Majorana Bands in Topological Superconductors

by

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Abstract

Majorana fermions can exist in condensed matter systems as quasi-particle excitations called Majorana bands. The details of Majorana bands will be the central concern of this thesis. In the thesis, Majorana bands are studied analytically and numerically in two square lattice systems with vortices. The p+ip superconductor, containing two vortices in each magnetic unit cell, exhibits slightly dispersing Majorana bands in the middle of the superconducting gap. With the same vortex geometry, the Fu-Kane model shows similar Majorana bands, which, however, can become completely flat when chemical potential is tuned to coincide with the Dirac point. By comparison to a tight binding model of vortex lattice, it is clear that the dispersion is mainly contributed by first and second nearest neighbor hoppings of Majorana fermions bound in vortices. The hoppings, which are extracted from numerical diagonalization, are not quite identical to the existing analytical prediction. Therefore, we built two simple equations that show the phenomenologically correct trends of the hoppings.
Preface

This thesis is a summary of the author’s M.Sc. project, formulated by Prof. Marcel Franz, focusing on the details of Majorana bands with the presence of vortex lattice. The author is in charge of generating all numerical data and figures as well as some of the analytical derivation.

In chapter 2, section 2.1 and section 2.2 are reproductions of the analytical results in the work [1] that Prof. Franz used to participate in. Figure 2.3 and Figure 2.6 are also reproductions, though the parameters may be slightly different. In chapter 3, the analytical derivation in section 3.1 is wholly developed by Prof. Franz. In chapter 4, Figure 4.1 and Figure 4.2 are reproductions of the work by D. J. J. Marchand and M. Franz [2] with same parameter settings. In appendix, Figure A.1 and Figure A.3 are both reproductions of the work [1] with same parameter settings.

All the other analytical and numerical work is original and done by the author under supervision of Prof. Franz. A rough draft containing analytical derivation and numerical results with details based on chapter 3 and chapter 4 has been prepared by the author and is being modified by Prof. Franz for future submission.
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To My Family
Chapter 1

Introduction

Our central concern in this thesis is the Majorana bands existing as quasi-particle excitations in p+ip superconductor and the Fu-Kane model. In the first section of this chapter, we will review some critical literatures on creating Majorana fermions theoretically and experimentally. In the second section, we will state our motivation and summarize our main results.

1.1 Majorana fermion

1.1.1 Background

In 1928, Dirac built his relativistic wave equation [5] for spin-1/2 particles predicting the existence of antimatter, which was confirmed later by the discovery of positrons [6]. In 1937, Ettore Majorana separated Dirac equation into a pair of real wave equations [7] named after him. The Majorana equation is satisfied by fermionic particle named Majorana fermion, which is theoretically defined as its own anti-particle. Thus, Majorana fermions are in a sense "real-valued" particles, while Dirac fermions are "complex-valued" particles. Mathematically, a Majorana fermion is understood as the real (imaginary) half of a Dirac fermion. And in return, a Dirac fermion can always be written as a superposition of two Majorana fermions. When the two Majorana fermions are spatially separated, their state is robust against local perturbations. However, the adiabatic exchange of two Majorana fermions does change the state up to a phase other than 0 or π by their non-Abelian anyonic nature [8], and leads to the idea of topological quantum computation [9,11] resorting to braiding of Majorana fermions. Also, with no intrinsic electric and magnetic moments [12,13], a Majorana fermion has little response to electromagnetic field, making it a potential candidate for dark matter [14,15].
1.1. Majorana fermion

1.1.2 Theoretical proposals

To realize the appealing properties of Majorana fermions, we shall figure out a way to create Majorana fermions first. Majorana fermions are never really observed as elementary particles in high energy physics. In condensed matter, however, many theoretical models have been developed to realize Majorana fermions as quasi-particle excitations, which are naturally expected to appear in superconductors where particle-hole symmetry is automatically satisfied.

For spin triplet superconductor, the pioneering work was done by Kitaev [16] with a toy model for 1D fermionic chain.

\[ H = \sum_{j=1}^{N} \left[ -t(c_{j}^\dagger c_{j+1} + c_{j+1}^\dagger c_{j}) - \mu (c_{j}^\dagger c_{j} - \frac{1}{2}) + (\Delta c_{j+1}^\dagger c_{j}^\dagger + \Delta^* c_{j} c_{j+1}) \right] \]  (1.1)

Kitaev’s model considers nearest neighbor hoppings and p-wave pairing for \(N\) fermionic particles and can be rewritten with \(2N\) Majorana operators \(\{\gamma_1, \ldots, \gamma_{2N}\}\). In a special case when hopping and pairing are identical and chemical potential is zero, there are two operators, \(\gamma_1\) and \(\gamma_{2N}\), not entering into the Hamiltonian. Therefore, Kitaev chain is a realization of spatially separated Majorana fermion pair, which is promising to be used as a qubit. Majorana fermions can also be realized in 2D \(p+ip\) superconductor (and superfluid) with vortices [17–19] or with electric defects [20].

![Figure 1.1: Kitaev’s toy model. Upper panel: trivial phase with \(\Delta = t = 0\) and \(\mu \neq 0\). Majorana fermions are paired to form a regular Dirac fermion chain. Lower panel: topological phase with \(\Delta = t\) and \(\mu = 0\). Majorana fermions are paired in a pattern that two unpaired Majorana fermions are left on the ends of the chain.](image)

For spin singlet superconductor, the breakthrough in searching Majorana fermions was made by Fu and Kane [21]. They patterned an s-wave superconductor to 3D strong topological insulator surface (the Fu-Kane model) such that both spin singlet pairing and strong spin orbital coupling can exist on the interface. The former will be deformed by the latter giving a \(p+ip\)
1.1 Majorana fermion

type low-energy spectrum potentially holding Majorana fermions. Generally, a Zeeman splitting is expected to break time reversal symmetry so that the Kramers’ degeneracy is relieved and the low-energy physics is recovered to be "spinless". The Zeeman splitting can enter the system by doping magnet in the Sc-TI interface [22], by patterning a magnetic insulator [9], or by external field [23]. After Fu and Kane’s groundbreaking development, many similar proposals were reported to realize Majorana fermions with s-wave superconductor [24–29]. It is worth noting that topological insulator is not a must in the Fu-Kane model. What really matters is the strong spin orbital coupling [9, 23, 30].

1.1.3 Experimental realization

As theoretical models come out prosperously, experimentalists have been attempting to confirm the correctness of the theories. The Fu-Kane model argues that we no longer need a p-wave superconductor, which is generally hard to fabricate. And further tests show that topological insulator is not necessary either, provided that there is strong spin orbital coupling. Therefore, it is feasible to assemble topological superconductors manually. Mourik et al. [31] put InSb semiconductor nanowire, which is proved to have strong spin-orbital coupling, in proximity to NbTiN s-wave superconductor, and found zero-bias peaks possibly to be Majorana fermions due to the fact that these zero-bias peaks disappear when any necessary ingredient of Majorana proposal is taken out and is robust when varying chemical potential and applied field in a large range. This is a nice check to models [28, 29] based on semiconductor. However, it is recently pointed out that some other trivial bound states [32] can highly mimic those zero-bias peaks.

Three similar works on semiconductor-superconductor structure were done in the same year with InSb/Nb [33, 34] and InAs/Al [35], respectively. The original Fu-Kane model was also realized later by considering Pb/Bi$_2$Se$_3$/Pb, which showed striking departure from the common Josephson junction behaviors. Such deviation can be easily explained by assuming a 1D Majorana chain along the width of the junction [36].

In late 2014, Nadj-Perge et al. [37] proposed a slightly different scheme by fabricating ferromagnetic iron atomic chains on the surface of superconducting lead. The major difference to semiconductor-superconductor model is that the strong spin orbital coupling is provided by the conventional superconductor instead of semiconductor nanowire. Low temperature scanning tunneling microscopy (STM) observation of the Fe/Pb system showed similar zero-bias peaks and zero-energy end states, which should be a strong
1.2 Motivation

In the preceding section, we have grasped basics on Majorana fermions including its origin, application, and realization. It is worth noting that Majorana fermions in those condensed matter systems are quasi-particles satisfying non-Abelian statistics instead of Fermi-Dirac statistics. Therefore, it is more rigorous to call the corresponding excitations as Majorana bands or Majorana zero modes. Although many proposals have been brought up to realize Majorana bands, the dispersion of these bands has not yet been studied so far. When vortex density is large, the inter-vortex tunnelings are inevitable. Therefore, the Majorana bands have to be dispersing. What the dispersion looks like is the central question worthy of further study since understanding and characterizing the electronic structure will be a prerequisite of manipulating these Majorana modes for topological quantum computation. Our motivation in this thesis will be to systematically study the dispersion of Majorana bands.

