Topological Superconductor

Yu-Cheng Shaw*
National Taiwan University, Taipei 10617, Taiwan

Topological superconductor is a state of matter such that the bulk state has a superconducting gap while the edge hosts gapless Majorana fermions [1]. In this essay, I aim to explain how do we define topological number for superconducting Hamiltonian, how does the superconducting bulk state and Majorana edge state appear, its application in quantum computing, the experimental signature and finally some approaches scientists have tried to achieve such a state.

A. Topological number in superconducting Hamiltonian

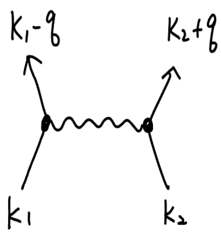
1. *Superconducting Hamiltonian*

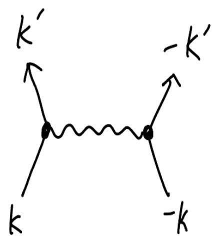
In order to understand how it is possible to define topological number for superconducting Hamiltonian, we need to first exploit the particle-hole symmetry it pocesses. A general spinless Hamiltonian consists of two electron channel effective potential due to electron-phonon coupling is

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{k_1 k_2 q} V(k_1, k_2, q) c_{k_1}^\dagger c_{k_1 - q} c_{k_2}^\dagger c_{k_2 + q} \tag{1}$$

If we look at pairing whose center of mass momentum is zero we'll get

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{k_1 k_2} V(k_1, k_2) c_{k_1}^\dagger c_{k_2} c_{-k_1}^\dagger c_{-k_2} \tag{2}$$





And if we consider pairing between electron $|k,\downarrow>$ and $|-k,\uparrow>$ with spin structure, we get the conventional BCS Hamiltonian

$$H = \sum_k \epsilon_k (c_{k,\uparrow}^\dagger c_{k,\uparrow} + c_{k,\downarrow}^\dagger c_{k,\downarrow}) + \sum_{k_1 k_2} V(k_1, k_2) c_{k_1,\uparrow}^\dagger c_{k_2,\uparrow} c_{-k_1,\downarrow}^\dagger c_{-k_2,\downarrow} \tag{3}$$

Note we can exchange (with a minus sign) the $c_{k_2,\uparrow} c_{-k_1,\downarrow}^\dagger$ in the second term and do the mean field approximation for previously mentioned $|k,\downarrow>$ and $|-k,\uparrow>$ pair. This will give us the Hamiltonian mentioned in class.

2. *Particle-hole symmetry*

For simplicity sake let us drop the spin degree of freedom and focus on the particle-hole symmetry. The Hamiltonian now takes the form

$$H = \frac{1}{2} \sum_k (c_k^\dagger, c_{-k}) \begin{pmatrix} \varepsilon(k) & d(k) \\ d^*(k) & -\varepsilon(-k) \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \tag{4}$$

* pbture102@gmail.com

we call the middle 2×2 matrix H'. With fermions being anti-commute and change of dummy index, we can prove that $d(k)$ is an odd function. We now check if the Hamiltonian obey the belowed transformation property of particle-hole symmetry [2]

$$CH'_{2\times 2}(k)C^{-1} = -H'_{2\times 2}(-k) \tag{5}$$

with

$$C = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} K \tag{6}$$

and K being the complex conjugate operator. This identity check if the Hamiltonian has symmetry when you exchange all the particles with holes (or equivalently, creation operators with annihilation operators with opposite momentum). After some algebra we confirmed the above Hamiltonian indeed pocesses particle-hole symmetry. We can also look at particle-hole symmetry in another way: in order to have the symmetry, the $d(k)$ in H' must be an odd function. While this may also be derived from the fermion statistic for conventional s-wave pairing, it is not guarenteed in all other spin structures (ex. p-wave pairing since electrons of the same spin can now couple to each other [6]).

