3 Symmetry Protected Topological Phase

3.1 Breakdown of noninteracting SPT phases with interaction

Building on our previous discussion of the Majorana chain and the Haldane chain, we are now going to talk about an interesting model which looks topological as a quadratic fermionic Hamiltonian but once interaction is added, it turns out to be topologically trivial.

Let’s start from the exactly solvable point of a single Majorana chain, with two Majorana modes $\gamma_{2j-1}$ and $\gamma_{2j}$ per each lattice site.

$$ H_M = \sum_j i\gamma_{2j}\gamma_{2j+1} \quad (1) $$

$\gamma_1$ and $\gamma_{2N}$ do not show up in the Hamiltonian and forms a two fold degeneracy, which is stable to any local perturbation.

If we have two Majorana chains in parallel which can couple to each other, the edge degeneracy can break down.

The Hamiltonian in the decoupled limit reads

$$ H_M = \sum_j i\gamma_{2j}^{(1)}\gamma_{2j+1}^{(1)} + \sum_j i\gamma_{2j}^{(2)}\gamma_{2j+1}^{(2)} \quad (2) $$

Giving rise to two Majorana zero modes on each edge: $\gamma_1^{(1)}$, $\gamma_1^{(2)}$; $\gamma_{2N}^{(1)}$, $\gamma_{2N}^{(2)}$. Between the two Majorana zero modes on each side, there can a local interaction term on each side which lifts the degeneracy

$$ i\gamma_{1}^{(1)}\gamma_{1}^{(2)}; i\gamma_{2N}^{(1)}\gamma_{2N}^{(2)} \quad (3) $$

Therefore, with two Majorana chains, the system is not topological any more. In fact, for all odd number of Majorana chains, the system is topological; with even number, trivial.

On the other hand, it is possible that with more symmetry, even two Majorana chains can be nontrivial. This happens when the interaction term is not allowed under the symmetry transformation. For example, let’s consider time reversal symmetry. In a usual spinful electronic system, time reversal acts by reversing the spin of the electron

$$ c^\dagger_{\uparrow} \rightarrow c^\dagger_{\downarrow}, \quad c^\dagger_{\downarrow} \rightarrow -c^\dagger_{\uparrow} \quad (4) $$

This time reversal symmetry action has the interesting property that acting twice on an electron operator gives $-1$. That is, $T^2 = -1$ on each electron. Moreover, time reversal in quantum
mechanical system has the weird property of acting nontrivially on complex numbers. In particular, under time reversal
\[ i \rightarrow -i \] (5)
Time reversal is hence an ‘anti-unitary’ symmetry, and acts on wave functions as
\[ \alpha|0\rangle + \beta|1\rangle = \alpha^*|0\rangle + \beta^*|1\rangle \] (6)
In the spinless Majorana chain example, time reversal has to be defined differently. We can define a fictitious time reversal symmetry action as
\[ i \rightarrow -i, \quad \gamma_{2j-1} \rightarrow \gamma_{2j-1}, \quad \gamma_{2j} \rightarrow -\gamma_{2j} \] (7)
Under this symmetry transformation, the Hamiltonian is symmetric and we can ask if it is topological.

For a single Majorana chain, it is always topological with or without the symmetry, because the Majorana zero mode cannot be removed with any local perturbation. With two parallel Majorana chains, things are different. Without time reversal symmetry, the coupling term
\[ i\gamma_1^{(1)}\gamma_1^{(2)} \] (8)
lifts the degeneracy. With time reversal symmetry, this term is not allowed. Because under time reversal, \( i\gamma_1^{(1)}\gamma_1^{(2)} \rightarrow -i\gamma_1^{(1)}\gamma_1^{(2)} \). Therefore, the two fold degeneracy remains stable with time reversal symmetry and the system is still topological protected by the time reversal symmetry.