With this motivation in mind, we have, both numerically and analytically, studied two specific models – the p+ip superconductor and the Fu-Kane model – in the presence of vortex lattice. By a singular gauge transformation, we avoided the difficulty in figuring out the phase field $\phi(r)$ of superconductor order parameter. We found dispersing Majorana bands for both models, which is contrary to the flat band prediction [38] in which magnetic field is simply neglected. We further found that a tight binding model of vortex lattice is capable to capture the dispersion of Majorana band provided that only first and second nearest neighbor hoppings are considered and matches highly with numerical results. Therefore, the hoppings can be extracted from numerical diagonalization by examining gaps at high symmetry points. These hoppings show oscillating behavior, with respect to chemical potential, whose period is well predicted by Cheng et al. [3, 4] but with different amplitude. Specifically, for the Fu-Kane model, both hoppings are zero when chemical potential $\varepsilon_F$ is tuned to coincide with Dirac point, leaving a completely flat Majorana band. We numerically tested the flat Majorana band under different vortex configuration and showed that such flat band possesses robustness, which is protected by chiral symmetry [39].
Chapter 2

The p+ip superconductor

In this chapter, we will reproduce some key results for the 2D spinless p+ip superconductor. We shall see that such chiral superconductor \[40\] can be described by a simple BCS type lattice Hamiltonian. A unitary transformation can move the phase of superconductor order parameter to the crystalline blocks, whose total phase then can be rewritten as a linear integral of the superfluid velocity along the crystalline lattice. The superfluid velocity is expressed as an infinite integral with integrand’s decay following the \( k^{-1} \) rule. Thus, the integral can be cut off softly and well approximated by a summation, making numerical diagonalization feasible. Most results in the chapter have been developed by Vafek et al. \[1\] and Franz and Tešanović \[41\]. However, it is worth reproducing them for the completeness and coherence of the thesis. The techniques in this chapter will be used again in the following chapters.

2.1 Hamiltonian of p+ip superconductor

The 2D spinless p+ip superconductor can be described by the following BCS type \[42\] lattice Hamiltonian in the basis of \( \Phi_r = (c_r, c^*_r)^T \) with \( r \) being the coordinates of lattice sites of the underlying crystalline lattice.

\[
H = \begin{pmatrix} \hat{h} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{h}^* \end{pmatrix}
\] (2.1)

where the Hamiltonian for the crystalline lattice is

\[
\hat{h} = -\tau \sum_{\delta} e^{-i(e/\hbar)c} f_{\delta r}^* \cdot A(r) \cdot dl \cdot s_{\delta} - \varepsilon_F
\] (2.2)

and superconductor order parameter \[43\] is

\[
\hat{\Delta} = \Delta_0 \sum_{\delta} e^{i\phi(r)/2} \eta_{\delta} e^{i\phi(r)/2}
\] (2.3)
2.1. Hamiltonian of \( p+ip \) superconductor

From now on, we will set the hopping \( \tau \) on crystalline lattice to be unity and measure all energies in this \( p+ip \) superconductor in unit of \( \tau \). Specifically, for \( p+ip \) superconductor, the operator \( \hat{\eta}_\delta \) is defined as

\[
\hat{\eta}_\delta = \begin{cases} 
\mp i \hat{s}_\delta & \text{if } \delta = \pm \hat{x} \\
\pm \hat{s}_\delta & \text{if } \delta = \pm \hat{y} 
\end{cases}
\] (2.4)

where the operator \( \hat{s}_\delta \) works as shift operator \( \hat{s}_\delta u(r) = u(r + \delta) \). Applying a proper magnetic field, a square vortex lattice \( \{ r_i \} \) is formed with two sets of sublattices \( \{ r_i^A \} \) and \( \{ r_i^B \} \). Square vortex lattice [44, 45] has been confirmed in \( \text{Sr}_2\text{RuO}_4 \), which shows \( p \)-wave pairing [46] similar to \( ^3\text{He}-\text{A} \) [47–49]. The superconductor order parameter phase field \( \phi(r) \) is constrained by topology to wind a phase of \( 2\pi \) around each vortex. Explicitly,

\[
\nabla \times \nabla \phi(r) = 2\pi \hat{z} \sum_i \delta(r - r_i) \] (2.5)

The summation is over both types of sublattices. As we have two sets of sublattices \( \{ r_i^A \} \) and \( \{ r_i^B \} \), we can separate the phase into two parts.

\[
\nabla \times \nabla \phi_\mu(r) = 2\pi \hat{z} \sum_i \delta(r - r_i^\mu) \quad \mu = A, B \] (2.6)

where the summation is now over a certain type of sublattice.

Figure 2.1: Two vortex sublattices. Each magnetic unit cell (orange square) encloses two different vortices on the diagonal with vortex spacing to be half of the diagonal length.

With the definition of the two phase fields \( \phi_A(r) \) and \( \phi_B(r) \), we can
2.2. Superfluid velocity

define a unitary matrix
\[ U = \begin{pmatrix} e^{i\phi_A(r)} & 0 \\ 0 & e^{-i\phi_B(r)} \end{pmatrix} \] (2.7)
and a singular gauge transformation \( H \rightarrow U^{-1}HU \) under which the eigenvalues of the Hamiltonian remain same. Such transformation may help remove the phase of \( \Delta(r) \) and brings mathematical simplicity, because of the fact that \( \phi_A(r) + \phi_B(r) = \phi(r) \). After the transformation, the Hamiltonian reads,
\[ U^{-1}HU = \begin{pmatrix} -\sum_{\delta} e^{i\mathcal{V}_\delta(r)} s_\delta - \varepsilon_F & \Delta_0 \sum_{\delta} e^{iA_\delta(r)} \eta_\delta \\ \Delta_0 \sum_{\delta} e^{iA_\delta(r)} \eta_\delta^* & \sum_{\delta} e^{-i\mathcal{V}_\delta(r)} s_\delta + \varepsilon_F \end{pmatrix} \] (2.8)
with the phase factors defined as
\[ \mathcal{V}_\delta(r) = \int_{r}^{r+\delta} \left( \nabla \phi_\mu - \frac{e}{\hbar c} A \right) \cdot dl \quad \mu = A, B \] (2.9)
and
\[ A_\delta(r) = \frac{1}{2} \int_{r}^{r+\delta} (\nabla \phi_A - \nabla \phi_B) \cdot dl = \frac{1}{2} [\mathcal{V}_\delta^A(r) - \mathcal{V}_\delta^B(r)] \] (2.10)

2.2 Superfluid velocity

To calculate the phase factors, we may rewrite the phase factor \( \mathcal{V}_\delta^\mu(r) \) in terms of superfluid velocity \( v_\delta^\mu(r) \).
\[ \mathcal{V}_\delta^\mu(r) = \frac{m}{\hbar} \int_{r}^{r+\delta} v_\delta^\mu(r) \cdot dl \] (2.11)
where
\[ v_\delta^\mu(r) = \frac{\hbar}{m} \left( \nabla \phi_\mu - \frac{e}{\hbar c} A \right) \] (2.12)
Without knowing \( \phi_\mu \) and \( A(r) \), we are not able to tell the value of \( v_\delta^\mu(r) \). Therefore, we will need to develop a more practical form of superfluid velocity. We first take the curl of the superfluid velocity
\[ \nabla \times v_\delta^\mu(r) = \frac{e}{m c} \left[ \hat{z} \phi_0 \sum_i \delta(r - r_i^\mu) - B \right] \] (2.13)
2.2. Superfluid velocity

where the flux quantum \( \phi_0 = \frac{hc}{e} \). We combine two velocities together to suppress index \( \mu \),

\[
2B + \frac{2mc}{e} \nabla \times v_s = \hat{z} \phi_0 \sum_i \delta(r - r_i) \tag{2.14}
\]

The Maxwell equation

\[
-\nabla^2 B = \nabla \times (\nabla \times B) = \nabla \times \left( \frac{4\pi J}{c} \right) = \nabla \times \frac{4\pi n_s e}{c} v_s \tag{2.15}
\]

