Topological Insulators 2 (Topological superconductors)
2020 Spring, Lecture 2
Kitaev chain as a topological insulator (v1)

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SUMMARY

In the first semester, we have demonstrated that the topological SSH chain has zero-energy edge modes, whose localization and zero-energy nature are both robust against adiabatic deformation of the Hamiltonian, including adding disorder, as long as those changes respect chiral symmetry. This observation brings up the possibility that the energy-degenerate quantum states could be used for robust storage of quantum information. Unfortunately, chiral symmetry is usually not guaranteed for real physical systems. Here, we will introduce a model analogous to SSH, the so-called Kitaev chain, where the symmetry guaranteeing robust degeneracies is much more 'physical' than chiral symmetry: it is the particle-hole symmetry that is inherently present in the mean-field description of superconductors. In this lecture, we focus on the bulk properties of this model, calculating the quasiparticle band structure and the topological classification. In subsequent lectures, we will describe their edge states, called Majorana zero modes, and their robustness and use for quantum information.

I. REMINDER: BOGOLIUBOV QUASIPARTICLES

1. Stationary states of a (mean-field) superconductor can be thought of a gas of non-interacting 'quasiparticles' or 'excitations', which are often called 'Bogoliubov quasiparticles' or 'Bogoliubov excitations' or 'bogoliubons'.

2. Eigenvectors ψ of the $2N \times 2N$ BdG matrix (or 'BdG Hamiltonian') $\mathcal{H}$ are called BdG wave functions. Here, N is the number of fermionic modes (single-particle wave functions) in our model. In Lecture 1, we have introduced $\mathcal{H}$ as having a 'electron-hole' (e-h) block structure, the top left $N \times N$ block called the electron block, the bottom right $N \times N$ block called the the hole block. Using the e-h block structure, we have introduced the N-element electron component u^* of the BdG wave function and the N-element hole component v^* of the BdG function via

$$\psi = \begin{pmatrix} u^* \\ v^* \end{pmatrix}. \tag{1}$$

II. THE BULK KITAEV CHAIN CAN BE A 'METAL' OR AN 'INSULATOR'

1. We will soon (re)introduce the bulk Kitaev chain and study its excitation spectrum, to reveal strong analogies between that and the band structure of non-interacting electrons in solids, and to discuss the topological properties of the excitation spectrum. Beforehand, we warm up with a minimal, finite-sized version, the 2-site Kitaev chain. The 2-site Kitaev chain is a model with two sites, each site hosting a single fermionic mode. (I.e., it is a spinless model.) It models, e.g., two quantum dots coupled to a superconductor hosting Cooper pairs. The Hamiltonian of this model reads:

$$H = -\mu c_1^\dagger c_1 - \mu c_2^\dagger c_2 + v(c_1^\dagger c_2 + h.c.) + \Delta(c_1^\dagger c_2^\dagger + h.c.), \tag{2}$$

where μ is the chemical potential of the superconductor, v is the hopping amplitude between the two dots, and Δ is the superconducting order parameter, describing the strength of Cooper-pair breaking and Cooper-pair unification. For simplicity, we consider $\mu, v, \Delta \geq 0$ here, and leave for the reader to generalize to the case of arbitrary real μ and arbitrary complex v and Δ.

For the original paper, see A. Yu. Kitaev, *Unpaired Majorana fermions in quantum wires*, Physics-Uspekhi 44, 131 (2001), or `https://arxiv.org/abs/cond-mat/0010440`.

2. The BdG Hamiltonian of a 2-site Kitaev chain, using the e-h block structure (1e, 2e, 1h, 2h), then reads:

$$\mathcal{H} = \begin{pmatrix} -\mu & v & 0 & \Delta \\ v & -\mu & -\Delta & 0 \\ 0 & -\Delta & \mu & -v \\ \Delta & 0 & -v & \mu \end{pmatrix}. \tag{3}$$

3. Later on, we'll use a different arrangement of $\mathcal{H}$, by re-ordering the rows and columns, e.g., to (1e, 1h, 2e, 2h), and call this the 'spatially ordered block structure. This is motivated by our future goal to describe translationally invariant models, whose BdG Hamiltonian resembles multi-orbital tight-binding models once written in the spatially ordered block structure. For our example in Eq. (3), the spatially ordered version with ordering (1e, 1h, 2e, 2h) reads

$$\mathcal{H} = \begin{pmatrix} -\mu & 0 & v & \Delta \\ 0 & \mu & -\Delta & -v \\ v & -\Delta & -\mu & 0 \\ \Delta & -v & 0 & \mu \end{pmatrix}. \tag{4}$$