So does this protection continue for even larger number of Majorana chains? This is so for odd number of Majorana chains because the dimension of the zero modes at each edge is fractional \((2^n\sqrt{2})\) and there is no way to fully gap it out without coupling the two edges. For even number of Majorana chains, there is a chance that the degeneracy can be lifted, but does not seem to be the case. In particular, any quadratic coupling term that can be written down at each edge
\[ i\gamma_1^{(m)}\gamma_1^{(n)} \] (9)
changes sign under time reversal symmetry. Therefore, if we restrict ourself to only quadratic coupling between the Majoranas, the system remains a stable topological phase for any number of chains. Moreover, for different number of chains, the topological order is different because there is no way to change the number of zero modes with quadratic coupling terms.

On the other hand, if we are allowed to add interacting (quartic or higher) terms to the Hamiltonian, we may be able to lift degeneracies that remain stable under quadratic coupling. We can start to have quartic terms with four chains. At the left end of chain, there are four Majorana zero modes \( \gamma_1^{(1)}, \gamma_1^{(2)}, \gamma_1^{(3)}, \gamma_1^{(4)} \) giving rise to a four fold degeneracy. Using the four Majorana modes, we can write a quartic term
\[ \gamma_1^{(1)\gamma_1^{(2)}\gamma_1^{(3)}\gamma_1^{(4)}} \] (10)
which remains invariant under time reversal symmetry. By adding this term to the Hamiltonian, the four fold degeneracy becomes two fold, but there is no way we can further remove the two fold degeneracy. This two fold degeneracy looks like a spin 1/2 at the edge of the Haldane chain. In particular, the quadratic terms
\[ \gamma_1^{(1)\gamma_1^{(2)}}, \gamma_1^{(2)\gamma_1^{(3)}}, \gamma_1^{(3)\gamma_1^{(4)}} \] (11)
all commute with the quartic term above and anti-commute with each other. Within the low energy subspace of $\gamma_{1}^{(1)} \gamma_{1}^{(2)} \gamma_{1}^{(3)} \gamma_{1}^{(4)}$, they act like the Pauli operators of a spin $1/2$, $\sigma_x$, $\sigma_y$, $\sigma_z$.

What about even higher number of chains? Does the free fermion topological phase ever breakdown due to interaction? We are going to explore this in the homework.

4 Matrix product states

Matrix product state (MPS) is a highly useful tool in the study of interacting quantum systems in one dimension, both analytically and numerically. In this lecture, we are going to present first some simple and important examples of matrix product state. From there we are going to discuss their symmetry properties, their power in representing 1D gapped ground states, and how to do numerical simulation with them.

4.1 Definition and examples

Matrix product states describe many-body entangled states of spins living on a one dimensional chain.

A matrix product state (MPS) of a chain of $N$ spins is described as

$$|\psi\rangle = \sum_{i_1, i_2, \ldots, i_N} \text{Tr}(A_{i_1}^{[1]} A_{i_2}^{[2]} \ldots A_{i_N}^{[N]}) |i_1 i_2 \ldots i_N\rangle$$ (12)

$i_k = 1 \ldots d$, $A_{i_k}^{[k]}$'s are $D \times D$ matrices on site $k$ with $D$ being the dimension of the MPS. $d$ is the dimension of the physical Hilbert space at each site and is called the physical dimension. $D$ is the dimension of the matrices used in the matrix product representation which does not correspond to physical Hilbert spaces. $D$ is called the inner dimension of the MPS. We suppress the normalization of the wave functions here. The representation is efficient as with fixed $D$ for a state of $N$ spins, the number of parameters involved is at most $N D^2$ as compared to $d^N$ in the generic case. If the set of matrices does not depend on site label $k$, then the state represented is translation invariant.

Taking the trace of all matrices $A^{[k]}$ corresponds to periodic boundary condition on the one dimensional chain. If the chain has open boundary condition, it may be more convenient to use a slightly different form of MPS.

$$|\psi\rangle = \sum_{i_1, i_2, \ldots, i_N} \langle l | A_{i_1}^{[1]} A_{i_2}^{[2]} \ldots A_{i_N}^{[N]} | r \rangle |i_1 i_2 \ldots i_N\rangle$$ (13)

where $|l\rangle$ and $|r\rangle$ are two $D$ dimensional vectors giving the left and right boundary conditions in the state.