Plugging this back to the curl of \( v_s \), we get the conventional London equation,

\[
B - \lambda^2 \nabla^2 B = \frac{1}{2} \hat{z} \phi_0 \sum_i \delta(r - r_i) \tag{2.16}
\]

where London penetration depth \( \lambda^2 = \frac{mc^2}{4\pi n_s e^2} \). Perform Fourier transform

\[
B(r) = \int \frac{d^2 k}{(2\pi)^2} e^{ik \cdot r} B_k \tag{2.17}
\]

to the London equation, we would get

\[
B_k + \lambda^2 k^2 B_k = \frac{1}{2} \hat{z} \phi_0 \sum_i e^{-ik \cdot r_i} \tag{2.18}
\]

and equivalently,

\[
B_k = \frac{\frac{1}{2} \hat{z} \phi_0 \sum_i e^{-ik \cdot r_i}}{1 + \lambda^2 k^2} \tag{2.19}
\]

Perform Fourier transform to the curl of \( v_s^\mu \) and plug in \( B_k \)

\[
i k \times v_s^\mu(r) = \frac{2\pi \hbar}{m} i k \times \hat{z} \left[ \hat{z} \sum_i e^{-ik \cdot r_i^\mu} - \frac{1}{2} \hat{z} \frac{\sum_i e^{-ik \cdot r_i^\mu}}{1 + \lambda^2 k^2} \right] \tag{2.20}
\]

We then perform a cross product

\[
i k \times (i k \times v_s^\mu) = \frac{2\pi \hbar}{m} i k \times \hat{z} \left[ \frac{\lambda^2 k^2}{1 + \lambda^2 k^2} \sum_i e^{-ik \cdot r_i^\mu} + \frac{1}{2(1 + \lambda^2 k^2)} \left( \sum_i e^{-ik \cdot r_i^\mu} - \sum_i e^{ik \cdot r_i^\mu} \right) \right] \tag{2.21}
\]
The second term can be safely dropped. We further apply transverse gauge $k \cdot v^\mu_{sk} = 0$, so that

$$v^\mu_{sk} = \frac{2\pi\hbar}{m} \frac{i \mathbf{k} \times \hat{z}}{1 + \lambda^2 k^2} \sum_i e^{-i \mathbf{k} \cdot \mathbf{r}^\mu_i} \tag{2.22}$$

Then the superfluid velocity in real space

$$v^\mu_s(\mathbf{r}) = \frac{2\pi\hbar}{m} \int \frac{d^2k}{(2\pi)^2} \frac{i \mathbf{k} \times \hat{z}}{k^2} \sum_i e^{i \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}^\mu_i)} \tag{2.23}$$

where we assume $\lambda \to \infty$. As $\mathbf{r}^\mu_i$ represents the position of the type $\mu$ vortex of the $i$-th magnetic unit cell, it can be rewrite as $\mathbf{r}^\mu_i = \mathbf{R}_i + \delta^\mu$, with $\mathbf{R}_i$ being the center of the $i$-th magnetic unit cell and $\delta^\mu$ being the position of type $\mu$ vortex with respect to the center. By this separation of index $i$ and index $\mu$, we can first conduct the summation and get

$$v^\mu_s(\mathbf{r}) = \frac{2\pi\hbar}{m} N \sum_G \int \frac{d^2k}{(2\pi)^2} \frac{i \mathbf{k} \times \hat{z}}{k^2} e^{i \mathbf{k} \cdot (\mathbf{r} - \delta^\mu)} \delta_{k,G} \tag{2.24}$$

where $N$ is the number of magnetic unit cells and we use the relation

$$\sum_i e^{-i \mathbf{k} \cdot \mathbf{R}_i} = \sum_G \delta_{k,G} \tag{2.25}$$

with $\mathbf{G}$ being the reciprocal lattice vector of lattice $\{\mathbf{R}_i\}$. For an $L \times L$ magnetic cell, where $\mathbf{G} = \frac{2\pi}{L} (n_x, n_y)$, we have

$$\int \frac{d^2k}{(2\pi)^2} \to \frac{1}{L^2N} \sum_k$$

This will help us further simplify the superfluid velocity to

$$v^\mu_s(\mathbf{r}) = \frac{2\pi\hbar}{m} \frac{1}{L^2} \sum_G \frac{i \mathbf{G} \times \hat{z}}{G^2} e^{i \mathbf{G} \cdot (\mathbf{r} - \delta^\mu)} \tag{2.26}$$

And finally, the phase factor will be

$$\psi^\mu_\delta(\mathbf{r}) = \frac{2\pi}{L^2} \sum_G \int_{\mathbf{r}}^{\mathbf{r} + \delta^\mu} e^{i \mathbf{G} \cdot (\mathbf{r} - \delta^\mu)} \frac{i \mathbf{G} \times \hat{z}}{G^2} \cdot d\mathbf{l} \tag{2.27}$$

Numerically, we cannot sum over all possible reciprocal vector $\mathbf{G}$. The summand decays as $G^{-1}$ so that we may perform a soft cut-off to the summation.
For a lattice problem, by plugging in $e^{\pm ik \cdot r}$, we may write the Bloch Hamiltonian $\mathcal{H}_k = e^{-ik \cdot r}UHU^{-1}e^{ik \cdot r}$.

\[
\mathcal{H}_k = \begin{pmatrix}
-\sum_\delta e^{i V_\delta(r)} e^{ik \cdot \delta \hat{s}_\delta} - \varepsilon_F & \Delta_0 \sum_\delta e^{i A_\delta(r)} e^{ik \cdot \delta \hat{\eta}_\delta} \\
\Delta_0 \sum_\delta e^{i A_\delta(r)} e^{ik \cdot \delta \hat{\eta}_\delta}^* & \sum_\delta e^{-i V_\delta(r)} e^{ik \cdot \delta \hat{s}_\delta} + \varepsilon_F
\end{pmatrix}
\]  

(2.28)

in which we use the fact that $e^{-ik \cdot \delta \hat{S}} e^{ik \cdot \delta \hat{S}} f(r) = e^{ik \cdot \delta \hat{S}} f(r + \delta) = e^{ik \cdot \delta \hat{S}} f(r)$  

(2.29)

Here $\hat{S}$ is a general shift operator that can be chosen among $\hat{s}_\delta$, $\hat{\eta}_\delta$, and $\hat{\eta}_\delta^*$. And $f(r)$ is an arbitrary function defined on the crystalline lattice. We write the Schrödinger equation for such Bloch Hamiltonian $\mathcal{H}_k \Phi_{nk} = \varepsilon_{nk} \Phi_{nk}$ with $\Phi_{nk} = [u_{nk}(r_j), v_{nk}(r_j)]^T$, where $r_j$ is the coordinates of the $j$-th crystalline site. Here we will choose a magnetic unit cell contains 100 sites with $10\delta \times 10\delta$ geometry and periodic boundary conditions in both directions. For $j = 1, 2, \ldots, 100$, when we plug $\Phi_{nk}(r_j)$ in Schrödinger equation, we will have 200 equations, which in return can be written as a $200 \times 200$ matrix of Hamiltonian. Such Hamiltonian is our final version that can be numerically diagonalized directly.

### 2.3 Majorana band and spectrum

Numeric diagonalization of the Bloch Hamiltonian will show us DOS and spectra. It can be seen that in zero magnetic field, which means no vortices will appear, the spectrum is fully gapped. However, a pair of slightly dispersing midgap states appear provided that a square vortex lattice is presented by some nonzero magnetic field. We denote the states as $\psi_{\pm}$ that satisfy Schrödinger equation $H \psi_{\pm} = \pm E \psi_{\pm}$. Due to the particle-hole symmetry, we have $\psi_+ = \sigma_x \psi_-^*$. By linear combination, we can separate two linearly independent states

\[
\psi_1 = \frac{1}{2}(1 - i)\psi_+ + \frac{1}{2}(1 + i)\psi_-
\]

(2.30)

\[
\psi_2 = \frac{1}{2}(1 + i)\psi_+ + \frac{1}{2}(1 - i)\psi_-
\]

(2.31)

with particle-hole symmetry $\psi_{1,2} = \sigma_x \psi_{1,2}^*$. which means the particle in such state is equal to its own antiparticle. Hence, the new states characterize Majorana fermions. Such midgap states hold non-Abelian statistics [50].
2.3. Majorana band and spectrum

Figure 2.2: Magnetic unit cell with $10\delta \times 10\delta$ geometry. The order $j$ of crystalline site is assigned row by row so that $r_j$ is explicitly defined. The vortices are located in the center of corresponding plaquettes on the diagonal of the unit cell. The spectrum does not rely on the specific positions of the vortices as long as they are on the diagonal with spacing to be $(5\delta, 5\delta)$. 