3. Hilbert space topology and Z_2 topological number

Now we know the particle-hole symmetry gives constraint to the superconducting Hamiltonian by requiring the $d(k)$ being an odd function, we seek its implication in topology. If we assume $\varepsilon(k)$ to be an even function, due to traceless property the above H' can be diagonalized into

$$U^\dagger(k)H'(k)U(k) = \begin{pmatrix} E(k) & 0 \\ 0 & -E(k) \end{pmatrix} \tag{7}$$

with $E(k) = \sqrt{\varepsilon^2(k) + |d(k)|^2}$, the manifold composed of matrix elements of the Hamiltonian (or equivalently, manifold of Hilbert space) is hence only related to the unitary transformation that diagonalize the Hamiltonian. After the gauge degree of freedom has been quotient out, we see the manifold is

$$\mathcal{M} = \frac{U(2)}{U(1) \times U(1)} = \mathcal{S}^2 \tag{8}$$

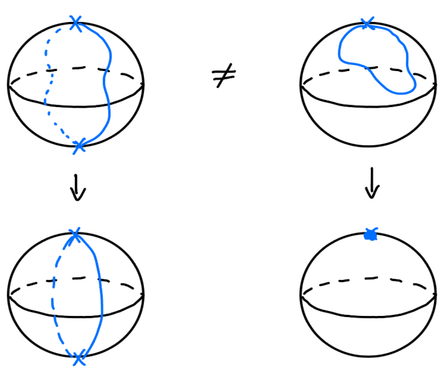
We can also write the Hamiltonian as

$$H'(k) = E(k)\vec{x}(k) \cdot \vec{\sigma} \tag{9}$$

where

$$\vec{x}(k) = (\frac{Re[d(k)]}{E(k)}, \frac{-Im[d(k)]}{E(k)}, \frac{\varepsilon(k)}{E(k)}) \tag{10}$$

with the fact that $x^2 = 1$ we see clairly it's a sphere. Since the 1D Brillouin zone has the topology of a ring, the mapping between k (Brillouin zone) and the Hamiltonian is from a ring to a sphere. Because $d(k) = -d(-k)$, $d(0) = d(\pi) = 0$, this mean the $k = 0$ and $k = \pi$ positions on the ring is mapped to either the northpole or southpole of the sphere. Two possibilities exit: you either have $k = 0$ and $k = \pi$ mapped to the same pole on $\mathcal{S}^2$ or the opposite pole. The two scenarios are topologically different since if $k = 0$ and $k = \pi$ are mapped to opposite pole, one cannot adiabatically shrink the ring into a point, while it could be done in the case where $k = 0$ and $k = \pi$ are mapped to the same pole.



We can hence define the topological number

$$(-1)^{\nu_{1d}} = sgn[\varepsilon(0)\varepsilon(\pi)] \tag{11}$$

the system is topological nontrivial if ν_{1d} is $+1$ and is topological trivial if ν_{1d} is -1.

B. Edge state of topological superconductor

1. *Majorana fermion*

One way to argue the Majorana fermion will appear at the edge of topological superconductor is as follow. 1. Whenever there is a boundary between materials that is topological trivial and nontrivial, a gapless edge state appear so that the real space energy gap could close and the band topology may change. 2. The spectrum of the quasi-particle in superconducting Hamiltonian crosses the Fermi level as long as the tight-binding model is in the topological nontrivial regime in terms of tigh-binding parameters. So it is natural to identify such low energy excitation as the gapless edge state. 3. The fact that the quasi-particle

$$\psi_k = \begin{pmatrix} c_{k,\uparrow} \\ c^\dagger_{-k,\uparrow} \end{pmatrix} \tag{12}$$

obey the Majorana condition [3]

$$\psi^\dagger_{-k} = \Gamma\psi_k, \Gamma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{13}$$

concludes that Majorana fermion will appear at the edge of topological superconductor.
However, we seek more explicit explanation including the real space wavefunction of such edge state, how it will become zero energy mode once the edge is now the border of defect-induced vertices and the analogy between quantum Hall system.

