Platforms for Quantum Technologies
Topological Materials - Exercises

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Exercise 1 - Majorana Zero Modes in the Kitaev Model

In this exercise you will get familiar with the physics of the famous Kitaev Model (A Yu Kitaev 2001 Phys.-Usp. 44 131). It predicts the appearance of Majorana Zero Modes at the ends of a topologically superconducting wire.

We consider the fermionic states on a one-dimensional chain of sites at positions x that are linked via hoppings t. The chemical potential μ and a superconducting pairing Δ and a superconducting phase ϕ are included as well. The resulting tight-binding Hamiltonian reads:

$$H = -\mu \sum_x c_x^\dagger c_x - \frac{1}{2} \sum_x \left(t c_x^\dagger c_{x+1} + \Delta e^{i\phi} c_x c_{x+1} + t c_{x+1}^\dagger c_x + \Delta e^{-i\phi} c_{x+1}^\dagger c_x^\dagger \right),$$

where the operator $c_x^\dagger$ (c_x) creates (annihilates) an electron at site x. It obeys the conventional fermionic relations:

$$\left\{ c_x, c_{x'}^\dagger \right\} = c_x c_{x'}^\dagger + c_{x'}^\dagger c_x = \delta_{x,x'}, \left\{ c_x, c_{x'} \right\} = \left\{ c_x^\dagger, c_{x'}^\dagger \right\} = 0, c_x^2 = (c_x^\dagger)^2 = 0$$

- Familiarize yourself with the terms in this Hamiltonian. Can you attribute a physical meaning to each of them? What degree of freedom is missing?

Before we study the properties of a finite chain, we first want to take a look at the bulk properties of such wires. For this purpose, it is convenient to consider a wire consisting of N sites, joined at the ends by periodic boundary conditions. Additionally we want to look at the Hamiltonian in momentum-space.

- Fourier transform the Hamiltonian given above. Use:

  $$c_x = \frac{1}{\sqrt{N}} \sum_{k \in BZ} e^{ikx} c_k$$

  Remember that:

  $$\sum_x e^{i(k-k')x} = N \delta_{k,k'}$$

  You should end up at:

  $$H = -\mu \sum_{k \in BZ} c_k^\dagger c_k - \frac{1}{2} \sum_{k \in BZ} \left(t \cos(k) (c_k^\dagger c_k - c_{-k} c_{-k}^\dagger) - i\Delta \sin(k) (e^{-i\phi} c_k^\dagger c_{-k}^\dagger - e^{i\phi} c_{-k} c_k) \right)$$

  If you end up with terms of type e^{ik}, the $\sin(k)$ and $\cos(k)$ terms can be obtained from linear combinations.

- Show that this can be rewritten to:

  $$H = \frac{1}{2} \sum_{k \in BZ} \left(c_k^\dagger, c_{-k} \right) \begin{pmatrix} \epsilon_k & \Delta_k^* \\ \Delta_k & -\epsilon_k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix},$$

  where $\epsilon_k = -t\cos(k) - \mu, \Delta_k = -i\Delta e^{i\phi} \sin(k)$.

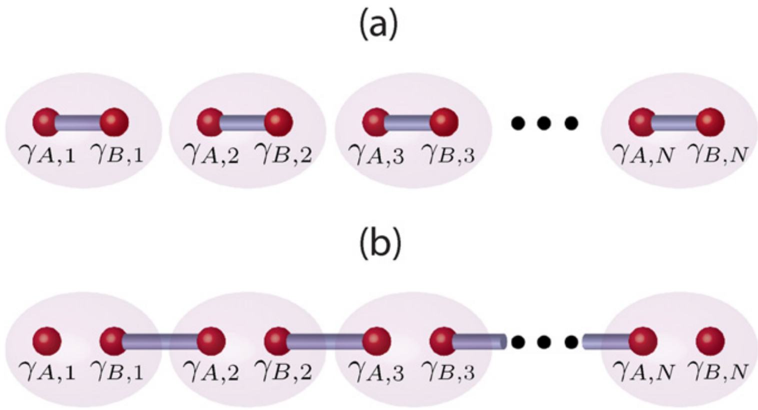

Figure 1: Visualization of the breaking of the original Kitaev chain. The fermionic operators at each site get split into two Majorana operators. The (a) and (b) part of the figure correspond to different parameter regimes as discussed in the exercises. Figure taken from Alicea, Rep. Prog. Phys. 75 (2012) 076501

- This Hamiltonian is now in the Bogoliubov-de Gennes shape. Calculate the eigenenergies of the corresponding quasiparticles. For which combinations of μ and t are there zero energy solutions?

Now we want to turn to the case of a chain of finite length. Consider again the Hamiltonian in real-space as given above. It can be rewritten by defining so called Majorana operators γ. They can be understood as the real and imaginery part of the ordinary fermion operator, i.e. $\gamma_{B,x} = e^{i\phi/2}c_x + e^{-i\phi/2}c_x^\dagger, \gamma_{A,x} = -i(e^{i\phi/2}c_x - e^{-i\phi/2}c_x^\dagger)$. Every site x has now two subsites A, B.