If $D = 1$, i.e. if $A$ are numbers, then $|\psi\rangle$ is a product state. For example, if $d = 2$ and $A_1^{[i]} = \frac{1}{\sqrt{2}}$ and $A_2^{[i]} = \frac{1}{\sqrt{2}}$, then $|\psi\rangle$ describes a product state of two level spins of the form

$$|\psi\rangle = \left[ \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle) \right] \left[ \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle) \right] \ldots \left[ \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle) \right]$$ (14)
However, if $D \geq 2$, then $|\psi\rangle$ would in general be an entangled state of many spins. As the simplest example, consider matrices

$$A_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \ A_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

(15)

which are independent of site. Then the matrix product state they produce is the many-body entangled GHZ state,

$$|GHZ\rangle = |0\rangle^\otimes N + |1\rangle^\otimes N$$

(16)

One of the most important examples of matrix product states is the AKLT state describing an anti-ferromagnetic ground state of spin 1 chains, which we discussed in the last lecture. For spin 1 chains, $d = 3$ and the three basis states can be chosen as the eigenstate of spin in the $z$ direction with $S_z = -1, 0$ and 1. The matrices defining the (unnormalized) AKLT state $|\psi\rangle_{AKLT}$ are site independent and are given by

$$A_{-1} = - (\sigma_x - i \sigma_y) / \sqrt{2}, \ A_0 = - \sigma_z, \ A_1 = (\sigma_x + i \sigma_y) / \sqrt{2}$$

(17)

We can also choose a different set of basis states for spin 1 as

$$|x\rangle = \frac{1}{\sqrt{2}} \left( -|1\rangle + |1\rangle \right), \ |y\rangle = \frac{-i}{\sqrt{2}} \left( |-1\rangle + |1\rangle \right), \ |z\rangle = -|0\rangle$$

(18)

where $|x\rangle$, $|y\rangle$ and $|z\rangle$ are eigenvalue 0 eigenstates of the spin in the $x$, $y$ and $z$ directions respectively. In this basis, the matrices for the AKLT state take the nice form

$$A_x = \sigma_x, \ A_y = \sigma_y, \ A_z = \sigma_z$$

(19)

Graphically, the set of matrices are represented as shown in Fig.1 (a) where the vertical bond denotes the physical index and the two horizontal bonds denote the inner indices. An MPS is then represented as in Fig.1 (b), with all the inner indices contracted between neighboring sites.

![Figure 1: Graphical representation of (a) the set of matrices (b) a matrix product state.](image)

### 4.2 Symmetry Protected Topological order in MPS

The symmetry protected topological order shows up in the matrix product state representation of the ground state in a particularly simple way. Let’s take the AKLT state as an example.

Recall that the Hamiltonian of the AKLT model reads

$$H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left( \vec{S}_i \cdot \vec{S}_{i+1} \right)^2$$

(20)
The Hamiltonian is invariant under time reversal symmetry which maps
\[ S_x \rightarrow -S_x, \quad S_y \rightarrow -S_y, \quad S_z \rightarrow -S_z \tag{21} \]
The operator that implements this mapping is
\[ T = e^{i\pi S_y K} \tag{22} \]
That is, complex conjugation followed by rotation around the $y$ axis by $\pi$. Note that complex conjugation here is done in the basis of $|1\rangle$, $|0\rangle$, $|-1\rangle$, because we have used the fact that $S_y$ is pure imaginary. If we change the basis to $|x\rangle$, $|y\rangle$, $|z\rangle$, its action becomes
\[ |x\rangle \rightarrow -|x\rangle, \quad |y\rangle \rightarrow -|y\rangle, \quad |z\rangle \rightarrow -|z\rangle \tag{23} \]
which in matrix form reads
\[ T = -IK \tag{24} \]
where now $K$ implements complex conjugation in the $|x\rangle$, $|y\rangle$, $|z\rangle$ basis.

