms in (9.2) are very small, and we conclude that

$$\langle\psi \mid \mathcal{O}_1\mathcal{O}_2 \mid \psi\rangle - \langle\mathcal{O}_1\rangle\langle\mathcal{O}_2\rangle \sim e^{-R/\xi}, \tag{9.3}$$

where $\xi \sim \tau_2$, the largest remaining component.

Thus matrix product states have exponentially decaying correlation functions and limited entanglement, which is exactly what we expect from the ground states of gapped Hamiltonians. In fact, in $d = 1$, there is a one-to-one correspondence: given a gapped Hamiltonian, there's a matrix product state representation of its ground state, and given a matrix product state one can reconstruct a gapped Hamiltonian. Since matrix product states are computationally efficient to work with, this is very fortunate.

Example 9.4. Consider a trivial state where the spins are alternating. We can represent this with a $\chi = 1$ matrix product state, where $M^s = \delta_{s,\uparrow}$ for i even and $M^s = \delta_{s,\downarrow}$ for i odd. ◂

Example 9.5. For a more interesting example, consider the GHZ state

$$\frac{|\uparrow\uparrow\uparrow\cdots\uparrow\rangle + |\downarrow\downarrow\downarrow\cdots\downarrow\rangle}{\sqrt{2}}. \tag{9.6}$$

This can be represented as a $\chi = 2$ matrix product state, where

$$M^\uparrow = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad M^\downarrow = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{9.7a}$$

and

$$V_L = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad V_R = \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{9.7b}$$

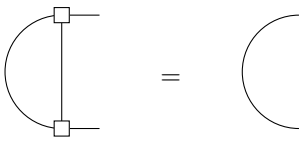
◂

In the exercises, you'll construct a matrix product state representation for the ground state of the AKLT chain (Example 7.1).

One can run a kind of renormalization on the tensor network where we take a few legs, say 3, and regard them as one larger node. Then we obtain a new transfer matrix $\widetilde{T} := T^3$. If we keep doing this, in the limit the eigenvalues τ_i for $i > 1$ will die off, and we'll just get the projector $T = V_1^\dagger V_1$.

Remark 9.8. The matrix product state representation of a ground state is not unique: for example, we can insert W^{-1}, then W, into the tensor network. This is sometimes called a *gauge redundancy*. One can cut down on this redundancy by asking for the chain to be in *(left) canonical form*, meaning...

(9.9)



This guarantees that the ground state is normalized correctly, even in infinite chains, and simplifies some other computations (TODO: I missed some of what came afterwards.) ◂

Since matrix product states describe ground states of gapped systems, we can use them to study SPTs. First, though, we need to understand how symmetries of a system are implemented for matrix product states. This will lead us to a complete understanding of 1d SPTs.

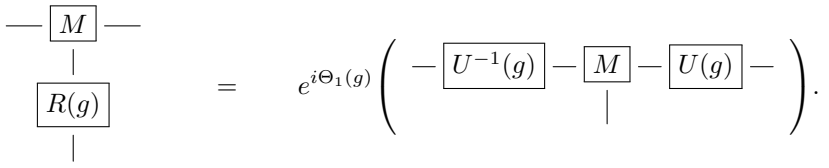
Let S be a symmetry group of a system, acting via a representation R on the Hilbert space. For now, we assume R is unitary (so no time-reversal symmetry), and that it represents an *internal symmetry*: R factors as a tensor product over all sites. Geometrically, the symmetry is just doing something independently to each site, rather than something like translation or reflection which exchanges sites. Spin rotation is a good example of such an R.

We want to describe the ground state $|\psi\rangle$ as a matrix product state, i.e. $R(g)|\psi\rangle = e^{i\Theta(g)}|\psi\rangle$. What does this mean for the matrices in the matrix product state description of $|\psi\rangle$? One clear sufficient condition is that

$$R_{ss'}(g)M^{s'}_{\alpha,\beta} = e^{i\Theta_1(g)}M^{s}_{\alpha,\beta}, \tag{9.10}$$

but this turns out to be too strong: one can write down symmetric ground states which do not have this property. This is related to the gauge redundancy that we discussed above: we can ask for