2. *Zero energy edge mode*

We start from BdG equation with a p-wave pairing gap function

$$\begin{pmatrix} \xi(k) & \hat{\Delta}(k_x - ik_y) \\ \hat{\Delta}(k_x + ik_y) & -\xi(-k) \end{pmatrix} \begin{pmatrix} u(k) \\ v(k) \end{pmatrix} = E(k) \begin{pmatrix} u(k) \\ v(k) \end{pmatrix} = i\frac{\partial}{\partial t} \begin{pmatrix} u(k) \\ v(k) \end{pmatrix} \tag{14}$$

It is called p-wave pairing because the gap function is proportional to $|L_z = \pm 1 >$ state (which in $(c_k, c_k^\dagger)^T$ basis is $L_\pm$ or $\hat{k_x} \pm i\hat{k_y}$ and using momentum space representation, it's just $k_x \pm ik_y$.) If we focus on small k excitations, $\xi(k) \approx -\mu$ since the single particle kinetic energy is roughly $k^2/2m^*$ and we'll get these coupled partial differential equations in real space

$$\begin{aligned} i\frac{\partial u}{\partial t} &= -\mu u + \hat{\Delta}^* i(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y})v \\ i\frac{\partial v}{\partial t} &= \mu v + \hat{\Delta} i(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y})u \end{aligned} \tag{15}$$

The more rigorous way to inspect the edge state will be to solve the self-consistent gap equation for the edge Hamiltonian, yet we seek a more convenient appoach by the observation of domain wall [4]. One can view the edge as the place chemical potential changes sign so that particles in the material will not tunnel through its edge much like the particle in a box (specifically, the chemical potential should be negative outside the material). Once we have this notion, let's consider a material with edge along y direction so that $\mu = \mu(x)$ while $\mu(y)$ is constant. In this case, the above set of equations has solution only if $\partial u/\partial y$ and $\partial v/\partial y$ are both zero (the condition is obtained by requiring the determinant of secular equation to be zero). We look into the zero energy state with assumption $\hat{\Delta}$ being real. This then gives a much simplified set of equatinos

$$\begin{aligned} \mu u &= \hat{\Delta} i\frac{\partial}{\partial x}v \\ -\mu v &= \hat{\Delta} i\frac{\partial}{\partial x}u \end{aligned} \tag{16}$$

After putting $u = iv$, the solution is obtained

$$u(x) \propto e^{i\pi/4} exp - \frac{1}{\hat{\Delta}} \int^{x} \mu(x')dx' \tag{17}$$

the phase factor is there to ensure the conjugate relation $u^* = v$ we have in the original set of equation (which is another way to manifest the Majorana condition of these modes) and the $u = iv$ assumption. This is certainly a wave function that localized at the edge.

3. *Helical edge mode*

If we seek solutions for higher energy edge modes, we'll have to break the previous $E = 0$ constraint. We then have to deal with slightly more complicated set of equation

$$\begin{aligned} Eu &= -\mu u + \hat{\Delta} i(\frac{\partial v}{\partial x} - k_y v) \\ Ev &= \mu v + \hat{\Delta} i(\frac{\partial u}{\partial x} + k_y u) \end{aligned} \tag{18}$$

yet by putting $E = -\hat{\Delta} k_y$, we obtain the same solution for the x coordinate part of the wavefunction. As for y coordinate, it is automatically solved by momentum eigenstate with fixed momentum k_y. This mean the solution of such excitations are edge state that has its density concentrate on the edge yet with momentum along y direction. This excitation with a pair of edge state propagating in opposite direction along the edge is called the chiral edge state.

