Lecture notes on topological insulators

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I. REVIEW OF BCS THEORY

Because of the superconducting gap, a superconductor (SC) is similar to an insulator (from the energy spectrum point of view). One thing that distinguishes a SC from an insulator is that the former has particle-hole symmetry near the gap. The ground state of a bulk SC *has a definite phase, but does not have a definite number of Cooper pairs* (some discussion can be found in Sec. 5.4 of Martin and Rothen, 2002). Therefore, adding an electron to a SC is the same as removing an electron (or adding a hole), as the two processes only differ by a Cooper pair. In this and following chapters we study the topology of such an "insulator".

A. Mean field Hamiltonian

Depending on detailed mechanism, the two electrons in a Cooper pair can form a spin-singlet (s-wave, d-wave) or spin-triplet (p-wave). The mean-field BCS Hamiltonian of a s-wave superconductor is,

$$H_{MF} = \sum_{\mathbf{k}s} \varepsilon_k c^\dagger_{\mathbf{k}s} c_{\mathbf{k}s} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} + \sum_{\mathbf{k}} \Delta^*_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \tag{1.1}$$

where $\varepsilon_k = \hbar^2 k^2/2m - \mu$, μ is the chemical potential, and $\Delta_{\mathbf{k}}$ is called the **gap function**. In the following, we simply write the subscript $\mathbf{k}$ as k, so that $c_{\pm ks}$ and $\Delta_{\pm k}$ represent $c_{\pm \mathbf{k}s}$ and $\Delta_{\pm \mathbf{k}}$.

Since c_{ks} are fermion operators, they satisfy anti-commutation relations,

$$\{c_{ks}, c^\dagger_{k's'}\} = \delta_{kk'}\delta_{ss'}, \tag{1.2}$$
$$\{c_{ks}, c_{k's'}\} = 0, \tag{1.3}$$

For the simplest type of s-wave SC, $\Delta_k = \Delta_0$. In general, the gap function of s-wave SC has even parity (and no node), $\Delta_{-k} = \Delta_k$.

To diagonalize the Hamiltonian, rewrite the first term of H_{MF} as,

$$\sum_k \varepsilon_k \left(c^\dagger_{k\uparrow} c_{k\uparrow} - c_{k\downarrow} c^\dagger_{k\downarrow} \right) + \sum_k \varepsilon_k, \tag{1.4}$$

then the Hamiltonian can be written as,

$$H_{MF} = \sum_k (c^\dagger_{k\uparrow} c_{-k\downarrow}) \begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta^*_k & -\varepsilon_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} + \sum_k \varepsilon_k. \tag{1.5}$$

The Hamiltonian with quadratic fermion operators can be solved easily. First, diagonalize the 2×2 matrix $\mathsf{H}(\mathbf{k})$ with an unitary transformation U,

$$\begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta^*_k & -\varepsilon_k \end{pmatrix} = U \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} U^\dagger, \tag{1.6}$$
$$U = \begin{pmatrix} \alpha_+ & \alpha_- \\ \beta_+ & \beta_- \end{pmatrix}, \tag{1.7}$$

where $\pm E_k = \pm\sqrt{\varepsilon_k^2 + |\Delta_k|^2}$ are the eigenvalues, and $(\alpha_\pm, \beta_\pm)$ are the corresponding eigen-vectors. We only keep the positive excitation energy $+E_k$.

It can be shown that, for example,

$$\begin{pmatrix} \alpha_+ \\ \beta_+ \end{pmatrix} = N \begin{pmatrix} \varepsilon_k + E_k \\ \Delta^*_k \end{pmatrix}, \tag{1.8}$$

in which N is a constant. After normalization,

$$\alpha_+ = \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_k}{E_k}\right)}; \quad \beta_+ = \sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right)} \frac{\Delta^*_k}{|\Delta_k|}. \tag{1.9}$$

Similarly, for $-E_k$,

$$\alpha_- = -\sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right)}; \quad \beta_- = \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_k}{E_k}\right)} \frac{\Delta^*_k}{|\Delta_k|}. \tag{1.10}$$

For a *homogeneous* SC, $\Delta_k = e^{i\phi}|\Delta_k|$. The k-*in*dependent phase ϕ is the SC phase mentioned in the Introduction.