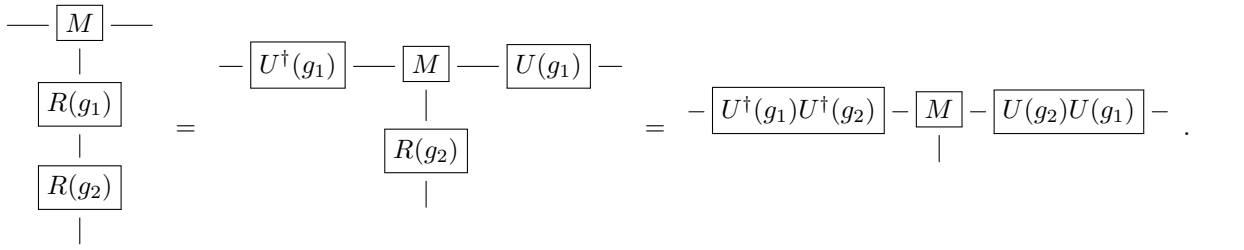
(9.11)



These compute the same ground state, as we described above, and one can show that this is both a necessary and a sufficient condition.

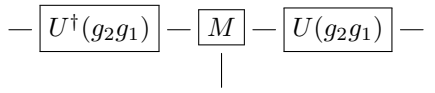
Now, what happens when we compose two elements of the symmetry group? We know $R(g_2)R(g_1) = R(g_2g_1)$, and can also compute what happens to the bond degrees of freedom, by first pulling $R(g_1)$ back into the bond space à la (9.11), then pulling back $R(g_2)$:

(9.12)



We can compare this to what happened if we combined $R(g_1)$ and $R(g_2)$ before pulling back into the bond space, in which case we obtain

(9.13)



It would be nice to say these are equal, but this is not always true: it could be the case that

$$U(g_2g_1) = \omega(g_1, g_2)U(g_2)U(g_1) \tag{9.14}$$

for some function $\omega\colon S \times S \to \mathrm{U}_1$.

Example 9.15. In the AKLT state, $S = \mathbb{Z}/2 \times \mathbb{Z}/2$. Let a denote the generator of the first copy of $\mathbb{Z}/2$ and b denote the generator of the second. Then $U(a)U(b) = -U(b)U(a)$, indicating that $\omega(a,b)\omega(b,a) = -1$, so ω is nontrivial. ◂

So we get a projective representation, which is reasonable. This can also explain something interesting: in a closed system, we get a unique ground state, but in a system with a boundary, there must be multiple ground states, which you can argue using the linear algebra of matrix product states. This is ultimately because we must choose boundary conditions, and in general have multiple choices. We say this ground state

degeneracy in both the Kitaev chain and the AKLT chains: in both cases, there's a unique ground state on the circle, but multiple on the interval.

This tensor product decomposition assumes that we're in a bosonic system, because locality is a little different. But the upshot is that to understand and classify 1d bosonic SPT phases for an internal symmetry group G, we should classify projective representations of the symmetry group.[13]

We arrived at projective representations through $\omega\colon S \times S \to \mathrm{U}_1$, but asking for ω to describe a projective representation puts both some conditions on ω and implies some redundancy. First, the condition: using associativity of multiplication in g,

$$\omega(g_1, g_2)\omega(g_1g_2, g_3)U(g_1g_2g_3) = \omega(g_1, g_2g_3)\omega(g_2, g_3)U(g_1g_2g_3). \tag{9.16}$$

Since $U(g_1g_2g_3)$ is invertible, we conclude that

$$\frac{\omega(g_1, g_2)\omega(g_1g_2, g_3)}{\omega(g_1, g_2g_3)\omega(g_2, g_3)} = 1. \tag{9.17}$$

This is called the 2-*cocycle condition*.

The redundancy arises as follows: given a phase $\beta \in \mathrm{U}_1$, we can conjugate $\mathrm{U}(g)$ by β and obtain what should be the same projective representation. Under this transformation,

$$\omega(g_1, g_2) \longmapsto \frac{\beta(g_1)\beta(g_2)}{\beta(g_2g_1)}\omega(g_1, g_2). \tag{9.18}$$

Therefore the group of isomorphism classes of projective representations into U_1 is the group of maps $\omega\colon S \times S \to \mathrm{U}_1$ satisfying the 2-cocycle condition, modulo the relation (9.18). This group is denoted $H^2(S; \mathrm{U}_1)$, the *second group cohomology of S with coefficients in* U_1. Here, "second" has to do with the fact that ω takes in two copies of S.