4. *Vortex and Majorana zero mode (MZM)*

Waht happens if the "edge" now is the boundary of topological defect? By topological defect we mean the region in the superconductor where magnetic flux may pierce through (Meissner effect no longer holds). The strategy is to treat the defect region as disk with samll raduis and with minus sign chemical potential. We thus first write Eq(15) in (r, θ) coordinate with the choice $E = 0$

$$\begin{aligned} \mu u &= \hat{\Delta} i e^{i\theta}(\frac{\partial}{\partial r} + \frac{i}{r}\frac{\partial}{\partial \theta})v \\ -\mu v &= \hat{\Delta} i e^{-i\theta}(\frac{\partial}{\partial r} - \frac{i}{r}\frac{\partial}{\partial \theta})u \end{aligned} \tag{19}$$

Different from the case where the edge is along y direction, we notice the Hamiltonian has no parts left out in the zero energy case now. This imply we do not have extra degree of freedom to change our wavefunction and solve the Schrodinger equation when the total energy is not zero [5]. Hence in the topological defect case, we only get one localized bound state with zero energy [4]. Another heuristic way to reason the vortex cannot hold a propagating excited state is as follow [5]. In Eq(19), we can view u and v as coefficients representing states with angular momentum $L_z = 1$ and $L_z = -1$ respectively. Since we have the Majorana condition which state $u = v^*$ due to symmetry in equation of motion, the expectation value of L_z operator evaluated for such superpositioned state

$$u|L_z = 1> + u^*|L_z = -1> \tag{20}$$

will be zero. We can explicitly solve through Eq(19) with the boundary condition $u(r, \theta + 2\pi) = -u(r, \theta)$ (likewise for v) [6] [4] and get

$$u = (i\bar{z})^{-1/2} f(r) \tag{21}$$

where $z = x + iy$. The radial part then becomes

$$\begin{aligned} &df/dr = -\mu f(r)/\hat{\Delta} \\ &f(r) \propto exp(-\int^{r} \mu(r')dr'/\hat{\Delta}) \end{aligned} \tag{22}$$

C. Application in quantum computing

The localized Majorana zero mode has interesting statistical property. Unlike fermions or bosons, when you exchange two MZM twice, their wavefunction will both aquire a minus sign rather than go back to its original form.

1. *Non-Abelian statistic*

We now call the above defined Majorana zero mode in vortex γ_0. Since it is its own anti-particle, we have

$$\gamma_0 = \gamma_0^\dagger \tag{23}$$

So if we want to construct a pair of creation and annihilation operator that obey

$$c \neq c^\dagger, \left\{c, c^\dagger\right\} = 1 \tag{24}$$

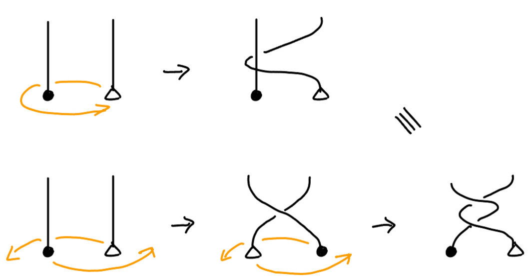
we have to seek combination of MZM at different defects. With the original fermionic statistic the zero mode also pocess, we have $\left\{\gamma_0^{(i)}, \gamma_0^{\dagger(j)}\right\} = 2\delta_{ij}$. This gives us hint to define

$$c_{12}^\dagger = \frac{\gamma_0^{(1)} + i\gamma_0^{(2)}}{2}, c_{12} = \frac{\gamma_0^{(1)} - i\gamma_0^{(2)}}{2} \tag{25}$$

such that

$$\left\{c_{12}, c_{12}^\dagger\right\} = 1 \tag{26}$$

Not only did we find out it's possible to define creation and annihilation operator from two different MZM, we notice one can actually bring creation operator to annihilation operator (and vise versa) via swapping or circling one MZM around another. It can be seen by the Aharonov-Bohm(A-B) phase that will appear if one state travel around a region with magnetic flux piercing through. Since both electron and hole gain an A-B phase of $e^{ie\phi_0} = e^{-ie\phi_0} = -1$ (ϕ_0 is unit magnetic flux π/e), after one moves a MZM around another, it gains a minus sign phase $\gamma_0 \to -\gamma_0$. It is important to point out that not only does the circling MZM change sign, the one being circled also changes sign. Since in the rest frame of the moving MZM, it is the other MZM that travel and gain an A-B phase. One can better understand this as a character of braiding: circling one around the other is equivalent to swapping the two in the same way twice.