There is some freedom in choosing the phases of $\alpha_\pm$ and $\beta_\pm$. If one writes (see Eq. (1.9))

$$\begin{pmatrix} \alpha_+ \\ \beta_+ \end{pmatrix} = \begin{pmatrix} u_k \\ v_k \end{pmatrix}, |u_k|^2 + |v_k|^2 = 1, \tag{1.11}$$

then, after adjusting an overall phase of (α_-, β_-),

$$\begin{pmatrix} \alpha_- \\ \beta_- \end{pmatrix} = \begin{pmatrix} -v^*_k \\ u_k \end{pmatrix}. \tag{1.12}$$

Now, define

$$\begin{pmatrix} \gamma_{k1} \\ \gamma^\dagger_{-k2} \end{pmatrix} = U^\dagger \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v^*_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} \tag{1.13}$$

or, $$\begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} = U \begin{pmatrix} \gamma_{k1} \\ \gamma^\dagger_{-k2} \end{pmatrix} = \begin{pmatrix} u_k & -v^*_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_{k1} \\ \gamma^\dagger_{-k2} \end{pmatrix} \tag{1.14}$$

They satisfy the anti-commutation relations ($s, s' = 1, 2$),

$$\{\gamma_{ks}, \gamma^\dagger_{k's'}\} = \delta_{kk'}\delta_{ss'}, \quad (1.15)$$
$$\{\gamma_{ks}, \gamma_{k's'}\} = 0. \quad (1.16)$$

The transformation between $(c_{k\uparrow}, c_{-k,\downarrow})$ and $(\gamma_{k1}, \gamma_{-k2})$ that preserves the (anti-)commutation relations is called as the **Bogoliubov-Valatin transformation**.

When written in new basis,

$$H_{MF} = \sum_k (\gamma^\dagger_{k1}\gamma_{-k2}) \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \gamma_{k1} \\ \gamma^\dagger_{-k2} \end{pmatrix} + \sum_k \varepsilon_k \quad (1.17)$$
$$= \sum_k E_k \left(\gamma^\dagger_{k1}\gamma_{k1} + \gamma^\dagger_{-k2}\gamma_{-k2}\right) + \text{const.} \quad (1.18)$$

Note that these quasiparticles (QPs) $(\gamma_{k1}, \gamma_{-k2})$ do not interact with each other (like phonons in a solid with harmonic vibrations), and that the excitation energy of one QP is E_k. Each QP has a definite energy, momentum, and spin, but does not have a definite charge (since it is a superposition of electron and hole states).

B. Particle-hole symmetry

The eigen-states in Eqs. (1.11),(1.12) are particle state and hole state. They can be related by a particle-hole (PH) transformation P. In next chapter, we will see that *spinless* p-wave SC has a Hamiltonian similar to the one in Eq. (1.1). One only needs to make the following changes: 1), Replace $(c_{k\uparrow}, c^\dagger_{-k\downarrow})$ by $(c_k, c^\dagger_{-k})$. This is merely a change of subscripts, without affecting the eigenstate solutions in Eqs. (1.11),(1.12). 2), Adopt a gap function with odd parity, $\Delta_{-k} = -\Delta_k$.

We now discuss the PH transformations in s-wave SC and in spinless p-wave SC. First, like the TR operator, the PH operator P is an anti-unitary operator: to flip the sign of charge, $P(\mathbf{p} + e\mathbf{A})P^{-1} = -(\mathbf{p} - e\mathbf{A})$, thus $PiP^{-1} = -i$ is required. Second, because of Eq. (1.9), if $\Delta_{-k} = \Delta_k$, then one has

$$u_{-k} = u_k, \; v_{-k} = v_k. \quad (1.19)$$

However, if $\Delta_{-k} = -\Delta_k$, then

$$u_{-k} = u_k, \; v_{-k} = -v_k. \quad (1.20)$$

For a s-wave SC,

if $\psi_k = \begin{pmatrix} u_k \\ v_k \end{pmatrix}$ has energy E_k,

then $P\psi_k = \begin{pmatrix} -v^*_k \\ u_k \end{pmatrix} = \begin{pmatrix} -v^*_{-k} \\ u_{-k} \end{pmatrix}$ has energy $-E_{-k}$.

Therefore, we choose

$$P = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K = -i\tau_y K, \quad (1.21)$$

where K is the operation of complex conjugation.