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2.3. Majorana band and spectrum

Figure 2.3: Density of states (DOS) for p+ip superconductor. The magnetic unit cell is chosen to be $10\delta \times 10\delta$, with $\delta$ being the lattice constant of the underlying crystalline lattice. The superconductor order parameter is $\Delta_0 = 0.5034$ and the chemical potential is $\varepsilon_F = -2.2$. The blue line is the DOS of magnetic field $B = 0$ so that no vortices will appear. The sudden drops at 1.8 and 6.2 result from band edges corresponding to the bottom and the top of the band respectively. The Van Hove singularity at 2.2 results from the saddle points of the band. The red line shows the DOS of magnetic field $B \neq 0$ and thus a vortex lattice appears. Landau levels show at the top of the spectrum.

Figure 2.4: Magnetic Brillouin zone for square vortex lattice with the notation of high-symmetry points used in plotting band structure.
2.3. Majorana band and spectrum

Figure 2.5: Band structure of \( p + ip \) superconductor with no vortices. The magnetic unit cell is chosen to be \( 10\delta \times 10\delta \), with \( \delta \) being the lattice constant of the underlying crystalline lattice. The superconductor order parameter is \( \Delta_0 = 0.5034 \) with chemical potential \( \varepsilon_F = -2.2 \).
2.3. Majorana band and spectrum

Figure 2.6: Band structure of p+ip superconductor with square vortex lattice. The magnetic unit cell is chosen to be $10\delta \times 10\delta$, with $\delta$ being the lattice constant of the underlying crystalline lattice. The superconductor order parameter is $\Delta_0 = 0.5034$ with chemical potential $\varepsilon_F = -2.2$. 
2.3. Majorana band and spectrum

Figure 2.7: Low-energy bands of p+ip superconductor in $10\delta \times 10\delta$ magnetic unit cell with $\Delta_0 = 0.5034$ and $\epsilon_F = -2.2$. The red lines show the Majorana bands with slight dispersion.
Chapter 3

Majorana lattice

As Majorana fermions are trapped in the cores of vortices, the vortex lattice will present us a lattice of Majorana fermions. Thus a tight binding model can be used here to find Majorana band analytically. In this chapter, we will first develop the tight binding Hamiltonian by considering first and second nearest neighbor hoppings. The hoppings are the origins of the dispersing Majorana bands and open gaps at high-symmetry points. Therefore, we can extract both hoppings from these points to plot the analytical dispersion, which is actually a good match with the numerical dispersion. We found that the hoppings oscillate with chemical potential, which is consistent with analytical prediction \[3, 4\] by Cheng et al. However, the dispersion developed by Cheng et al. can only capture the period of the oscillation. This may be because Cheng et al. obtained the dispersion from continuous model of p+ip superconductor. It seems that a linearly varying amplitude is good enough to fit our numerical data.

3.1 Tight binding Hamiltonian

We first consider a generic case about vortex lattice with each vortex carrying a flux quantum \(\Phi_0 = \pi \hbar c/e\) and a Majorana fermion in the core. The Hamiltonian, due to its own hermicity, can be written as

\[ H = it \sum_{i,j} s_{ij} \gamma_i \gamma_j \]

with \(s_{ij} = -s_{ji} = \pm 1\). The elements of \(s\) matrix can only be determined up to a sign, because a local \(Z_2\) transformation \(\gamma_i \rightarrow -\gamma_i\) will not affect the Majorana commutation relation. Although \(s_{ij}\) is gauge dependent, the product of \(s_{ij}\) along a closed loop is not. It has been proved \[51\] that for any lattice whose plaquette is a polygon of \(n\) vortices, the flux enclosed in the plaquette is

\[ \sum_{\text{polygon}} \phi_{ij} = \frac{\pi}{2} (n - 2) \]
indicating the product of hopping terms around the plaquette to be $t^n \exp[i(n - 2)\pi/2] = -i^n t^n$. Therefore, the product of the $s_{ij}$ around the plaquette is -1. Specifically, in our vortex lattice (Figure 2.1), a possible gauge is shown in Figure 3.1. The dispersion can then be found analytically by diagonalizing the following tight binding Hamiltonian

$$H = H_{fn} + H_{sn,A} + H_{sn,B}$$

(3.1)

with the first nearest neighbor hopping $H_{fn}$ and second nearest neighbor hopping $H_{sn,A(B)}$ to be

$$H_{fn} = it \sum_R \gamma_{R,A}(\gamma_{R,B} - \gamma_{R-\hat{x},B} + \gamma_{R-\hat{x},B} + \gamma_{R-\hat{y},B})$$

(3.2)

$$H_{sn,A} = it' \sum_R \gamma_{R,A}(-\gamma_{R+\hat{x},A} + \gamma_{R+\hat{y},A})$$

(3.3)

$$H_{sn,B} = it' \sum_R \gamma_{R,B}(\gamma_{R+\hat{x},B} - \gamma_{R+\hat{y},B})$$

(3.4)

with $t$ and $t'$ to be the hoppings. Perform Fourier transform,

Figure 3.1: Gauge of tight binding model of square vortex lattice. Each triangular plaquette has a phase factor of $\pi/2$. 
3.1. Tight binding Hamiltonian

![Figure 3.2: Diamond-shape reduced Brillouin zone (solid lines) in tight binding model with $Q = (\pi/2, -\pi/2)$.](image)

The first nearest neighbor hopping Hamiltonian is

$$H_{fn} = 4t \sum_{k} e^{i(k_x+k_y)/2} \left[ \sin \left( \frac{k_x+k_y}{2} \right) - i \sin \left( \frac{k_x-k_y}{2} \right) \right] \gamma_{k,A}^\dagger \gamma_{k,B}$$ (3.6)

The two second nearest neighbor hoppings are

$$H_{sn,A} = -2t' \sum_{k} (e^{-ik_x} + e^{-ik_y}) \gamma_{k,A}^\dagger \gamma_{k,A}$$ (3.7)

$$H_{sn,B} = 2t' \sum_{k} (e^{-ik_x} + e^{-ik_y}) \gamma_{k,B}^\dagger \gamma_{k,B}$$ (3.8)

By using $Q$, we can rewrite all three Hamiltonians in a diamond-shape reduced Brillouin zone (Figure 3.2) such that there will be a single Dirac cone coinciding with the $\Gamma$ point. Then the nearest neighbor hopping is

$$H_{fn} = - \sum_{k \in RBZ} h_k^* \gamma_{k,A}^\dagger \gamma_{k,B} - \sum_{k \in RBZ} h_k \gamma_{k,B}^\dagger \gamma_{k,A}$$ (3.9)
3.1. Tight binding Hamiltonian

with the parameter

\[ h_k = 4te^{i(k_x+k_y)/2} \left( \sin \frac{k_x+k_y}{2} - i \sin \frac{k_x-k_y}{2} \right) \]  

(3.10)

And the second nearest neighbor hoppings are

\[ H_{sn,A} = 2t' \sum_{k \in RBZ} (e^{-ik_x} + e^{-ik_y}) - \sum_{k \in RBZ} h'_k \gamma^\dagger_k,A \gamma_k,A \]  

(3.11)

\[ H_{sn,B} = -2t' \sum_{k \in RBZ} (e^{-ik_x} + e^{-ik_y}) + \sum_{k \in RBZ} h'_k \gamma^\dagger_k,B \gamma_k,B \]  

(3.12)

with the parameter

\[ h'_k = -4t'(\cos k_x + \cos k_y) \]  

(3.13)

Therefore, we can write the total tight binding Hamiltonian in the space of \( \Gamma_k = (\gamma_k,A, \gamma_k,B)^T \) as

\[ H = H_{fn} + H_{sn,A} + H_{sn,B} = \sum_{k \in RBZ} \Gamma_k^\dagger H_k \Gamma_k \]  

(3.14)

where

\[ H_k = \begin{pmatrix} -h'_k & -h_k^* \\ -h_k & h'_k \end{pmatrix} \]  

(3.15)

Diagonalization gives the analytical solution of dispersion of Majorana band

\[ \epsilon(k) = \pm \sqrt{ |h_k|^2 + |h'_k|^2 } \]  

(3.16)

Therefore, at Dirac point \( \Gamma \) the Hamiltonian opens a gap \( \Delta_\Gamma = 8t' \). At point \( X \), it opens a gap \( \Delta_X = 4\sqrt{2}t \). We can rewrite the dispersion in terms of \( \Delta_\Gamma \) and \( \Delta_X \).

\[ \epsilon(k) = \pm \sqrt{ \frac{\Delta_X^2}{2} \left( \sin^2 \frac{k_x+k_y}{2} + \sin^2 \frac{k_x-k_y}{2} \right) + \frac{\Delta_\Gamma^2}{4} (\cos k_x + \cos k_y)^2 } \]  