As the ground state (on a closed chain) is gapped and unique, it has to be invariant under the time reversal symmetry action. That is,
\[ |\psi\rangle \rightarrow |\psi\rangle \tag{25} \]
But how does the set of matrices transform in the MPS representation of the wave function? Let’s take the three matrices $A_x = \sigma_x$, $A_y = \sigma_y$, $A_z = \sigma_z$ and see how they transform under the symmetry. Under complex conjugation, the wave function becomes
\[ |\psi\rangle = \sum_{i_1,i_2,\ldots,i_N} \text{Tr}(A_{i_1}A_{i_2}\ldots A_{i_N})|i_1i_2\ldots i_N\rangle \rightarrow |\psi'\rangle = \sum_{i_1,i_2,\ldots,i_N} \text{Tr}((A_{i_1})^*(A_{i_2})^* \ldots (A_{i_N})^*)|i_1i_2\ldots i_N\rangle \tag{26} \]
so that the matrices transform as
\[ A_x = \sigma_x \rightarrow A_x^1 = \sigma_x, \quad A_y = \sigma_y \rightarrow A_y^1 = -\sigma_y, \quad A_z = \sigma_z \rightarrow A_z^1 = \sigma_z \tag{27} \]
Under the $-I$ part of the symmetry transformation, the matrices change as
\[ A_x^1 = \sigma_x \rightarrow \bar{A}_x = -\sigma_x, \quad A_y^1 = -\sigma_y \rightarrow \bar{A}_y = \sigma_y, \quad A_z^1 = \sigma_z \rightarrow \bar{A}_z = -\sigma_z \tag{28} \]
Therefore, under the full time reversal symmetry action, the matrices change as
\[ A_x = \sigma_x \rightarrow \bar{A}_x = -\sigma_x, \quad A_y = \sigma_y \rightarrow \bar{A}_y = \sigma_y, \quad A_z = \sigma_z \rightarrow \bar{A}_z = -\sigma_z \tag{29} \]
The matrices obvious do change under time reversal. How is this consistent with the fact that the wave function does not? This can be understood by noticing that the matrices change by conjugation with $\sigma_y$
\[ \bar{A}_x = \sigma_y A_x \sigma_y^\dagger, \quad \bar{A}_y = \sigma_y A_y \sigma_y^\dagger, \quad \bar{A}_z = \sigma_y A_z \sigma_y^\dagger \tag{30} \]
so that when contracted together, they produce the same coefficients for the wave function
\[ |\bar{\psi}\rangle = \sum_{i_1,i_2,\ldots,i_N} \text{Tr}(\bar{A}_{i_1}\bar{A}_{i_2}\ldots \bar{A}_{i_N})|i_1i_2\ldots i_N\rangle \tag{31} \]
\[ = \sum_{i_1,i_2,\ldots,i_N} \text{Tr}(\sigma_y A_{i_1} \sigma_y \sigma_y A_{i_2} \sigma_y^\dagger \ldots \sigma_y A_{i_N} \sigma_y^\dagger)|i_1i_2\ldots i_N\rangle \tag{32} \]
\[ = \sum_{i_1,i_2,\ldots,i_N} \text{Tr}(A_{i_1}A_{i_2}\ldots A_{i_N})|i_1i_2\ldots i_N\rangle \tag{33} \]
\[ = |\psi\rangle \tag{34} \]
Applying time reversal symmetry twice should be equivalent to doing nothing, which shows up as an interesting effect on the matrices. Applying the symmetry once, we have

\[ A \rightarrow \sigma_y A \sigma_y^\dagger \]  

(35)

When applying the symmetry for the second time, first of all, everything gets complex conjugated

\[ \sigma_y A \sigma_y^\dagger \rightarrow \sigma_y^* A^* \left( \sigma_y^\dagger \right)^* \]  

(36)

