2

Problem set #2

2.1. Spin orbit coupling

Consider a 2D electron gas with Rashba spin-orbital coupling

$$H = \sum_k \frac{k^2}{2\,m} c_{k\uparrow}^{\dagger} c_{k\uparrow} + \sum_k \frac{k^2}{2\,m} c_{k\downarrow}^{\dagger} c_{k\downarrow} + \alpha \sum_k \left(k_y + i\ k_x\right) c_{k\uparrow}^{\dagger} c_{k\downarrow} + \alpha \sum_k \left(k_y - i\ k_x\right) c_{k\downarrow}^{\dagger} c_{k\uparrow} \tag{2.1}$$

The first two terms are standard $k^2/2\,m$ kinetic energy (here $k^2 = {k_x}^2 + {k_y}^2$). The last two terms are spin-orbit coupling terms as we showed in the lecture notes. This Hamiltonian can be written in terms of a 2×2 matrix

$$H = \sum_k \begin{pmatrix} c_{k,\uparrow}^{\dagger} & c_{k,\downarrow}^{\dagger} \end{pmatrix} \begin{pmatrix} k^2/2\,m & \alpha\,k_y + \alpha\,i\ k_x \\ \alpha\,k_y - \alpha\,i\ k_x & k^2/2\,m \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \end{pmatrix} \tag{2.2}$$

2.1.1. Band structure

Diagonal this 2×2 matrix and find the energy spectrum. It should contain two bands $E_+(k)$ and $E_-(k)$

2.1.2. Fermi surface

Let's fix the chemical potential μ as a positive number. With a fixed $\mu>0$, these system has two Fermi surfaces, which are two circles with radius k_{F+} and k_{F-}. Here, k_{F+} is the solution to the equation $E_+(k) = \mu$ and k_{F-} is the solution to the equation $E_-(k) = \mu$. Find k_{F+} and k_{F-}

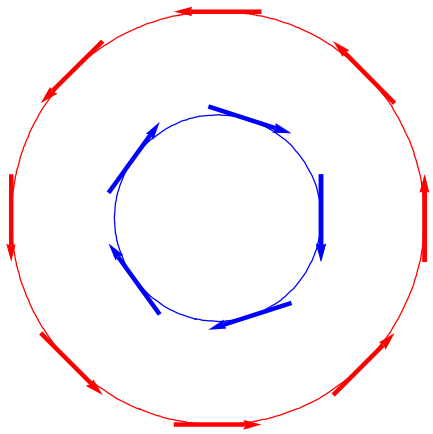
2.1.3. Spin configuration

Find the eigen-vectors of this 2×2 matrix. Show that at the momentum point $\vec{k} = \left(k_x,\ k_y\right)$, the two eigenvectors of the 2×2 matrix are eigenstates of the spin operator $\vec{\sigma}\cdot\vec{n}$ with $\vec{n} = \left(k_y \Big/ \sqrt{{k_x}^2 + {k_y}^2}\ ,\ -k_x \Big/ \sqrt{{k_x}^2 + {k_y}^2}\right)$.

Prove that $\vec{n}$ is perpendicular to $\vec{k} = \left(k_x,\ k_y\right)$

2.1.4. Implication of 2.1.3 (no question for this part)

The results found in 2.1.3 means that near the two Fermi surfaces, the directions of the spins are locked with the direction of the momentum as shown in the figure below. In fact, the spin is always perpendicular to the direction of $\vec{k}$.



The spin structure near the Fermi surfaces.

2.2. d-wave superconductivity (high T_c)

Consider a superconductor whose mean-field Hamiltonian is

$$H_{\text{MF}} = \sum_k \left[\epsilon(k)\, c_{k,\uparrow}{}^\dagger\, c_{k,\uparrow} + \epsilon(k)\, c_{k,\downarrow}{}^\dagger\, c_{k,\downarrow} + \Delta_k{}^*\, c_{k\downarrow}\, c_{-k\uparrow} + \Delta_{-k}\, c_{k\uparrow}{}^\dagger\, c_{-k\downarrow}{}^\dagger\right] \tag{2.3}$$

For simplicity, we assume that Δ_k is real ($\Delta_k{}^* = \Delta_k$) and Δ_k is an even function of k ($\Delta_k = \Delta_{-k}$), so that we can simplify the last term slightly

$$H_{\text{MF}} = \sum_k \left[\epsilon(k)\, c_{k,\uparrow}{}^\dagger\, c_{k,\uparrow} + \epsilon(k)\, c_{k,\downarrow}{}^\dagger\, c_{k,\downarrow} + \Delta_k\, c_{k\downarrow}\, c_{-k\uparrow} + \Delta_k\, c_{k\uparrow}{}^\dagger\, c_{-k\downarrow}{}^\dagger\right] \tag{2.4}$$