(3.17)

As long as we extract the gap parameters \( \Delta_\Gamma \) and \( \Delta_X \) from the numerical diagonalization, we can plot the whole dispersion of Majorana bands. For a \( 10\delta \times 10\delta \) magnetic unit cell with superconductor order parameter \( \Delta_0 = 0.5034 \), the match between the analytical results and numerical results is good (Figure 3.3).
3.2. Hoppings of p+ip superconductor

In the section, we are going to study the hoppings in p+ip superconductor. For simplicity, we will set $\hbar = 1$ and crystalline lattice constant $\delta = 1$. The hoppings in p+ip superconductor will show exponentially decaying behavior in the regime $\Delta_0^2 > 2m\varepsilon_F v_F^2$ and oscillating behavior in the regime $\Delta_0^2 < 2m\varepsilon_F v_F^2$. The chemical potential $\varepsilon_F$ is counted from the bottom of the band and therefore is always positive. We are more interested in the latter regime with large vortex spacing $R \gg \max(k^{-1}, \xi)$, where the superconducting coherence length is $\xi = v_F/\Delta_0$ and the momentum is
3.2. Hoppings of p+ip superconductor

\[ k^2 = 2m\varepsilon_F^2 - \Delta_0^2/v_F^2. \]  

Analytically, the energy splitting is predicted [3, 4] as

\[ E = \sqrt{\frac{2}{\pi} \Delta_0} \left| \cos \left( \frac{k_F R + \frac{\pi}{4}}{\sqrt{k_F R}} \right) \right| \exp \left( - \frac{R}{\xi} \right) \]  \hspace{1cm} (3.18)

if we temporarily ignore the sign. Such energy splitting is obtained by evaluating an overlap integral associated with zero modes at two vortices [3, 4], which are separated by a distance of \( R \). In the language of second quantization, this energy splitting \( E \) is identical to the hopping \( t(t') \) in the tight binding model in the preceding section [3.1] when first(second) nearest neighbor spacing is substituted. By plotting this hopping, we will be able to tell how well such hopping, which is calculated from continuous p+ip model, fits our numerical data. But the first task will be figuring out all corresponding parameters. The dispersion for the underlying crystalline lattice that we are using is

\[ \epsilon = -2(\cos k_x + \cos k_y) \]  \hspace{1cm} (3.19)

with the energy scaled in unit of \( \tau \) and momentum scaled in unit of \( \delta^{-1} \). The first nearest neighbor hopping happens along the diagonal in magnetic unit cell between different sublattices. Therefore, we take

\[ k_x = k_y = \frac{k_F}{\sqrt{2}} \]  \hspace{1cm} (3.20)

when calculating chemical potential \( \epsilon_F \). We may write the dispersion as

\[ \epsilon_F = -2 \left[ 2 - 4 \sin^2 \left( \frac{k_F}{2\sqrt{2}} \right) \right] \]  \hspace{1cm} (3.21)

Equivalently,

\[ k_F = 2\sqrt{2} \arcsin \sqrt{\frac{\epsilon_F + 4}{8}} \]  \hspace{1cm} (3.22)

The Fermi velocity is

\[ v_F = \frac{\partial \epsilon_F}{\partial k_F} = 4\sqrt{2} \sin \frac{k_F}{\sqrt{2}} \cos \frac{k_F}{\sqrt{2}} = \frac{16 - \epsilon_F^2}{2} \]  \hspace{1cm} (3.23)

By plugging in all parameters, we can plot

\[ E(\epsilon_F) = \sqrt{\frac{2}{\pi} \Delta_0} \left| \cos \left( 2\sqrt{2} \arcsin \frac{\epsilon_F + 4}{8} \frac{\sqrt{R} + \frac{\pi}{4}}{\sqrt{16 - \epsilon_F^2}} \right) \right| \exp \left( - \frac{\sqrt{2} R \Delta_0}{\sqrt{16 - \epsilon_F^2}} \right) \]  \hspace{1cm} (3.24)
3.2. Hoppings of p+ip superconductor

with the parameter $\Delta_0 = 0.1$ and $R = 25\sqrt{2}$. It looks that such analytical equation can capture the period of our numerical data when $\varepsilon_F$ is not so small, while at the bottom of the band the fitting is not very good. The second problem is that $E$ cannot fit the amplitude of our numerical data (Figure 3.4, blue line). To improve the fitting at low energy, we can use the real momentum $k$, but in a more practical form,

$$ k = \sqrt{k_F^2 - \frac{\Delta_0^2}{v_F^2}} $$

(3.25)

At low energy, this approximated expression of momentum will fix the fit of period. At high energy, this expression reduces to the Fermi momentum $k_F$, which is proved to fit the period very well. Phenomenologically, by using such momentum, a linearly varying amplitude $A + BkR$ combined with $\cos (kR + \pi/4)$ is good enough to fit our numerical data. The explicit relation is

$$ t(\varepsilon_F) = \left( A + B \sqrt{8R^2 \arcsin^2 \left( \frac{\varepsilon_F + 4}{8} - \frac{2R^2\Delta_0^2}{16 - \varepsilon_F^2} \right) } \right) $$

$$ \times \cos \left( \sqrt{8R^2 \arcsin^2 \left( \frac{\varepsilon_F + 4}{8} - \frac{2R^2\Delta_0^2}{16 - \varepsilon_F^2} + \frac{\pi}{4} \right) } \right) $$

(3.26)

with the parameter $\Delta_0 = 0.1$ and $R = 25\sqrt{2}$. Such function will fit both period and amplitude very well for all chemical potential $\varepsilon_F > -3.95$, where oscillating behavior is expected (Figure 3.4 red line). For the regime $\varepsilon_F < -3.95$, the exponentially decaying behavior is expected other than oscillation.
3.2. Hoppings of p+ip superconductor

Figure 3.4: First nearest neighbor hopping $t$ in p+ip superconductor with $50\delta \times 50\delta$ magnetic unit cell and $\Delta_0 = 0.1$. Black dots show how $t$ varies with chemical potential $\varepsilon_F$ numerically. The red line (Equation 3.26) is the phenomenological fit with the oscillation characterized by $\cos(kR + \pi/4)$ as is suggested by Cheng et al. [3,4]. The linearly varying amplitude is $A + BkR$ with parameters $A = 2.438 \times 10^{-4}$, $B = 3.981 \times 10^{-6}$, and $R = 25\sqrt{2}$. The blue line (Equation 3.24) is analytical result given by Cheng et al. [3, 4].

For second nearest neighbor hopping, the hopping is along either $x$ or $y$, giving a slightly different dispersion

$$\varepsilon_F = -2(1 + \cos k_F) = -4 + 4\sin^2\left(\frac{k_F}{2}\right) \quad (3.27)$$

And the Fermi momentum is changed to

$$k_F = 2\arcsin\sqrt{\frac{\varepsilon_F + 4}{4}} \quad (3.28)$$

The Fermi velocity is then given as

$$v_F = \frac{\partial \varepsilon_F}{\partial k_F} = 2\sin k_F = \sqrt{-\varepsilon_F^2 - 4\varepsilon_F} \quad (3.29)$$
3.2. Hoppings of $p+ip$ superconductor

By plugging in all parameters, we can plot

$$E(\varepsilon_F) = \sqrt{\frac{2}{\pi} \Delta_0} \frac{\cos \left( \frac{2 \arcsin \sqrt{\frac{\varepsilon_F + 4}{4} R'} + \pi}{4} \right)}{\sqrt{2 \arcsin \frac{\varepsilon_F + 4}{4} R'}} \exp \left( - \frac{R' \Delta_0}{\sqrt{-\varepsilon_F^2 - 4 \varepsilon_F}} \right)$$  \hspace{1cm} (3.30)

where superconducting order parameter $\Delta_0 = 0.1$ and the spacing between second nearest neighbors $R' = 50$. Still, this function cannot capture the amplitude (Figure 3.5, blue line). Phenomenologically, by using the real momentum $k$, the second nearest neighbor hopping can be written as a product of a linear function and an oscillating function

$$t'(\varepsilon_F) = \left( A + B \sqrt{4 R'^2 \arcsin^2 \frac{\varepsilon_F + 4}{4} - \frac{R'^2 \Delta_0^2}{-\varepsilon_F^2 - 4 \varepsilon_F}} \right)$$

$$\times \cos \left( \sqrt{4 R'^2 \arcsin^2 \frac{\varepsilon_F + 4}{4} - \frac{R'^2 \Delta_0^2}{-\varepsilon_F^2 - 4 \varepsilon_F}} + \frac{\pi}{4} \right)$$  \hspace{1cm} (3.31)