- Find the expressions for c_x and $c_x^\dagger$ in terms of $\gamma_{B,x}$ and $\gamma_{A,x}$. Show that it holds:

$$\gamma_{\alpha,x} = \gamma_{\alpha,x}^\dagger, \left\{\gamma_{\alpha,x}, \gamma_{\alpha',x'}\right\} = 2\delta_{\alpha,\alpha'}\delta_{x,x'}, \gamma^2 = 1$$

- Rewrite the Hamiltonian in terms of Majorana operators. Your result should read:

$$H = -\frac{\mu}{2}\sum_{x=1}^{N}\left(1 + i\gamma_{B,x}\gamma_{A,x}\right) - \frac{i}{4}\sum_{x=1}^{N-1}\left((\Delta + t)\gamma_{B,x}\gamma_{A,x+1} + (\Delta - t)\gamma_{A,x}\gamma_{B,x+1}\right)$$

To study the properties of this Hamiltonian, we now consider two limiting cases.

1. $\mu < 0$ and $t = \Delta = 0$
2. $\mu = 0$ and $t = \Delta \neq 0$

- Compare for both cases, which terms remain in the Hamiltonian. Which Majorana operators are coupled and which are potentially left out?

The second case corresponds to the topological regime with unpaired Majorana zero modes at the ends. With the help of numerical simulations, it can be shown, that this remains valid for a broader range of parameters μ, Δ, t as long as the system remains topological. The exact conditions for this will be calculated in exercise two.
Finally, we want to reformulate the Hamiltonian of the second limiting case again with the help of ordinary fermionic operator according to $d_x = \frac{1}{2}(\gamma_{A,x+1} + i\gamma_{B,x})$ and $f = \frac{1}{2}(\gamma_{A,1} + i\gamma_{B,N})$.

- What is the energy cost of adding a d-type fermion, and what is it for adding a f-type fermion? What does this say about the degeneracy of the ground state and its parity?

Exercise 2 - Topological invariant of a 2D chiral p-wave superconductor

The topology of a material can be characterized by an invariant. This number can only change discontinuously as a function of the system parameters and is stable against small perturbations. When the topological invariant of a system is equal to that of the vacuum, we call it trivial and topological otherwise.

In this exercise we want to study a continuous two-dimensional chiral p-wave superconductor. Its Hamiltonian in real-space is given by:

$$H = \int d\vec{r} \left\{ \psi(\vec{r})^\dagger \left(-\frac{\nabla^2}{2m} - \mu \right) \psi(\vec{r}) + \frac{\Delta}{2} \left[e^{i\phi}\psi(\vec{r}) \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y} \right) \psi(\vec{r}) + e^{-i\phi}\psi(\vec{r})^\dagger \left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \right) \psi(\vec{r})^\dagger \right] \right\},$$

where the operator $\psi(\vec{r})^\dagger$ creates an electron at position $\vec{r}$. At first, some mathematical preparations are necessary.

- Transform this Hamiltonian to momentum-space, similar to the previous exercise.
- Show that the resulting Hamiltonian can be transformed into BdG shape,

$$H = \frac{1}{2} \int \frac{d^2\vec{k}}{(2\pi)^2} \Psi^\dagger(\vec{k}) \mathcal{H} \Psi(\vec{k}), \tag{1}$$

  where $\Psi^\dagger(\vec{k}) = \left(\psi^\dagger(\vec{k}), \psi(-\vec{k}) \right)$.
  Your result should read:

$$\mathcal{H} = \begin{pmatrix} \epsilon_k & \Delta_k^* \\ \Delta_k & -\epsilon_k \end{pmatrix}, \tag{2}$$

  where $\epsilon_k = k^2/2m - \mu$ and $\Delta_k = i\Delta e^{i\phi}(k_x + ik_y)$.
- Show that $\mathcal{H}$ can be written with the help of the Pauli matrices:

$$\mathcal{H} = \vec{h} \cdot \vec{\sigma} = h_x\sigma_x + h_y\sigma_y + h_z\sigma_z, \tag{3}$$

  where

$$\vec{h} = \left(\mathrm{Re}(\Delta_k), \mathrm{Im}(\Delta_k), \epsilon_k \right) \tag{4}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{5}$$

The topological invariant is now defined in terms of this vector $\vec{h}$. It is defined as the number of times the normalized vector $\hat{h} = \vec{h}/|\vec{h}|$ covers the whole unit sphere as $\vec{k}$ is varied.

- For given values of μ and k^2, what does a variation of the relative weights of h_x and h_y correspond to?
- For a given value of μ, what does $\hat{h}$ look like for $k = 0$? How does it evolve for increasing k?
- What is the condition, that determines, whether the whole solid angle is covered by $\hat{h}$ upon variation of $\vec{k}$? Can you deduce from limiting cases, what situation is trivial or topological, respectively?

Now we can also step back and examine the Hamiltonian of the first exercise for its topology. The discussion is very similar, but since the system is discrete, k can only take values from the first Brillouin zone.

- Apply an analogous analysis to the BdG-Hamiltonian of exercise one. What is the condition for non-trivial topology in terms of μ and t?