Let's use the grand canonical ensemble (fixing μ), so we shall consider $\tilde{H}_{\text{MF}} = H_{\text{MF}} - \mu\, N$, instead of H_{MF}

$$\tilde{H}_{\text{MF}} = H_{\text{MF}} - \mu\, N = \sum_k \left[(\epsilon_k - \mu)\, c_{k,\uparrow}{}^\dagger\, c_{k,\uparrow} + (\epsilon_k - \mu)\, c_{k,\downarrow}{}^\dagger\, c_{k,\downarrow} + \Delta_k\, c_{k\downarrow}\, c_{-k\uparrow} + \Delta_k\, c_{k\uparrow}{}^\dagger\, c_{-k\downarrow}{}^\dagger\right] = \sum_k \begin{pmatrix} c_{k,\uparrow}{}^\dagger & c_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} \epsilon(k) - \mu & \Delta_k \\ \Delta_k & \mu - \epsilon(k) \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}{}^\dagger \end{pmatrix} \tag{2.5}$$

2.2.1. energy spectrum and superconducting gap

Diagonalize the matrix $\begin{pmatrix} \epsilon(k) - \mu & \Delta_k \\ \Delta_k & \mu - \epsilon(k) \end{pmatrix}$ to find the energy spectrum. The spectrum should contain two bands with energy $E_+(k)$ and $E_-(k)$ respectively.

Show that $E_+(k) \geq 0$ and $E_-(k) \leq 0$. In addition, show that $E_+(k) = -E_-(k)$.

Compute the superconducting gap $\Delta_{\text{SC}}(k) = E_+(k) - E_-(k)$

2.2.2. s-wave superconductor

Here, we consider a s-wave superconductor with Δ_k being a constant (independent of k) $\Delta_k = \Delta$. Find the minimum value of $\Delta_{\text{SC}}(k)$. Prove that the minimum is reach at the Fermi surface $\epsilon_k = \mu$.

Prove that the minimum value of $\Delta_{\text{SC}}(k)$ only relies on the value of Δ. As long as Δ>0, the two band never cross, so the system is always gaped.

2.2.3. d-wave superconductor

Now, let's consider a d-wave superconductor with $\Delta_k = \Delta\left(k_x{}^2 - k_y{}^2\right)$. We further assume that $\epsilon_k = \frac{k^2}{2\,m}$.

Find the minimum value of $\Delta_{\text{SC}}(k) = E_+(k) - E_-(k)$. Prove that the minimum value is reached when two conditions are satisfied (1) at the Fermi surface $\epsilon_k = \mu$ and (2) along the diagonal directions $k_x = \pm k_y$.

Show that there are four k-points at which Δ_k reaches its minimum value. These points are known as "nodes" or "nodal points".

Expand $E_+(k)$ and $E_-(k)$ near one of nodal points and show that the dispersion is linear near this point. (i.e. this is a Dirac point).

2.3. Majorana fermions

In general a complex number z is usually different from its complex conjugate z^*, $z \neq z^*$. For the special case where $z = z^*$, we call them "real numbers".

Very similarly, for operators, in general, the Hermitian conjugate of an operator O is different from O itself, $O \neq O^\dagger$. For the special case $O = O^\dagger$, these operators are known as Hermitian operators.

For fermion creation and annihilation operators c and $c^\dagger$, typically, they are NOT Hermitian, so $c^\dagger \neq c$. The fermions created and annihilated by these non-Hermitian operators are known as "complex" fermions. Most of the fermions we studied in condensed matter physics are "complex": e.g. Dirac fermions. In principle, their fermion creation and annihilation operators could be Hermitian with $c^\dagger = c$. These fermions are known as "Majorana fermions".

For ordinary fermions, we know that $\{c_i, c_j^\dagger\} = \delta_{ij}$, where i and j are site indices indicating different lattice sites. For Majorana fermions $c_i = c_i^\dagger = \gamma_i$ (let us define γ here for simplicity), the anti-commutation relation takes a very similar form $\{\gamma_i, \gamma_j\} = 2\,\delta_{ij}$. Here the normalization factor 2 is adopted for historical reasons. This normalization factor implies that $\{\gamma_i, \gamma_i\} = \gamma_i\,\gamma_i + \gamma_i\,\gamma_i = 2\,\gamma_i\,\gamma_i = 2$. So we can write $\gamma_i\,\gamma_i = 1$. (The square of a Majorana operator is the identity).