4. The BdG Hamiltonian of a 2-site Kitaev chain can also be written using the bra-ket notation followed in the preceding course 'Topological insulators':

$$\mathcal{H} = -\mu \left(|1e\rangle \langle 1e| + |1h\rangle \langle 1h| + |2e\rangle \langle 2e| + |2h\rangle \langle 2h| \right) \tag{5}$$
$$+ v \left(|1e\rangle \langle 2e| - |1h\rangle \langle 2h| + h.c. \right) + \Delta \left(|1e\rangle \langle 2h| - |2e\rangle \langle 1h| + h.c. \right). \tag{6}$$

5. This implies that the BdG Hamiltonian of an infinite Kitaev chain can be written as

$$\begin{aligned} \mathcal{H} = \sum_{m=-\infty}^{\infty} & \left[-\mu \left(|m,e\rangle \langle m,e| + |m,h\rangle \langle m,h| \right) \right. \\ & + v \left(|m,e\rangle \langle m+1,e| - |m,h\rangle \langle m+1,h| + h.c. \right) \\ & \left. + \ \Delta \left(|m,e\rangle \langle m+1,h| - |m+1,e\rangle \langle m,h| + h.c. \right) \right]. \end{aligned} \tag{7}$$

6. Notice that $\mathcal{H}$ in Eq. (7) looks like a Hamiltonian of a homogeneous, non-disordered tight-binding model with a unit cell of two orbitals, labelled by $|e\rangle$ and $|h\rangle$. Using terminology from the previous semester, we say that the dimension of the internal degree of freedom of this tight-binding model is 2.

7. To determine the excitation spectrum, we can use the machinery of the Bloch theorem. With that, we convert the real-space BdG Hamiltonian to the bulk momentum-space Hamiltonian as

$$\mathcal{H}(k) = (-\mu + 2v \cos k)\sigma_z - 2\Delta \sin k \sigma_y \equiv \boldsymbol{d}(k) \cdot \boldsymbol{\sigma}, \tag{8}$$

where

$$\boldsymbol{d}(k) = \begin{pmatrix} 0 \\ -2\Delta \sin k \\ -\mu + 2v \cos k \end{pmatrix}. \tag{9}$$

Hence, the Kitaev chain (and any other homogeneous, non-disordered mean-field superconductor) can be described by an effective band structure. The Bloch energies of the band structure , that is, the eigenvalues of $\mathcal{H}(k)$, provide the excitation energies of the bogoliubons:

$$E_{\pm}(k) = \pm\sqrt{(2v \cos k - \mu)^2 + 4\Delta^2 \sin^2 k}. \tag{10}$$

8. Let's see the spectrum for a few examples in Fig. 1:
   (a) $\mu = 0$, $v = \Delta = 1$: It is an 'insulator', i.e., it has a gap. It has flat bands.
   (b) $\mu = v = 1$, $\Delta = 0$: It is a 'metal', i.e., it has no gap.
   (c) $\mu = \Delta = 1$, $v = 0$: It is an 'insulator'.
   (d) $\mu = v = \Delta = 1$: It is an 'insulator'.

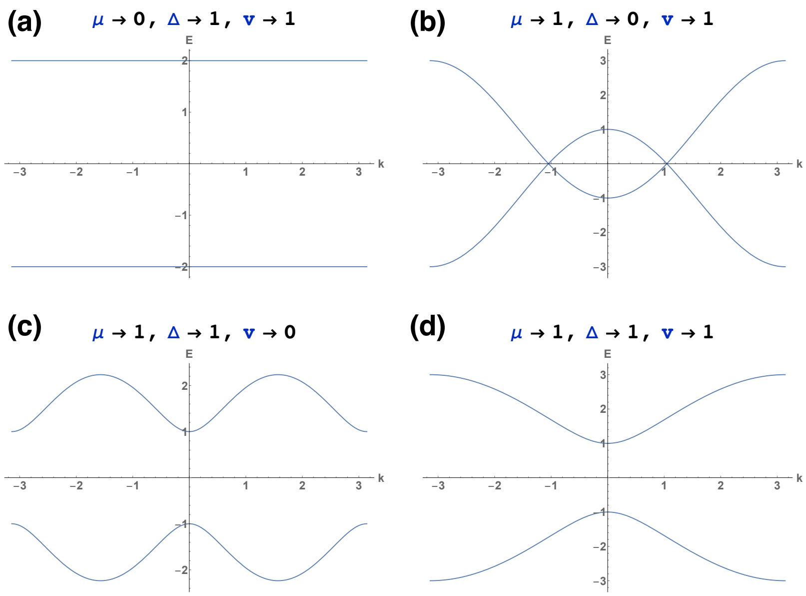

FIG. 1. Dispersion relations of the Kitaev chain for various parameters.