The braiding character is originated from the Dirac string in the sense of A-B effect.

2. *Logic gate for qubit*

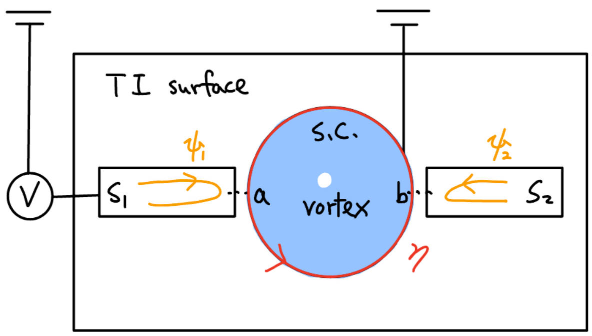
So if we wish to only change sign of $\gamma_0^{(2)}$ in c_{12} we can introduce a $\gamma_0^{(3)}$. In this case, if we define the initial state as $c_{12}|i>=0$, after we braid $\gamma_0^{(2)}$ with $\gamma_0^{(3)}$ we have $c_{12} \to c_{12}^\dagger$ and $|i> \to |f>$. In total, we have $c_{12}^\dagger|f>=0$ hence the final state is completely different from the initial state (they even are orthogonal). Via the above observation, we know how to change from $|i>$ to $|f>$ and this procedure is the "NOT gate" if we use $|i>$ and $|f>$ as the basis. Further more, if we have more then three MZM we would be able to entangle all of the pairs by simple swapping/ braiding. The best part is that the MZM are protected by topology hence is insensitive to perturbation and noise that may cause the breaking of delicate quantum state.

D. Routes to achieve topological superconductivity

Being such an interesting playground for theory while pocessing such promising application, we have to know how to spot a Majorana zero mode when we saw one. We also would like to know some of the promising system physicists have been trying to manifest the above-mentioned physics.

1. *Zero-bias conductance peak (ZBCP)*

Among experimental signatures for MZM, the zero-bias conductance peak is one of the most discussed both theoretical and experimental-wise. In the experiment, we try to measure the tunneling conductance dI/dV curve under point contact of a material. The shape should be Lorentzian centered at $V = 0$ and the peak value of the spectrum should be $2e^2/h$ for $1D$ topological superconductor [7]. To see how it is the case, we consider the following setup with a superconductor island on the surface of a topological insulator.



The superconductor and the lead has a point contact with a voltage difference of V. There are two electronic states we consider in the picture: the red arrow (η) represents chiral Majorana edge mode while the orange ones (ψ) represent chiral fileds in the lead (which is a combination of incoming and reflecting electron and hole). The coupling strength between η and ψ (ψ_2) is t_1 (t_2). We then write the total Hamiltonian as the sum of η and ψ with interaction only between S_1

$$H = H_{L1} + H_M + H_{t1} \tag{27}$$

where

$$\begin{aligned} H_{L1} &= -iv_f \int_{-\infty}^{\infty} \psi_1^\dagger(x)\partial_x\psi_1(x)dx \\ H_M &= -iv_m \int_{-\infty}^{\infty} \eta(x)\partial_x\eta(x)dx \\ H_{t1} &= -it_1\eta(a)[\psi_1^\dagger(0) + \psi_1(0)] \end{aligned} \tag{28}$$

Here, $\psi_1 = (\xi_\uparrow\psi_\uparrow + \xi_\downarrow\psi_\downarrow), |\xi_\sigma| = 1$ is the chiral field with triplet spin structure that does interact with Majorana mode.
From the Hamiltonian we then obtain the scattering matrix by the means of

$$S = \frac{1}{< 0|U(\infty)|0 >}\mathcal{T}exp(-i\int H_{int}(\tau)d\tau)) \tag{29}$$

using electron and hole as the basis

$$\begin{pmatrix} \psi_{1k}(0_+) \\ \psi_{1-k}^\dagger(0_+) \end{pmatrix} = S \begin{pmatrix} \psi_{1k}(0_-) \\ \psi_{1-k}^\dagger(0_-) \end{pmatrix} \tag{30}$$