The idea is that $H^2(S; \mathrm{U}_1)$ classifies 1d bosonic SPTs with internal symmetry S: such an SPT has edge modes transforming in the given projective representation.

Lecture 10.

The field-theoretic perspective: 10/3/19

In condensed-matter systems, we can compute partition functions by a sort of path integral:

$$U_{fi} = \langle f \mid e^{-iHt} \mid i\rangle = \sum_{i\to f} e^{iS_{cl}(\text{path})}, \tag{10.1}$$

where the sum is over all classical paths $i \to f$, and S_{cl} is the classical action, $\int_0^\beta \mathrm{d}\tau\, L$, where L is the Lagrangian.

We're not always so interested in time evolution in condensed-matter physics, but if we rotate to imaginary time, this tells you information about thermal behavior:

$$H \longrightarrow H + \frac{1}{\beta}\int \mathrm{d}x\, \lambda(x)\phi(x). \tag{10.2}$$

This is a sort of generating function: if

$$Z_\lambda \coloneqq \mathrm{tr}\Big(e^{-\beta H - \int \lambda\phi}\Big), \tag{10.3}$$

then, e.g.,

$$\frac{\partial^2 \ln Z_\lambda}{\partial\lambda(x_1)\partial\lambda(x_2)}\bigg|_{\lambda\to 0} = \frac{\partial}{\partial\lambda(x_1)}\left(\frac{\mathrm{tr}\big(-\phi(x_2)\exp\big(-\beta H - \int\lambda\phi\big)\big)}{\mathrm{tr}\exp\big(-\beta H - \int\lambda\phi\big)}\right) \tag{10.4}$$

$$= \frac{\mathrm{tr}\,\phi(x_1)\phi(x_2)e^{-\beta H}}{\mathrm{tr}\,e^{-\beta H}} - \frac{\mathrm{tr}\,\phi(x_1)e^{-\beta H}\,\mathrm{tr}\,\phi(x_2)e^{-\beta H}}{(\mathrm{tr}\,e^{-\beta H})^2} \tag{10.5}$$

$$= \langle\phi(x_1)\phi(x_2)\rangle - \langle\phi(x_1)\rangle\langle\phi(x_2)\rangle, \tag{10.6}$$

which is telling you thermal information.

[13] This is really a 1d story. One can generalize this to higher dimensions, where there's a generalization of the notion of a projective representation, but even then this misses some SPT phases. Still, it's an interesting story.

Today, we'll study a very simple example from this field-theoretic perspective, which will be surprisingly involved and technical. After that we'll apply this formalism to the AKLT spin chain.

We begin with the path integral for spins. There are various ways to derive the answer, but going into them would take us a little far off course, so we'll just write down the answer for now and see that it works.

The first question is, what do we do with open paths in the path integral? Defining the Berry phase doesn't work terribly well here, and we can't just write down a Lagrangian, because what Lagrangian defines a Berry phase?

Anyways, if we write $\mathbf{S} = s\mathbf{n}$, where s is the spin size and $|\mathbf{n}|^2 = 1$, we'll think of $|\mathbf{n}\rangle$, which is on the Bloch sphere, evolving by a phase, $|\mathbf{n}\rangle \mapsto e^{i\phi(\mathbf{n})}|\mathbf{n}\rangle$. Write $\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. Then the answer for the classical action is

$$S = s\int \mathrm{d}t\,(1-\cos\theta)\frac{\partial\phi}{\partial t}. \tag{10.7}$$

The derivative is a total derivative, so we don't have to worry about how fast a given path goes. A general path can be approximated by a bunch of small rectangles, so let's focus on a rectangular path given by four segments s_1, s_2, s_3, s_4. Then the contribution of, e.g., $s_1 + s_3$ is

$$s_1 + s_3 = s((1-\cos\theta_1)\,\Delta\Phi + (1-\cos\theta_3)(-\Delta\phi)) \tag{10.8}$$

$$= \Delta\left(-\frac{\partial}{\partial\theta}(1-\cos\theta)\,\Delta\theta\,\Delta\phi\right) \tag{10.9}$$

$$= s\sin\theta\,\Delta\theta\,\Delta\phi. \tag{10.10}$$

This works, but is awkward in that we had to choose coordinates for $\mathbf{n}$, and there's no global coordinate system that works. The solution, which manages to write this in a more invariant way, is due to Wess, Zumino, and Witten. We'll have to make a choice of a reference value $\mathbf{n}_0$, but any two choices will give the same answer.