For a spinless p-wave SC,

if $\psi_k = \begin{pmatrix} u_k \\ v_k \end{pmatrix}$ has energy E_k,

then $P\psi_k = \begin{pmatrix} v^*_k \\ u_k \end{pmatrix} = \begin{pmatrix} -v^*_{-k} \\ u_{-k} \end{pmatrix}$ has energy $-E_{-k}$.

Therefore, we choose

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} K = \tau_x K. \quad (1.22)$$

Note that for a s-wave SC, $P^2 = -1$; for a p-wave SC, $P^2 = 1$.

If a system has particle-hole symmetry, then

$$P\mathsf{H}(\mathbf{k})P^{-1} = -\mathsf{H}(-\mathbf{k}). \quad (1.23)$$

You can verify that the 2×2-matrix $H(\mathbf{k})$ in Eq. (1.5), and its p-wave version with $\Delta_{-k} = -\Delta_k$, do have the PH symmetry.

If one writes $P = U_P K$, where U_P is an unitary operator, then

$$U_P\mathsf{H}^*(\mathbf{k})U_P^{-1} = -\mathsf{H}(-\mathbf{k}). \quad (1.24)$$

In comparison, under TR transformation,

$$T\mathsf{H}(\mathbf{k})T^{-1} = \mathsf{H}(-\mathbf{k}). \quad (1.25)$$

If one writes $T = U_T K$, where U_T is an unitary operator, then

$$U_T\mathsf{H}^*(\mathbf{k})U_T^{-1} = \mathsf{H}(-\mathbf{k}). \quad (1.26)$$

Recall that for a particle with half-integer spin, $T^2 = -1$; for a particle with integer spin, $T^2 = 1$.

Note: for an *anti-unitary* operator like T or P, its square can only be ± 1. The proof is as follows. Applying either of the transformation twice, the system should go back to the state before the transformation, differing at most by a phase factor, $Q^2 = z, |z| = 1$. It follows that,

$$zQ = Q^2 Q = QQ^2 \quad (1.27)$$
$$= Qz = \bar{z}Q, \quad (1.28)$$
$$\to z = \bar{z} = \pm 1. \quad (1.29)$$

C. Real space formulation

To deal with SC systems without spatial homogeneity (e.g., those with edges, vortices ... etc), one needs the mean-field Hamiltonian in real space (see Chap 5 of de Gennes, 1989). For s-wave SC, it is

$$H_{eff} = \int d^3r \left\{ \sum_{s=\uparrow,\downarrow} \psi^\dagger_s H_0 \psi_s + \Delta(\mathbf{r})\psi^\dagger_\uparrow \psi^\dagger_\downarrow + \Delta^*(\mathbf{r})\psi_\downarrow\psi_\uparrow \right\}, \quad (1.30)$$

where

$$H_0 = \frac{1}{2m}\left(\mathbf{p}+e\mathbf{A}\right)^2 + V(\mathbf{r}) - \mu, \tag{1.31}$$

$V(\mathbf{r})$ is an external potential, and

$$\begin{aligned}\{\psi_s(\mathbf{r}), \psi_{s'}(\mathbf{r}')^\dagger\} &= \delta(\mathbf{r}-\mathbf{r}')\delta_{ss'}, &(1.32)\\ \{\psi_s(\mathbf{r}), \psi_{s'}(\mathbf{r}')\} &= 0. &(1.33)\end{aligned}$$

We wish to diagonalize H_{eff} using a generalized Bogoliubov-Valatin transformation,

$$\begin{aligned}\psi_\uparrow(\mathbf{r}) &= \sum_{n\geq 0}\left(u_n(\mathbf{r})\gamma_{n\uparrow} - v_n^*(\mathbf{r})\gamma_{n\downarrow}^\dagger\right), &(1.34)\\ \psi_\downarrow^\dagger(\mathbf{r}) &= \sum_{n\geq 0}\left(v_n(\mathbf{r})\gamma_{n\uparrow} + u_n^*(\mathbf{r})\gamma_{n\downarrow}^\dagger\right). &(1.35)\end{aligned}$$