2.3.1. $\gamma_i\,\gamma_j$: Hermitian or anti-Hermitian?

Prove $(\gamma_i\,\gamma_j)^\dagger = -\gamma_i\,\gamma_j$, assuming $i \neq j$.

This relation implies that $\gamma_i\,\gamma_j$ is anti-Hermitian. In other words, it is NOT a physical observable, which must be Hermitian.

Prove $(i\,\gamma_i\,\gamma_j)^\dagger = i\,\gamma_i\,\gamma_j$, assuming $i \neq j$.

This relation implies that $i\,\gamma_i\,\gamma_j$ is Hermitian. In other words, for any physical observables that are the products of two Majorana fermions, the Coefficient must be pure imaginary.

2.3.2. Majorana fermion as real and imaginary part of a complex fermion.

Consider "complex" fermions, which we are very familiar with. We assume the creation and annihilation operators for the complex fermions are $c^\dagger$ and c.

Define the "real part" of $c^\dagger$ as

$$\gamma_1 = c^\dagger + c \tag{2.6}$$

Define the "imaginary part" of $c^\dagger$ as

$$\gamma_2 = \frac{c^\dagger - c}{i} \tag{2.7}$$

Check that

$$c^\dagger = \frac{\gamma_1 + i\,\gamma_2}{2} \quad \text{and} \quad c = \frac{\gamma_1 - i\,\gamma_2}{2} \tag{2.8}$$

These γ_1 and γ_2 operators are two Majorana fermion operators. Check that they satisfies all the properties of Majorana fermions by showing the following relations

$$(1)\ \gamma_1^\dagger = \gamma_1 \quad \text{and} \quad (2)\ \gamma_2^\dagger = \gamma_2 \tag{2.9}$$

$$(3)\ \{\gamma_1, \gamma_1\} = \{\gamma_2, \gamma_2\} = 2 \text{ and } (4)\ \{\gamma_1, \gamma_2\} = \{\gamma_2, \gamma_1\} = 0 \tag{2.10}$$

The equations (1) and (2) here tell us that γ_1 and γ_2 are both Hermitian (they are "real fermions"). The last two equations imply that they satisfy the anti-commutation relation for Majorana fermions: $\{\gamma_i, \gamma_j\} = 2\,\delta_{ij}$

2.3.3. 1D superconducting chain

Consider a 1D superconducting chain.

$$H = -t \sum_{j=1}^{N} \left(c_j^\dagger\, c_{j+1} + c_{j+1}^\dagger\, c_j\right) - \mu \sum_{j=1}^{N} c_j^\dagger\, c_j + \Delta \sum_{j=1}^{N} \left(c_j\, c_{j+1} + c_{j+1}^\dagger\, c_j^\dagger\right) \tag{2.11}$$

The first term here is the kinetic energy (hoppings between nearest neighbors). The second term is the chemical potential and the last term is pairing (which breaks the particle number conservation). Here, for simplicity, we assume Δ is a positive real number.

Define Majorana fermion operators:

$$\gamma_{2\,j-1} = c_j^\dagger + c_j \tag{2.12}$$

and

$$\gamma_{2\,j} = \frac{c_j^\dagger - c_j}{i} \tag{2.13}$$

Rewrite the Hamiltonian using the Majorana operators. This definition split each fermion sites into two Majorana fermion sites. If we start from a model with N sites, the mapping gives us a Majorana fermion Chain with 2N sites.

2.3.4. special case I: Δ=t=0 and μ<0.

Consider a special case with $\Delta = t = 0$ and $\mu < 0$. Prove that the Hamiltonian is

$$H = -\frac{\mu}{2}\sum_{j=1}^{N} i\,\gamma_{2\,j-1}\,\gamma_{2\,j} \tag{2.14}$$

Please notice that here each term of the Hamiltonian contains a complex i in the coefficients. Please compare it with the problem 2.3.1. This complex i is crucial to keep the Hamiltonian a Hermitian operator.

2.3.5. special case II: Δ=t>0 and μ=0.

Consider a special case with $\Delta = t > 0$ and $\mu = 0$. Prove that the Hamiltonian is

$$H = t\sum_{j=1}^{N-1} i\,\gamma_{2\,j}\,\gamma_{2\,j+1} \tag{2.15}$$

Again we noticed the complex i here, which is important for the Hermitian condition.