Such phenomenological fit is good (Figure 3.5, red line) for $\varepsilon_F < -1$. When we keep going up to the corner of the reduced Brillouin zone, the numerical data becomes slightly disordered. And the fit shows a little deviation.
3.2. Hoppings of $p+ip$ superconductor

Figure 3.5: Second nearest neighbor hopping $t'$ in $p+ip$ superconductor with $50\delta \times 50\delta$ magnetic unit cell and $\Delta_0 = 0.1$. Black dots show how $t'$ varies with chemical potential $\varepsilon_F$ numerically. The red line (Equation 3.31) is the phenomenological fit with the oscillation characterized by $\cos(kR' + \pi/4)$ as is suggested by Cheng et al. [3, 4]. The linearly varying amplitude is $A + BkR'$ with parameters $A = 5.91 \times 10^{-5}$, $B = 3.904 \times 10^{-8}$, and $R' = 50$. The blue line (Equation 3.30) is analytical result given by Cheng et al. [3, 4].
Chapter 4

The Fu-Kane model

The Fu-Kane model [21] may be realized by patterning a topologically trivial s-wave superconductor (see Appendix) to a surface of a strong topological insulator. The Cooper pairs can tunnel to the interface of superconductor and topological insulator, which will modify the surface Hamiltonian to one that resembles the p+ip superconductor Hamiltonian. Thus, Majorana fermions are possible to appear. In this chapter, we will start from a simplified Hamiltonian [2] with all bulk degrees of freedom being integrated out. Physically, such a Hamiltonian represents two parallel surfaces of the topological insulator coupled by some interaction. It is proven that such Hamiltonian captures the low-energy physics of a realistic strong topological insulator. By adding in an s-wave superconducting term and a mass term, one builds a lattice Hamiltonian realizing Fu-Kane model. Diagonalization of such Hamiltonian in the same vortex geometry (Figure 2.1) shows midgap states indicating Majorana fermions. For non-zero chemical potential, such Majorana bands show dispersion that is consistent with what we expect from the tight binding Majorana lattice. For zero chemical potential, the Majorana bands are flat to high numerical accuracy. The flat bands are protected by chiral symmetry [39] and therefore are robust when bringing two vortices closer.

4.1 The Fu-Kane Hamiltonian

The simplified Hamiltonian [2] for 3D strong topological insulator is

\[
H_{k, TI} = \begin{pmatrix} h_k & \bar{M}_k \\ \bar{M}_k & -h_k \end{pmatrix}
\]  

(4.1)

with blocks defined as

\[
h_k = 2\lambda(s_y \sin k_x - s_x \sin k_y)
\]

(4.2)

\[
\bar{M}_k = 2\bar{t}(2 - \cos k_x - \cos k_y)
\]

(4.3)

The Hamiltonian is written in basis \(\Psi_k = (c_{k,1,\uparrow}, c_{k,1,\downarrow}, c_{k,2,\uparrow}, c_{k,2,\downarrow})^T\). Here \(s_x\) and \(s_y\) are Pauli matrices in spin space. \(H_{k, TI}\) considers the two parallel
4.1. The Fu-Kane Hamiltonian

surfaces denoted by $h_k$ and $-h_k$ coupled by matrix $\bar{M}_k$. From now on, we will take $\lambda$ to be unity and measure all energies in terms of $\lambda$. The spectrum of $H_{k,\text{TI}}$ is

$$\epsilon(k) = \pm \sqrt{4(\sin^2 k_x + \sin^2 k_y) + \bar{M}_k^2}$$

which is doubly degenerate because of the fact that each surface will have a gapless Dirac cone.

Figure 4.1: Spectrum of the simplified topological insulator model with $\bar{t} = 0.5$. The spectrum is doubly degenerate with a single Dirac point at $\Gamma$.

An interesting modification is to open a gap at one of the surface by adding a mass term

$$H_{k,\text{Mag}} = m(c_{k,1,\uparrow}^\dagger c_{k,1,\uparrow} - c_{k,1,\downarrow}^\dagger c_{k,1,\downarrow})$$

such that the low-energy physics is completely determined by the ungapped surface. Due to the additional mass term, the Hamiltonian is now

$$H_{k,\text{TI}} + H_{k,\text{Mag}} = \begin{pmatrix} h_k + ms_z & \bar{M}_k \\ \bar{M}_k & -h_k \end{pmatrix}$$
4.1. The Fu-Kane Hamiltonian

The non-degenerate spectrum is

\[ \epsilon(k) = \pm \sqrt{4(\sin^2 k_x + \sin^2 k_y) + M_k^2 + \frac{1}{2} m^2 \pm \sqrt{\frac{1}{4} m^4 + m^2 M_k^2}} \] (4.7)

![Figure 4.2: Spectrum of the simplified topological insulator model with \( \bar{t} = 0.5 \). One of the surfaces is gapped by mass \( m = 0.2 \).](image)

We now pattern a slab of s-wave superconductor to the ungapped surface. The tunneling of Copper pair will introduce another term to the TI Hamiltonian

\[ H_{k,Sc} = \Delta c_{k;2,\uparrow}^\dagger c_{-k;2,\downarrow} + \Delta^* c_{-k;2,\downarrow}^\dagger c_{k;2,\uparrow} \] (4.8)

This term will open a gap and is the last piece of the Fu-Kane model. The full Hamiltonian is

\[ H_{FK} = \frac{1}{2} \sum_k \Phi_k^\dagger H_{k,FK} \Phi_k \] (4.9)
4.1. The Fu-Kane Hamiltonian

with

\[
H_{k,FK} = \begin{pmatrix}
  h_k + m s_z & M_k & 0 & 0 \\
  M_k & -h_k - \mu & 0 & i \Delta \sigma_y \\
  0 & 0 & h_k^* - m s_z & -M_k \\
  0 & -i \Delta^* \sigma_y & -M_k & -h_k^* + \mu
\end{pmatrix}
\] (4.10)

in the basis \( \Phi_k = (c_{k,1,\uparrow}, c_{k,1,\downarrow}, c_{k,2,\uparrow}, c_{k,2,\downarrow}, c_{-k,1,\uparrow}, c_{-k,1,\downarrow}, c_{-k,2,\uparrow}, c_{-k,2,\downarrow})^T \).

Figure 4.3: Spectrum of the simplified topological insulator model with \( \bar{t} = 0.5 \). The mass is \( m = 0.2 \), the superconductor order parameter is \( \Delta = 0.5 \), and the chemical potential is \( \mu = 0 \).

We would expect Majorana bands to appear provided that there is a non-zero magnetic field to create a set of vortex lattice (Figure 2.1). The vortices will break the translational symmetry of the underlying crystalline lattice. Thus, the momentum \( k_{x(y)} \) is not a good quantum number, indicating that we will need to solve this in real space. Perform Fourier transform,

\[
c_{k,\alpha} = \frac{1}{\sqrt{N}} \sum_r e^{-i k \cdot r} c_{r,\alpha}
\] (4.11)
where $\alpha$ specifies surface and spin. In an 8-component Nambu spinor $\Phi_r = (c_{r,1,\uparrow}, c_{r,1,\downarrow}, c_{r,2,\uparrow}, c_{r,2,\downarrow}, c_{r,1,\uparrow}^\dagger, c_{r,1,\downarrow}^\dagger, c_{r,2,\uparrow}^\dagger, c_{r,2,\downarrow}^\dagger)^T$, the Hamiltonian reads

$$H_{FK} = \frac{1}{2} \sum_r \Phi_r^\dagger \left( \begin{array}{cc} \hat{h}_r & \hat{\Delta}_r \\ \hat{\Delta}_r^\dagger & -\hat{h}_r^\dagger \end{array} \right) \Phi_r$$

(4.12)

with the blocks

$$\hat{h}_r = \left( \begin{array}{cccc} m & i \sum_\delta \hat{\eta}^\dagger_\delta & 4\tilde{t} - \tilde{t} \sum_\delta \hat{s}_\delta & 0 \\ i \sum_\delta \hat{\eta}_\delta & -m & 0 & 4\tilde{t} - \tilde{t} \sum_\delta \hat{s}_\delta \\ 4\tilde{t} - \tilde{t} \sum_\delta \hat{s}_\delta & 0 & -\varepsilon_F & -i \sum_\delta \hat{\eta}^\dagger_\delta \\ 0 & 4\tilde{t} - \tilde{t} \sum_\delta \hat{s}_\delta & -i \sum_\delta \hat{\eta}_\delta & -\varepsilon_F \end{array} \right)$$