Introduce a fictitious extra coordinate $u \in [0,1]$, which we'll think of as interpolating smoothly from some fixed configuration $\mathbf{n}(0,t) \coloneqq \mathbf{n}_0$ to $\mathbf{n}(1,t) \coloneqq \mathbf{n}(t)$, the configuration we're actually in. (So the two coordinates together form a ball instead of a sphere, with $(0,t)$ at the center.) Now the action looks like

$$S_{\mathrm{WZW}} = \frac{s}{2}\int_0^1 \mathrm{d}u \int_{t_i}^{t_f} \mathrm{d}t\,\mathbf{n}\cdot(\partial_\mu\mathbf{n}\times\partial_\nu\mathbf{n})\epsilon^{\mu\nu}, \tag{10.11}$$

where $\epsilon = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0\end{smallmatrix}\right)$.

Remark 10.12. Sometimes we also add a magnetic term $-\int sg\mathbf{B}\cdot\mathbf{n}|_{u=1}\,\mathrm{d}t$ to the action. ◂

Exercise 10.13. This is a bit of gory algebra, but check that if you introduce a specific coordimate system, letting $\theta(u,t) = u\theta(t)$ and keeping $\phi(t)$, then you get the coordinate-dependent action (10.7).

Now let's compute the variation of S_{WZW}.

$$\Delta S_{\mathrm{WZW}} = \frac{s}{2}\int_D \epsilon^{\mu\nu}\Big(\underbrace{3\delta n\cdot\partial_\mu n\times\partial_\nu n}_{(*)} + 2\partial_\mu(\mathbf{n}\cdot\delta\mathbf{n}\times\partial_\nu\mathbf{n})\Big). \tag{10.14}$$

A priori, there are additional terms, but they disappear because of the antisymmetrizer. I also missed another step in the computation; sorry about that.

The term $(*)$ vanishes, because δn cannot be linearly independent from the derivatives of n, and therefore we get only the boundary term. We're trying to collapse the u-direction, so we set $\mu = u$, forcing $\nu = t$. The result is

$$(10.14) = -s\oint \mathrm{d}t\,\delta n\cdot\left(\mathbf{n}\times\frac{\partial\mathbf{n}}{\partial t}\right). \tag{10.15}$$

So the mysterious extra coordinate u drops out as soon as we compute something physically relevant. If we added the magnetic term as in Remark 10.12, we get an extra factor of $\delta n g\mathbf{B}$.

Now let's study this a little more carefully. What if you and I picked different reference configurations $\mathbf{n}_0$ and $\mathbf{n}_0'$? Call the corresponding actions S_{WZW} and S'_{WZW}. Then

$$S_{\mathrm{WZW}} - S'_{\mathrm{WZW}} = \int_H L(\mathbf{n}) + \int_H L(\mathbf{n}'), \tag{10.16}$$

where H is a hemisphere and L is the Lagrangian density. We know the Lagrangians agree at $u = 1$, so we can glue these hemispheres together and conclude

$$= \int_{S^2} L(\mathbf{n}) = \frac{s}{2} \int_{S^2} n \cdot (\partial_\mu n \times \partial_\nu n) \epsilon^{\mu\nu}, \tag{10.17}$$

where n comes from the two choices of n and n' on the two hemispheres.

Now (10.17) isn't obviously zero, so let's look a little closer. The cross product is the oriented area of the parallelogram spanned by $\partial_\mu n$ and $\partial_\nu n$. Now, μ and ν are coordinates on the sphere, so (10.17) computes the surface area of the sphere, times the degree $N \in \mathbb{Z}$ of the map $S^2 \to S^2$ from the sphere with coordinates (u, t) to the Bloch sphere n.[14]

The key point is that the degree is a rigid invariant: if you wiggle the input data to (10.16), you get the same answer: the degree is a topological invariant of maps $S^2 \to S^2$, so it cannot change under small perturbations. Therefore the variation of the difference vanishes, which is good. It might seem weird that the actions differ by some number, but this is actually OK — we care about the partition function (and correlation functions) in order to actually compute physically meaningful information. This means we exponentiate the action: $Z \coloneqq e^{iS_{\mathrm{WZW}}}$. If Z' is the corresponding value for S'_{WZW},[15]

$$\frac{Z}{Z'} = e^{iS_{\mathrm{WZW}} - S_{\mathrm{WZW}'}} = e^{i4\pi s N}, \tag{10.18}$$

and since s is either an integer or a half-integer, this is always equal to 1.