In addition, it is important to notice that γ_1 and $\gamma_{2\,N}$ do NOT appear in the Hamiltonian. In other words, $[\gamma_1,\ H] = [\gamma_{2\,N},\ H] = 0$

2.3.6. Zero-energy Majorana modes at the end of the chain.

Let's focus on the special case studied in 2.3.5. Suppose the ground state wavefunction for our system is |G⟩ with energy E_0.

$$H\,|G\rangle = E_0\,|G\rangle \tag{2.16}$$

Using the commutation relation we find in 2.3.5 ($[\gamma_1,\ H] = [\gamma_{2\,N},\ H] = 0$) to prove that

$$H\,\gamma_1\,|G\rangle = E_0\,\gamma_1\,|G\rangle \tag{2.17}$$

$$H\,\gamma_{2\,N}\,|G\rangle = E_0\,\gamma_{2\,N}\,|G\rangle \tag{2.18}$$

These two formulas tell us that we can create one Majorana fermion at each of the two ends of this 1D superconducting chain. After we create this Majorana fermion, the new state is still the ground state with the same eigen energy as |G⟩. In other words, it costs no energy to create a Majorana fermion at any of the two ends of this chain.

2.3.7. More general statement (no question for this part)

In fact, for this 1D superconducting chain, there are two different phases (assuming Δ>0). For 2|t|<μ, it is a topologically trivial phase with no extra modes at the two ends. For 2 |t|<μ, it is a topological phase, which contains one zero-energy Majorana modes at each of the two ends. The two cases mentioned above in 2.3.4 and 2.3.5 are examples for the topologically trivial and topological phases, respectively.

Here, the meaning of the word "topological" is similar to what we learned in higher dimensions. In 2D and 3D, topological insulator/superconductors have low-energy edge/surface modes. In 1D, they have zero energy modes near the two ends.

2.3.8. Topological degeneracy part I: How many ground states do we have for a 1D topological superconducting chain?

For the 1D superconducting chain studied in 2.3.5, we can define a complex fermion operator using γ_1 and $\gamma_{2\,N}$

$$c = \frac{\gamma_1 + i\,\gamma_{2N}}{2} \tag{2.19}$$

and

$$c^\dagger = \frac{\gamma_1 + i\,\gamma_{2N}}{2} \tag{2.20}$$

Because $H\,\gamma_1\,|G\rangle = E_0\,\gamma_1\,|G\rangle$ and $H\,\gamma_{2N}\,|G\rangle = E_0\,\gamma_{2N}\,|G\rangle$, it is easy to check that

$$H\,c\,|G\rangle = E_0\,c\,|G\rangle \tag{2.21}$$

$$H\,c^\dagger\,|G\rangle = E_0\,c^\dagger\,|G\rangle \tag{2.22}$$

Therefore, the space formed by all the ground states of this Hamiltonian can be written using the operators c and $c^\dagger$

Define a state $|0\rangle$, which is a ground state of the Hamiltonian $H\ |0\rangle = E_0\,|0\rangle$ and in addition it satisfies the condition $c|0\rangle=0$.

Another ground state $|1\rangle$ can be defined as $|1\rangle = c^\dagger\,|0\rangle$.

Prove that $c^\dagger\,|1\rangle = 0$ and $c\,|1\rangle = |0\rangle$, so that we cannot get any extra ground states from $|0\rangle$ using c and $c^\dagger$ operators.

Prove that $\langle 1|0\rangle=0$, so that $|1\rangle$ and $|0\rangle$ are two different ground state.

Therefore, we conclude that there are two degenerate ground state for the case studied in 2.3.5.

2.3.9. Topological degeneracy part II: How many ground states do we have, if we have many Majorana chains?

Assume that we have n Majorana chains. For each chain, we can define c_i and $c_i^\dagger$ operator as we did in 2.3.8, with i=1,2,…n. Now, we can start from a state $|000...0\rangle$, which is a ground state of the system and satisfies the condition

$$c_i\,|00\ldots\ 0\rangle = 0 \tag{2.23}$$

for any c_i.

Now, it is easy to check that any states like this is a new ground states.

$$c_{i1}^\dagger\,c_{i2}^\dagger\,c_{i3}^\dagger\ldots c_{im}^\dagger\,|00\ldots0\rangle \tag{2.24}$$

Show that there are 2^n ground states.

This conclusion is very generic. For a system with 2n Majorana fermions., the number of ground states is 2^n. (Majorana fermions always appears in pairs, so the total number is always even. This is why we consider a system with 2n Majorana fermions here, instead of 2n+1).