Then the \(-I\) part acts as

\[ \sigma_y^* A^* \left( \sigma_y^\dagger \right)^* \rightarrow \sigma_y^* - A^* \left( \sigma_y^\dagger \right)^* = \sigma_y^* \sigma_y A \sigma_y^\dagger \left( \sigma_y^\dagger \right)^* \]  

(37)

The transformation on the left hand side is

\[ \sigma_y^* \sigma_y = -1 \]  

(38)

and similarly on the right hand side is

\[ \sigma_y^\dagger \left( \sigma_y^\dagger \right)^* = -1 \]  

(39)

When combined together, they keep the matrices \( A \) invariant. But on each side, acting time reversal twice gives rise to a \(-1\) phase factor. This is exactly the same as the \( T^2 = -1 \) symmetry action on the edge spin 1/2 of the AKLT chain. In general, if the ground state of a symmetry protected topological phase can be represented as a matrix product state, the projective symmetry action on the physical edge state is going to show up as the transformation on one side of the matrices in the MPS formalism. Based on this, SPT order in 1D can be classified.

### 4.3 Gapped Ground States

MPS is useful analytically because it provides an efficient and sufficient representation of ground states of one dimensional gapped Hamiltonians. We are going to state, but not prove, some of the most important theorems showing the power of MPS in representing gapped ground states.

The power of MPS to represent gapped ground state is related, first of all, to the entanglement area law in MPS.

**In a matrix product state with finite bond dimension, if we take out a continuous segment and calculate its entanglement entropy, the entanglement entropy is going to be upper bounded by a constant (that depends on the finite bond dimension).**

This is left as a homework problem. Because of the entanglement area law, it is expected that MPS provides a good representation for gapped ground states because Hastings proved in ‘An area law for one-dimensional quantum systems’, Journal of Statistical Mechanics: Theory and Experiment, Volume 2007, August 2007:

**Gapped ground states in 1D satisfy an entanglement area law.**

The power of using MPS to simulate gapped ground states has been demonstrated in ‘Entropy Scaling and Simulability by Matrix Product States’ by Schuch et al, where it is stated that
1D states satisfying an entanglement (Renyi entropy) area law can be efficiently represented as matrix product states.

Moreover, not only does this efficient representation exist, it can be found in an efficient way. In particular, a polynomial time algorithm has been proposed based on the MPS formalism to find the ground state of one-dimensional gapped local Hamiltonians (Landau et. al. Nature Physics 11, 566-569 (2015), ‘A polynomial time algorithm for the ground state of one-dimensional gapped local Hamiltonians’.)

On the other hand, it is known that generic MPS are indeed gapped ground states of local Hamiltonians. That is, MPS which satisfy a condition called ‘injectivity’ have short range correlation and is the unique ground state of a gapped Hamiltonian. If we randomly pick an MPS, it is going to satisfy the injectivity condition which is defined as follows (see ‘Matrix Product State Representations’ by Perez-Garcia et al Quantum Information and Computation Volume 7 Issue 5, July 2007 Pages 401-430)

Consider the set of matrices on \( l \) sites \( A_{i_1,...,i_l} = A_{i_1}...A_{i_l} \). The MPS is called injective if there exists a finite \( l_0 \) such that the set of matrices \( A_{i_1,...,i_{l_0}} \) spans the full space of \( D \times D \) matrices.

It was then proven that

An injective matrix product state has a finite correlation length and is the gapped ground state of a local Hamiltonian.

There is an explicit way to construct this so-call ‘parent Hamiltonian’.

### 4.4 Numerical Algorithm

Numerically, even before the notion of matrix product state was proposed, similar ideas has been used for simulation since the early 90s under the name of ‘Density Matrix Renormalization Group’ (DMRG) algorithm. With the development of the MPS theory, new algorithms have been proposed. We are going to briefly describe one of them, the ‘Time Evolving Block Decimation’ (TEBD) algorithm which can be used to find the ground state wave function in MPS form (see Guifre Vidal, ‘Efficient Classical Simulation of Slightly Entangled Quantum Computations’, PRL 91, 147902 (2003)).