one can obtain the tunneling current due to the Majorana mode by

$$I = \frac{2e}{h}\int_0^{eV} |S_{eh}(E)|^2 \, dE \tag{31}$$

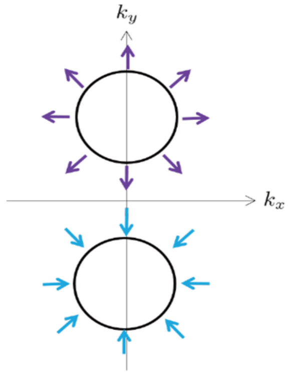
If the phase aquired by Majorana fermion after circling a vortex and its wave vector meet the condition $kL + \pi = 2m\pi, m \in Z$, the se-called "resonance" happens and $|S_{eh}(E)|$ has its largest value. So near the resonance condition, $|S_{eh}(E)|^2$ can be written in resonance Lorentz form as a function of energy, hence the tunneling conductance dI/dV curve. In short, the phase of Majorana fermion effect the scattering process. We tune the electron wave vector of in-coming electron in lead by the voltage difference and we expect to see the dI/dV curve shows zero bias peaks of various values (ex. $2e^2/h$ in $1D$).

To be precise, the ZBCP here is demonstrated via a chiral Majorana mode rather then actual MZM with zero energy. Yet this effect is quite a general phenomenon in this kind of setup [7] [6].

Beside the zero-bias conductance peak, other experimental evidences include ARPES which probe the dispersive relation of Majorana edge state and STM which probe the edge/ surface density.

2. Candidates for realizing Majorana fermion

We are now ready to look into systems that are candidates for manifesting these experimental features predicted by theorists. Here we briefly go through two kinds of system mentioned in [2]. Superconductor with odd parity has spin triplet state and may host p-wave pairing hence is a good candidate. Further, there are some theorem which says that if the fermi surface encloses an odd number of time-reversal-invariant-momenta (TRIM), the odd-parity superconductor will be topological [2]. Based on these theorem, one can use first principle density functional calculation to pin down promising materials. Another possible choice is Weyl semimetal with break of time-reversal symmetry($\mathcal{T}$). Either time-reversal or inversion symmetry($\mathcal{P}$) must be broken in order to form Weyl semimetal, so the $\mathcal{P}$ need not be broken in this case. Additionally, one of $\mathcal{P}$, $\mathcal{T}$ must exist for the Cooper pair to have the same energy so it is necessary for $\mathcal{P}$ to hold here. In such system, the simplest Hailtonian composed of a Weyl node and an anti-Weyl node with opposite Chern number will give a special spin structure on fermi surface. The structure suggests if a pair of electron is to have zero momentum combined (like the case of Cooper pair), their spin must be in the same direction. This is also a character of a p-wave pairing.



The above two creiteria greatly reduce the possible set of materials that may exhibit topological superconductivity, allowing both theorists and experimentalists to dig further into some specific materials and hopefully one day realize the Majorana fermion and its relavent application.

[1] Jian Wang, Superconductivity in topological semimetals, Natl. Sci. Rev. Vol.6, No.2 199 (2019).
[2] M. Sato and Y. Ando, Topological superconductors: a review, Rep. Prog. Phys. **80**, 076501 (2017).
[3] Y. Tanaka, M. Sato and N. Nagaosa, Symmetry and Topology in Superconductors Odd-Frequency Pairing and Edge States, J. Phys. Soc. Jpn. **81**, 011013 (2012).
[4] N. Read and D. Green, Paired states of fermions in two dimensions with breaking of parity and time-reversal symmetries and the fractional quantum Hall effect, Phys. Rev. B. **61**, 10267 (2000).
[5] I think of the explanation myself.
[6] I'm not sure about the reason or the entire picture.
[7] K. Law, P. Lee and T. Ng, Majorana Fermion Induced Resonant Andreev Reflection, Phys. Rev. L. **103**, 237001 (2009).