9. Let's see the 3D phase diagram. For simplicity, focus on positive parameter values. Before drawing it, let's use the dispersion relation Eq. (10) to find the metallic points (surfaces), i.e., the points in parameter space where the gap closes.

   (a) If $\Delta = 0$ and $2v \geq \mu$, then the spectrum is metallic. If $\Delta = 0$ and $2v < \mu$, then the spectrum is insulating.

   (b) If $\Delta > 0$, then the gap closes as $k = 0$ $(k = \pi)$ if $2v = \mu$ $(2v = -\mu)$. Since we work with $v, \mu \geq 0$ for now, we can disregard the options in the brackets.

Based on these observations, the 3D phase diagram is shown in Fig. 2. There are two metallic surfaces, one in the v-μ plane, and one separating the volumes labelled insulator$_0$ and insulator$_1$.

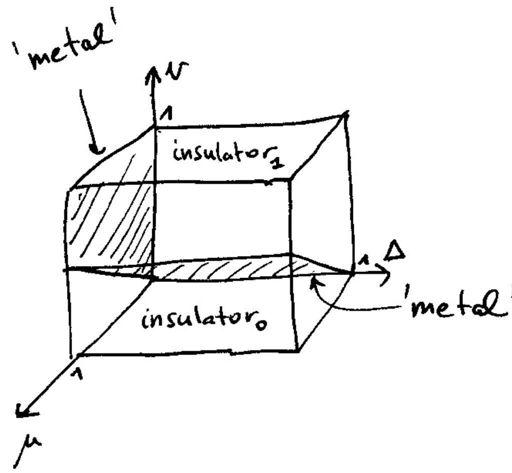

FIG. 2. Phase diagram of the Kitaev model (with positive parameters).

III. PARTICLE-HOLE SYMMETRY AND THE BULK TOPOLOGY OF THE KITAEV CHAIN

1. Notice that the spectrum is up-down symmetric in all cases: for a state with momentum k and energy E, there is a partner state with the same momentum and opposite energy $-E$. (This is the consequence of the fact that the unitary operator $\Sigma_x = \sigma_x \otimes 1_{N\times N}$ is a chiral symmetry of the model.) The spectrum is also left-right symmetric in all cases: for a state with momentum k and energy E, there is a partner state with the same energy E and opposite momentum $-k$. (This is a consequence of the fact that the antiunitary operator K of complex conjugation is a time-reversal symmetry of the model.) As a consequence of the above two observations, it is also true that for any state with momentum k and energy E, there is a partner state with opposite energy $-E$ and opposite momentum $-k$ (*diagonal* symmetry).

2. We claim that the diagonal symmetry of the quasiparticle band structure is a consequence of the particle-hole symmetry built in the BdG formalism. This also implies that for generalizations of our Kitaev chain model, where the chiral symmetry and the time-reversal symmetry are broken, and therefore the up-down and left-right symmetries of the quasiparticle band structure are broken, even then the diagonal symmetry would remain there.

3. Recall that for a BdG Hamiltonian, the antiunitary transformation $\Sigma_x K$ is always a particle-hole symmetry, that is,

$$\Sigma_x K \mathcal{H} \Sigma_x K = -\mathcal{H}. \tag{11}$$

   Note also that $(\Sigma_x K)^2 = +1$.

4. To prove the claim in item 2 above, we first prove a lemma, which tells the consequence of particle-hole symmetry on the bulk momentum-space Hamiltonian:

$$\mathcal{H}(k) = -\sigma_x \mathcal{H}^*(-k)\sigma_x. \tag{12}$$

   This is proven as

$$\left[\mathcal{H}(k)\right]_{pp'} = \langle k,p|\mathcal{H}|k,p'\rangle = \langle k,p| - \Sigma_x \mathcal{H}^* \Sigma_x |k,p'\rangle = -\langle -k,p|\Sigma_x \mathcal{H} \Sigma_x| -k,p'\rangle^* = \left[\sigma_x \mathcal{H}^*(-k)\sigma_x\right]_{pp'}. \tag{13}$$

   Here, $p,p' \in \{e,h\}$, the plane wave $|k\rangle = \frac{1}{\sqrt{N}}\sum_{m=1}^{N} e^{ikm}|m\rangle$ is defined in the usual way, and the second equality uses Eq. (11).