(4.13)

and

$$\hat{\Delta}_r = \left( \begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Delta \\ 0 & 0 & -\Delta & 0 \end{array} \right)$$

(4.14)

where $\Delta = \Delta_0 e^{i\phi}$. When a magnetic field is applied, a vortex lattice is formed, and the hoppings, which are characterized by shift operators, should be modified by Peierls phase $\theta_r = \frac{e}{\hbar c} \int_{r}^{r+\delta} A(r) \cdot dl$. The diagonal block $\hat{h}_r(\theta_r)$ is now

$$\left( \begin{array}{cccc} m & i \sum_\delta e^{-i\theta_r \hat{\eta}^\dagger_\delta} & 4\tilde{t} - \tilde{t} \sum_\delta e^{-i\theta_r \hat{s}_\delta} & 0 \\ i \sum_\delta e^{-i\theta_r \hat{\eta}_\delta} & -m & 0 & 4\tilde{t} - \tilde{t} \sum_\delta e^{-i\theta_r \hat{s}_\delta} \\ 4\tilde{t} - \tilde{t} \sum_\delta e^{-i\theta_r \hat{s}_\delta} & 0 & -\varepsilon_F & -i \sum_\delta e^{-i\theta_r \hat{\eta}^\dagger_\delta} \\ 0 & 4\tilde{t} - \tilde{t} \sum_\delta e^{-i\theta_r \hat{s}_\delta} & -i \sum_\delta e^{-i\theta_r \hat{\eta}_\delta} & -\varepsilon_F \end{array} \right)$$

Working in same vortices geometry (Figure 2.1), the similar singular gauge transformation will remove the phase of superconductor order parameter and make the Hamiltonian easy to be diagonalized numerically. A natural choice of such transformation may be

$$U = diag(e^{i\phi A,1,\uparrow}, e^{i\phi A,1,\downarrow}, e^{i\phi A,2,\uparrow}, e^{i\phi A,2,\downarrow},$$

$$e^{-i\phi B,1,\uparrow}, e^{-i\phi B,1,\downarrow}, e^{-i\phi B,2,\uparrow}, e^{-i\phi B,2,\downarrow})$$

(4.15)
4.1. The Fu-Kane Hamiltonian

As for our topological insulator, only one surface is connected to superconductor, \( \phi_{A(B),1,1} \) does not have real physical meaning, because for a zero superconductor order parameter its phase can be arbitrary. We further assume phase is independent on spin orientation. By setting \( \phi_{A,1}(2,1) = \phi_A \) and \( \phi_{B,1}(2,1) = \phi_B \), where \( \phi_A + \phi_B = \phi \), we may get a more convenient unitary transformation

\[
U = \begin{pmatrix}
    e^{i\phi_A} & 0 \\
    0 & e^{-i\phi_B}
\end{pmatrix}
\]  

(4.16)

with each block being a 4 \times 4 matrix. After the unitary gauge transformation, we further plug in \( e^{-ik \cdot r} \) and \( e^{ik \cdot r} \), arriving at an \( 8 \times 8 \) Bloch Hamiltonian

\[
\mathcal{H}_{k,FK} = e^{-ik \cdot r} U^{-1} \begin{pmatrix}
    \hat{h}_r(\theta_r) & \Delta_r \\
    \Delta_r^* & -\hat{h}_r^*(\theta_r)
\end{pmatrix} U e^{ik \cdot r}
\]  

(4.17)

where the diagonal blocks \( \mathcal{H}^{(1,1)}_{k,FK} \) and \( \mathcal{H}^{(2,2)}_{k,FK} \) are defined as

\[
\begin{pmatrix}
    m & i \sum_{\delta} e^{i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\eta}_\delta & 4l - l \sum_{\delta} e^{i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\delta}_\delta & 0 \\
    i \sum_{\delta} e^{i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\eta}_\delta & -m & 4l - l \sum_{\delta} e^{i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\delta}_\delta & 0 \\
    4l - l \sum_{\delta} e^{i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\delta}_\delta & 4l - l \sum_{\delta} e^{i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\delta}_\delta & -\varepsilon_F & -i \sum_{\delta} e^{i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\eta}_\delta \\
    0 & -i \sum_{\delta} e^{i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\eta}_\delta & -\varepsilon_F & \delta \\
\end{pmatrix}
\]

and

\[
\begin{pmatrix}
    -m & i \sum_{\delta} e^{-i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\eta}_\delta & i \sum_{\delta} e^{-i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\delta}_\delta & 0 \\
    i \sum_{\delta} e^{-i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\eta}_\delta & m & 0 & i \sum_{\delta} e^{-i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\delta}_\delta \\
    i \sum_{\delta} e^{-i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\delta}_\delta & 0 & \varepsilon_F & -i \sum_{\delta} e^{-i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\eta}_\delta \\
    0 & i \sum_{\delta} e^{-i\sqrt{\delta} \cdot \delta} e^{ik \cdot \delta} \hat{\delta}_\delta & -\varepsilon_F & \delta \\
\end{pmatrix}
\]

respectively. And off-diagonal blocks are

\[
\mathcal{H}^{(1,2)}_{k,FK} = -\mathcal{H}^{(2,1)}_{k,FK} = \begin{pmatrix}
    0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 \\
    0 & 0 & \Delta_0 & 0 \\
    0 & 0 & -\Delta_0 & 0 \\
\end{pmatrix}
\]  

(4.18)

This is our final version of Fu-Kane Hamiltonian that can be numerically diagonalized.
4.2 Majorana band and spectrum

We will focus on the regime $\delta \epsilon_0 < \Delta_0 < \lambda$, where $\delta \epsilon_0$ is the energy difference between the lowest two Landau levels. In the regime $\delta \epsilon_0 < \Delta_0$, the low-energy bands are mainly determined by superconductor instead of magnetic field. On the other hand, for $\delta \epsilon_0 > \Delta_0$, the magnetic field dominates. And one will see flat Landau levels. Accordingly, $\delta \epsilon_0$ is obtained by diagonalizing the Bloch Hamiltonian $\mathcal{H}_{k, FK}$ with $\Delta_0 = 0$ and finding the gap between two lowest flat bands. As we are interested in the low-energy physics, we shall restrict both $\delta \epsilon_0$ and $\Delta_0$ within the bulk gap of topological insulator. The bulk gap is roughly measured by energy unit $\lambda$ (Figure 4.1). In this regime, the low-energy bands should resemble those of $p+ip$ superconductor.

By diagonalizing the Bloch Hamiltonian (Equation 4.17) with some non-zero chemical potential, one can confirm that Majorana bands (Figure 4.4, 4.5) have the same dispersion as the one in $p+ip$ superconductor (Figure 3.3), which can be explained by first and second nearest neighbor hoppings in the tight binding model. Specifically, when the chemical potential is tuned to coincide with Dirac point, namely, $\varepsilon_F = 0$, the Majorana bands become flat to high numeric accuracy (Figure 4.6), which is protected by chiral symmetry. Therefore, such flat band is robust when one brings two vortices in a magnetic unit cell closer until they merge into a double vortex. It can be shown numerically that the bandwidth of Majorana band does not have qualitative change in the merging process (Figure 4.6, 4.7, 4.8, 4.9).
4.2. Majorana band and spectrum

Figure 4.4: Majorana bands in the Fu-Kane model in a $30\delta \times 30\delta$ magnetic unit cell with $\varepsilon_F = 0.25$, $m = 0.5$, $\Delta_0 = 0.4$, $\tilde{t} = 0.5$, and $\delta \varepsilon_0 = 0.23$. Black dots represent numerical data while red lines are $\epsilon(k)$ given by tight binding model (Equation 3.17) with gaps $\Delta_\Gamma = 2.76 \times 10^{-4}$ and $\Delta_X = 1.336 \times 10^{-2}$ extracted from numerical data.
4.2. Majorana band and spectrum

Figure 4.5: Low-energy bands in the Fu-Kane model in a $30\delta \times 30\delta$ magnetic unit cell with $\varepsilon_F = 0.25$, $m = 0.5$, $\Delta_0 = 0.4$, $\bar{t} = 0.5$, and $\delta\varepsilon_0 = 0.23$. The red lines are dispersing Majorana bands.
4.2. Majorana band and spectrum