Suppose that we want to find the ground state of a local Hamiltonian. WLOG, we consider Hamiltonian with nearest neighbor two-body interactions.

\[
H = \sum_i h_{i,i+1} \tag{40}
\]

The ground state can be obtained by applying the ‘imaginary time evolution’ to a generic starting state \( e^{-\beta H} \). When \( \beta \) is positive and large enough, \( e^{-\beta H} \) becomes a projector onto the ground state with the weight on the excited states being exponentially small. \( e^{-\beta H} \) is a complicated operator. To implement it, we can approximate it with a ‘Trotterized’ form

\[
e^{-\beta H} = \left[ e^{-\Delta \beta \sum_i h_{i,i+1}} \right]^{\beta/\Delta \beta} \approx \left[ \prod_{j=2i-1}^{\beta/\Delta \beta} e^{-\Delta \beta h_{j,j+1}} \prod_{j=2i}^{\beta/\Delta \beta} e^{-\Delta \beta h_{j,j+1}} \right]^{\beta/\Delta \beta} \tag{41}
\]
That is, the evolution can be decomposed into small time steps $\Delta \beta$. Within each time step, the $e^{-\Delta \beta h_{j,j+1}}$ terms approximately commute with each other. We can separate them into two layers, one with even site terms and one with odd site terms, so that the terms within each layer exactly commute with each other and we can write each layer as a product of local exponential terms.

Applying this Trotterized evolution process to a generic state can lead to the ground state of the system. In the MPS formalism, this is realized in the following step. The graphical representation of the steps is given in the figure below.

1. Initialize the state in the MPS formalism. The initial state can be chosen simply as product state but it has to be generic enough to have a nonzero overlap with the ground state. Separate the odd and even lattice sites into $A$, $B$ sub-lattices. We can think of the set of matrices on each lattice site as a rank three tensor which we denote as

$$A^i_{\alpha,\gamma}, \quad B^i_{\alpha,\gamma} \quad (42)$$

2. Combine the matrices on site $2j - 1$ and $2j$, perform one step of imaginary time evolution $e^{-\Delta \beta h_{2j-1,2j}}$ on these two sites.

$$\left(AB\right)^{ik}_{\alpha,\lambda} = \sum_{i'k'} \left[ e^{-\Delta \beta h_{2j-1,2j}} \right]^{ik}_{i'k'} \sum_{\gamma} A^i_{\alpha,\gamma} B^k_{\gamma,\lambda} \quad (43)$$

3. Perform an SVD decomposition between matrices on site $2i - 1$ and site $2i$. That is, decompose $(AB)^{ik}_{\alpha,\lambda}$ as

$$\left(AB\right)^{ik}_{\alpha,\lambda} = \sum_{\gamma} U^i_{\alpha,\gamma} \rho_{\gamma} V^k_{\gamma,\lambda} \quad (44)$$

where $U$ is a unitary matrix from $i, \alpha$ to $\gamma$, $V$ is a unitary matrix from $k, \lambda$ to $\gamma$, $\rho_{\gamma}$ are non-negative numbers. If the number of nonzero $\rho$ exceeds a ‘cut-off’ dimension $N_0$, keep only the largest $N_0$ of them in the decomposition. Update the matrices in $A$, $B$ sub-lattices as

$$\tilde{A}^i_{\alpha,\gamma'} = U^i_{\alpha,\gamma'} \sqrt{\rho_{\gamma'}}, \quad \tilde{B}^k_{\gamma',\lambda} = \sqrt{\rho_{\gamma'}} V^k_{\gamma',\lambda} \quad (45)$$

where $\gamma'$ is the truncated index.

4. Repeat steps 2 and 3 but with lattice sites $2j$ and $2j + 1$ using matrices $\tilde{B}$ and $\tilde{A}$.

5. Repeat steps 2, 3, 4.