5. We now rephrasing the claim in item 2. For a Bloch bogoliubon ψ at momentum k and energy E, there is a particle-hole partner $\psi' = \sigma_x K\psi$ with opposite momentum $-k$ and opposite energy $-E$. To prove this, we take $\mathcal{H}\psi = E\psi$ as the starting point, and act with $\sigma_x K$ on this from the left. Thereby we obtain

$$\sigma_x K\mathcal{H}(k)\psi = E\sigma_x K\psi. \tag{14}$$

Now we insert unity in the form of $\sigma_x K\sigma_x K$ after $\mathcal{H}$:

$$\sigma_x K\mathcal{H}(k)\sigma_x K\sigma_x K\psi = E\sigma_x K\psi. \tag{15}$$

We use $\psi' = \sigma_x K\psi$:

$$\sigma_x K\mathcal{H}(k)\sigma_x K\psi' = E\psi' \tag{16}$$
$$\sigma_x \mathcal{H}^*(k)\sigma_x\psi' = E\psi'. \tag{17}$$

Finally, we use our lemma (12):

$$-\mathcal{H}(-k)\psi' = E\psi', \tag{18}$$
$$\mathcal{H}(-k)\psi' = -E\psi'. \tag{19}$$

which concludes the proof.

6. Remark: In the above consideration, if $E > 0$, then the particle-hole partners ψ and ψ are orthogonal, $\langle\psi|\psi'\rangle = 0$, since they are eigenvectors belonging to two different eigenvalues. On the other hand, if $E = 0$, then ψ' might have an overlap with ψ, or they might even be identical. Usually, ψ is called a *Majorana zero mode*, if $\sigma_x K\psi = \psi$.

7. Being familiar with topological insulators, it is natural to ask: are the two insulating phases of the positive-parameter Kitaev chain ($2v < \mu$ and $2v > \mu$) topologically different? A naive answer is based on the observation that σ_x is a chiral symmetry of $\mathcal{H}(k)$, or, in other words, the $\boldsymbol{d}$-vector is lying in a plane (the yz plane). As known from Chapter 1 of the book, this implies that the $\boldsymbol{d}$ map is characterized by an integer winding number, which tells how many times does the endpoint of vector $\boldsymbol{d}$ wind around the origin of the yz plane as k runs around the Brillouin zone from $-\pi$ to π.

8. The above argument can be used to classify the two insulating phases $2v < \mu$ and $2v > \mu$. Look at one representative for each case:

$$\text{trivial dimerized limit} : \mu = 1, v = \Delta = 0, \tag{20}$$
$$\text{topological dimerized limit} : \mu = 0, v = \Delta = 1. \tag{21}$$

We show the curve drawn by the function $\boldsymbol{d}$ for each case in Fig. 3, and observe that the winding number is 0 for the trivial case, and 1 for the topological case. Now it might be clear why these special cases are called trivial and topological. Why they're called 'dimerized' might become clearer in a short while.

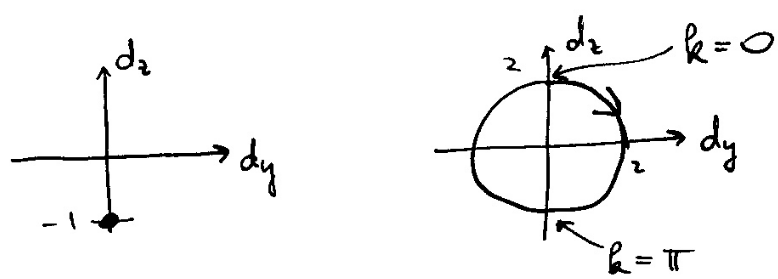

FIG. 3. Trajectories of the $\boldsymbol{d}$-vector endpoint for the trivial (left) and the topological (right) dimerized limit of the Kitaev chain.