Figure 4.6: Low-energy bands in the Fu-Kane model in a $30\delta \times 30\delta$ magnetic unit cell with $\varepsilon_F = 0$, $m = 0.5$, $\Delta_0 = 0.4$, $\tilde{t} = 0.5$, and $\delta \epsilon_0 = 0.23$. The spacing of two vortices in the magnetic unit cell is $\mathbf{d} = (15\delta, 15\delta)$. The bandwidth of Majorana band (red line) is $5.7 \times 10^{-5}$. 
4.2. Majorana band and spectrum

Figure 4.7: Low-energy bands in the Fu-Kane model in a $30\delta \times 30\delta$ magnetic unit cell with $\varepsilon_F = 0$, $m = 0.5$, $\Delta_0 = 0.4$, $\tilde{t} = 0.5$, and $\delta \epsilon_0 = 0.23$. The geometry is changed by bringing two vortices closer to $d = (10\delta, 10\delta)$ along the diagonal. The bandwidth of Majorana band (red line) is $5.6 \times 10^{-5}$. 
4.2. Majorana band and spectrum

Figure 4.8: Low-energy bands in the Fu-Kane model in a $30\delta \times 30\delta$ magnetic unit cell with $\varepsilon_F = 0$, $m = 0.5$, $\Delta_0 = 0.4$, $\tilde{t} = 0.5$, and $\delta \varepsilon_0 = 0.23$. The geometry is changed by bringing two vortices further closer to $d = (5\delta, 5\delta)$ along the diagonal. The bandwidth of Majorana band (red line) is $4.9 \times 10^{-5}$. 
4.2. Majorana band and spectrum

Figure 4.9: Low-energy bands in the Fu-Kane model in a $30\delta \times 30\delta$ magnetic unit cell with $\varepsilon_F = 0$, $m = 0.5$, $\Delta_0 = 0.4$, $\tilde{t} = 0.5$, and $\delta\epsilon_0 = 0.23$. The geometry is changed by merging two vortices along the diagonal into a double vortex. The bandwidth of Majorana band (red line) is $4.9 \times 10^{-5}$.
4.3 Hoppings in Fu-Kane model

As working in the same vortex geometry (Figure 2.1), the analytical dispersion (Equation 3.17) of Majorana band will still be unchanged. The first nearest neighbor hopping is $t = \Delta x / 4\sqrt{2}$ and second nearest neighbor hopping is $t' = \Delta \Gamma / 8$. It is easy to test that such hoppings still hold oscillating behaviors that can be characterized by simple sine functions. Phenomenologically, we will use an exponentially decaying amplitude, which explicitly is $e^{-B[k(\varepsilon_F)]}$, with momentum $k = \varepsilon_F + D\varepsilon_F^3$. The s-wave superconductor is patterned to the surface characterized by surface Hamiltonian $h_k = -2(s_y \sin k_x - s_x \sin k_y)$, which only depends on sine functions. Thus, only odd powers should enter $k(\varepsilon_F)$. Therefore, the explicit fitting equation for our hopping will be

$$\epsilon = |Ae^{-B(|\varepsilon_F| + D|\varepsilon_F|^3)} \sin[R(|\varepsilon_F| + D|\varepsilon_F|^3)]| \quad (4.19)$$

with $\epsilon$ representing either $t$ or $t'$. 

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4.3. Hoppings in Fu-Kane model

Figure 4.10: First nearest neighbor hopping $t$ of the Fu-Kane model in a $30\delta \times 30\delta$ magnetic unit cell with $m = 0.5$, $\Delta_0 = 0.4$, $\bar{t} = 0.5$, and $\delta\epsilon_0 = 0.23$. Black dots are numerical data and red line is phenomenological fit. Fitting parameters are $A = 7.85 \times 10^{-3}$, $B = 1.79$, $D = 0.341$, and $R = 7.87$. 
4.3. Hoppings in Fu-Kane model

Figure 4.11: Second nearest neighbor hopping $t'$ of the Fu-Kane model in a $30\delta \times 30\delta$ magnetic unit cell with $m = 0.5$, $\Delta_0 = 0.4$, $\bar{t} = 0.5$, and $\delta \epsilon_0 = 0.23$. Black dots are numerical data and red line is phenomenological fit. Fitting parameters are $A = 5.87 \times 10^{-4}$, $B = 2.05$, $D = 0.26$, and $R = 12.06$. 
In this thesis, our research question is successfully accomplished. We systematically studied the dispersion of Majorana bands in topological superconductors. For both p+ip superconductor and the Fu-Kane model with vortices, we found the dispersion by numerical diagonalization of the Bloch Hamiltonian and by analytical diagonalization of the tight binding Hamiltonian. The two methods showed good consistency. The dispersion implies inter-vortex tunneling of Majorana fermions and is mainly contributed by first and second nearest neighbor hoppings of Majorana fermions. The hoppings are not identical to the previous analytical prediction [3, 4]. Thus, we used simplified equations to phenomenologically show the trends of the hoppings.

Although showing dispersing Majorana bands similar to p+ip superconductor at nonzero chemical potentials, the Fu-Kane model distinguishes itself by exhibiting flat Majorana bands at neutrality point where chemical potential is zero, coinciding with Dirac point. We also found that this additional feature is robust under different vortex configuration due to the extra chiral symmetry. This finding is consistent with previous theoretical prediction [39] on topological classification of the zero mode.

Our work may contribute to a better understanding of electronic structures of p+ip superconductor and the Fu-Kane model and should be beneficial to manipulating Majorana modes for topological quantum computation. Most analytical and numerical techniques in our work may be transplanted to study other "Fu-Kane model like" lattice systems, i.e., interface between a 3D strong topological insulator and a d-wave superconductor. A further step may be to consider a realistic model for 3D strong topological insulator by adding bulk layer Hamiltonians and corresponding couplings to the simplified Hamiltonian (Equation [4.1]), which will allow us to study the bulk physics of the topological insulator in proximity to a conventional superconductor.
Bibliography


Bibliography


Appendix A

The s-wave superconductor

In this appendix, we will show that s-wave superconductor is topologically trivial. Namely, there are no midgap states when vortex lattice is provided. The s-wave superconductor can also be described by the BCS type lattice Hamiltonian (Equation 2.1) that we used for p+ip superconductor. The only difference is that the off-diagonal shift operator is now a constant $\eta_\delta = \frac{1}{4}$. The lattice Bloch Hamiltonian is now,

$$H_{k,s} = \begin{pmatrix} -t \sum_\delta e^{i\mathcal{V}_\delta^A(r)} e^{ik \cdot \delta} \hat{s}_\delta - \varepsilon_F & \Delta_0 \\ \Delta_0 & t \sum_\delta e^{-i\mathcal{V}_\delta^B(r)} e^{ik \cdot \delta} \hat{s}_\delta + \varepsilon_F \end{pmatrix} \quad (A.1)$$

The definitions of $\mathcal{V}_\delta^A$ and $\mathcal{V}_\delta^B$ keep unchanged (Equation 2.9). By using the same technique (Equation 2.27) to calculate these two phase factors, the Hamiltonian $H_{k,s}$ can be diagonalized numerically so that both DOS and spectrum are able to be checked. We can see that the ground state is lowered if the s-wave superconductor possesses a vortex lattice, which is reflected in DOS as several discrete peaks below the superconducting gap $\Delta_0 = 1$. However, the spectrum is gapped regardless of the appearance of vortices.
Appendix A. The s-wave superconductor

Figure A.1: Density of states for an s-wave superconductor. The magnetic unit cell is chosen to be $10\delta \times 10\delta$, with $\delta$ being the lattice constant of the underlying crystalline lattice. The superconductor order parameter is $\Delta_0 = 1$ and the chemical potential is $\varepsilon_F = -2.2$. The blue line is the DOS with magnetic field $B = 0$ so that no vortices will appear. The sudden drops at 2.1 and 6.3 result from the edges of the band corresponding to the bottom and the top of the band respectively. The Van Hove singularity at 2.4 results from the saddle points of the band. The red line shows the DOS with non-zero magnetic field $B \neq 0$ and thus a vortex lattice appears. Landau levels show at the top of the spectrum.
Figure A.2: Band structure of s-wave superconductor with no vortices. The magnetic unit cell is chosen to be $10\delta \times 10\delta$, with $\delta$ being the lattice constant of the underlying crystalline lattice. The superconductor order parameter is $\Delta_0 = 1$ with chemical potential $\varepsilon_F = -2.2$. 
Figure A.3: Band structure of s-wave superconductor with square vortex lattice. The magnetic unit cell is chosen to be $10\delta \times 10\delta$, with $\delta$ being the lattice constant of the underlying crystalline lattice. The superconductor order parameter is $\Delta_0 = 1$ with chemical potential $\varepsilon_F = -2.2$. 

Appendix A. The s-wave superconductor