When we care about imaginary time (to study thermal behavior), we replace t with $i\tau$, and replace $e^{iS_{\mathrm{WZW}}}$ with $e^{-S_{\mathrm{therm}}}$.

$$\sim \cdot \sim$$

Now let's study a spin chain. We'll have to tack on one of these WZW actions for every node in the chain. We look at a 1d spin chain with Hamiltonian $H = J \sum_i \mathbf{s}_i \cdot s_{i+1}$. If we perturb this, we get the AKLT phase as before; that's still true for this simpler Hamiltonian, at least for $J > 0$, which we assume. This Hamiltonian prefers states in which neighboring spins point in opposite directions. But this is the local description, and there might be a few blips in this globally.

The goal of quantum field theory is to cook out slowly fluctuating changes. So let's let $\mathbf{m}_j \coloneqq (-1)^j \mathbf{n}_j$: on even sites, it's positive on $\uparrow$ and negative on $\downarrow$, but on odd states the opposite is true. This is a better object than $\mathbf{n}_j$ to feed to field theory, because $\mathbf{n}_j$ changes at most sites, but changing $\mathbf{m}_j$ reflects a change in something physical in the system. So we rewrite the Hamiltonian as

$$H = -J \frac{s^2}{2} \sum_i \left((\mathbf{m}_i - \mathbf{m}_{i+1})^2 - \mathbf{m}_i^2 - \mathbf{m}_{i+1}^2 \right) \approx -J s^2 a \int \mathrm{d}x \left(\frac{\partial \mathbf{m}}{\partial \mathbf{x}} \right)^2, \tag{10.19}$$

as the sum approximates an integral and the difference approximates a derivative. So we have

$$\sum_j S_{\mathrm{WZW}}(\mathbf{n}_j) = \sum_j (-1)^j S_{\mathrm{WZW}}(\mathbf{m}_j) \tag{10.20}$$

$$= \frac{s}{2} \int_D \sum_{j \text{ even}} (m_{j+1} \cdot \partial_\mu m_{j+1} \times \partial_\nu m_{j+1} - m_j \cdot \partial_\mu m_j \times \partial_\nu m_j) \tag{10.21}$$

$$= a \frac{s}{2} \sum_{j \text{ even}} \int \mathrm{d}\tau \left(\frac{\partial \mathbf{m}}{\partial x} \right) \cdot \left(\mathbf{m} \times \frac{\partial \mathbf{m}}{\partial \tau} \right) \tag{10.22}$$

$$= \frac{s}{4} \int \mathrm{d}x \, \mathrm{d}\tau \, \epsilon_{\mu\nu} \mathbf{m} \cdot (\partial_\mu \mathbf{m} \times \partial_\nu \mathbf{m}), \tag{10.23}$$

where $\mu, \nu \in \{x, t\}$. Thus the partition function is

$$Z = \sum_{\mathbf{m}} e^{i \frac{s}{2} \Gamma_{\mathrm{WZW}}[\mathbf{m}]} e^{- \int \mathrm{d}\tau \, \mathrm{d}x \, \frac{1}{2g} (\partial \mathbf{m} / \partial x)^2}. \tag{10.24}$$

[14] In differential topology, one can prove that a smooth map $S^n \to S^n$ is almost d-to-one for some integer d: for a set of full measure in the codomain, the preimage of a point is d points, counted with sign (meaning that oppositely oriented points cancel out, for example). This d is called the *degree* of the map.

[15] Well, really, we should sum over paths, but the point is that once we exponentiate, the difference disappears.

This will have a contribution from the degree again, and will behave differently for integer and half-integer spins. We'll then study how this behaves under symmetries and how to see that this is a topological phase from this perspective.

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