9. One might imagine a generalization of this Kitaev chain model, still in the mean-field approximation (quadratic Hamiltonian), still with 2 bands, but such that chiral symmetry and time-reversal symmetry are broken. For example, a particular such generalization yields the following function $\boldsymbol{d}$:

$$\boldsymbol{d}(k) = \begin{pmatrix} 2\Delta' \sin(2k) \\ -2\Delta \sin(k) \\ -\mu + 2v \cos(k) \end{pmatrix}. \tag{22}$$

In such a case, the above argument leading to a $\mathbb{Z}$ invariant does not work. Is there still a nontrivial topological classification? Yes, there is one, where topological invariant is not a $\mathbb{Z}$ invariant, but a $\mathbb{Z}_2$ invariant, taking a value of 0 or 1. This is a consequence of particle-hole symmetry, as shown here.

First, particle-hole symmetry implies that the x and y components of the vector $\hat{\boldsymbol{d}} = \boldsymbol{d}/|\boldsymbol{d}|$ are odd functions of k, whereas the z component is an even function of k:

$$\hat{d}_x(k) = -\hat{d}_x(-k), \tag{23}$$
$$\hat{d}_y(k) = -\hat{d}_y(-k), \tag{24}$$
$$\hat{d}_z(k) = -\hat{d}_z(-k). \tag{25}$$

These follow directly from $\mathcal{H} = \boldsymbol{d}(k) \cdot \boldsymbol{\sigma}$ and Eq. (12). (I.e., we do not need to specify the form of $\boldsymbol{d}(k)$ explicitly to show this.) (These relations are also fulfilled for the components of $\boldsymbol{d}$.)

The above even-odd relations imply that at $k = 0$ and $k = \pi$, the vector $\boldsymbol{d}$ is parallel to the z axis. This leaves two different topologies for the image of the function $\boldsymbol{d}$ map: either $\boldsymbol{d}(0) = \boldsymbol{d}(\pi)$, and then the image consists of two loops, both glued to one of the poles, or $\boldsymbol{d}(0) = \boldsymbol{d}(\pi)$, and then the image consists of two paths, both connecting the north pole and the south pole. Two simple examples are the trivial and topological dimerized limits introduced above. The model in Eq. (22) can also be used to illustrate these $\boldsymbol{d}$-vector trajectories, see Fig. 4.

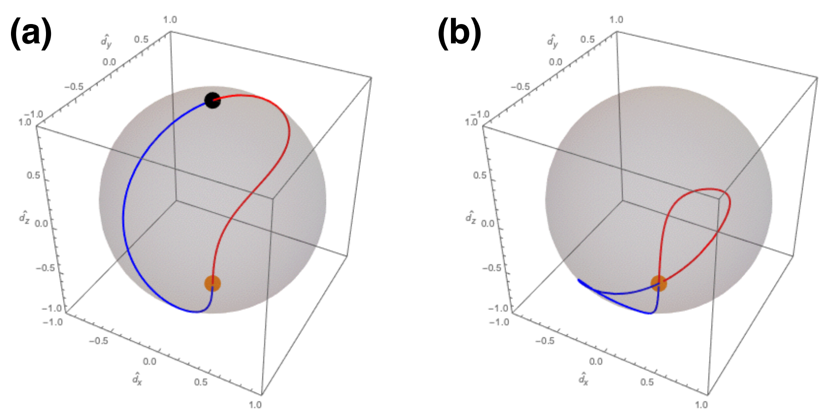

FIG. 4. Trajectories of the $\boldsymbol{d}$-vector endpoint for the trivial (left) and the topological (right) dimerized limit of the extended Kitaev chain model, Eq. (22). Blue/red curves show the trajectory for $k \in [-\pi, 0]$ / $k \in [0, \pi]$, and black/orange points correspond to $k = 0$ / $k = \pi$. (In (b), the black and orange points coincide.) Parameters: (a) $v = \Delta = \mu = 1$, $\Delta' = 1/2$ (trivial insulator), (b) $v = 1/4$, $\Delta = \mu = 1$, $\Delta' = 1/2$ (topological insulator).

EXAM QUESTIONS, EXERCISES

1. Write down the Hamiltonian of the N-site Kitaev chain with (a) open and (b) periodic boundary conditions.

2. Write out the Fock-space Hamiltonian of a 4-site Kitaev chain. Specify that in the trivial and topological fully dimerized limits. Repeat all these with the BdG matrix.

3. What is the dimension of the Fock space of a 5-site Kitaev chain? What is the dimension of the BdG Hamiltonian?

4. Draw the 3D phase diagram of the infinite Kitaev chain for positive-valued model parameters.
5. Draw the 3D phase diagram of the infinite Kitaev chain for real-valued model parameters.
6. Write out the real-space BdG Hamiltonian and the Fock-space Hamiltonian of the extended Kitaev chain model introduced in Eq. (22).