Note: One could start with a restricted version without the summation, but the superposition helps lowering the free energy and produces a more accurate solution (p.259 of Ketterson and Song, 1999). Choose u_n and v_n such that

$$H_{eff} = \sum_{n,s} E_n \gamma_{ns}^\dagger \gamma_{ns}, \tag{1.36}$$

and demand that

$$\begin{aligned}\{\gamma_{ns}, \gamma_{n's'}^\dagger\} &= \delta_{nn'}\delta_{ss'}, &(1.37)\\ \{\gamma_{ns}, \gamma_{n's'}\} &= 0. &(1.38)\end{aligned}$$

This leads to the equations of motion,

$$\begin{aligned}i\hbar\dot{\gamma}_{ns} &= [\gamma_{ns}, H_{eff}] = E_n\gamma_{ns}, &(1.39)\\ i\hbar\dot{\gamma}_{ns}^\dagger &= \left[\gamma_{ns}^\dagger, H_{eff}\right] = -E_n\gamma_{ns}^\dagger. &(1.40)\end{aligned}$$

Note that it is *commutators*, instead of anti-commutators in the equations of motion, so the following identity helps,

$$[a, bc] = \{a, b\}c - b\{a, c\}. \tag{1.41}$$

On the other hand, one has

$$\begin{aligned}i\hbar\dot{\psi}_\uparrow(\mathbf{r}) &= [\psi_\uparrow(\mathbf{r}), H_{eff}] = H_0\psi_\uparrow(\mathbf{r}) + \Delta(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}), &(1.42)\\ i\hbar\dot{\psi}_\downarrow(\mathbf{r}) &= [\psi_\downarrow(\mathbf{r}), H_{eff}] = H_0\psi_\downarrow(\mathbf{r}) - \Delta(\mathbf{r})\psi_\uparrow^\dagger(\mathbf{r}) &(1.43)\end{aligned}$$

Rewrite ψ's using γ's, and compare with Eqs. (1.39),(1.40), we get

$$\begin{aligned}H_0 u_n(\mathbf{r}) + \Delta(\mathbf{r})v_n(\mathbf{r}) &= E_n u_n(\mathbf{r}), &(1.44)\\ H_0^* v_n(\mathbf{r}) - \Delta^*(\mathbf{r})u_n(\mathbf{r}) &= -E_n v_n(\mathbf{r}). &(1.45)\end{aligned}$$

These are called the **Bogoliubov-de Gennes** (BdG) equations. They can be written in matrix form,

$$\begin{pmatrix} H_0 & \Delta \\ \Delta^* & -H_0^* \end{pmatrix}\begin{pmatrix} u_n \\ v_n \end{pmatrix} = E_n \begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{1.46}$$

The $*$ for H_0 is required if there is vector potential $\mathbf{A}$.

That is, the coefficients (u_n, v_n) turn out to be eigenstates of the Hamiltonian. Thus, they are orthonormal to each other,

$$\begin{aligned}\int d^3r\,(u_n^*(\mathbf{r}), v_n^*(\mathbf{r}))\begin{pmatrix} u_{n'}(\mathbf{r}) \\ v_{n'}(\mathbf{r}) \end{pmatrix} &= \delta_{nn'}, &(1.47)\\ \int d^3r\,(u_n^*(\mathbf{r}), v_n^*(\mathbf{r}))\begin{pmatrix} -v_{n'}^*(\mathbf{r}) \\ u_{n'}^*(\mathbf{r}) \end{pmatrix} &= 0. &(1.48)\end{aligned}$$

The first equation is for particle-state and particle-state; the second for particle-state and hole-state. With the help of Eqs. (1.47),(1.48), we have,

$$\begin{aligned}\gamma_{n\uparrow} &= \int d^3r\left(u_n^*(\mathbf{r})\psi_\uparrow(\mathbf{r}) + v_n^*(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\right), &(1.49)\\ \gamma_{n\downarrow}^\dagger &= \int d^3r\left(-v_n(\mathbf{r})\psi_\uparrow(\mathbf{r}) + u_n(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\right). &(1.50)\end{aligned}$$

Furthermore, the completeness relations are (see Exercise 4),

$$\begin{aligned}\sum_n [u_n(\mathbf{r})u_n^*(\mathbf{r}') + v_n^*(\mathbf{r})v_n(\mathbf{r}')] &= \delta(\mathbf{r}-\mathbf{r}'), &(1.51)\\ \sum_n [u_n(\mathbf{r})v_n^*(\mathbf{r}') - v_n^*(\mathbf{r})u_n(\mathbf{r}')] &= 0, &(1.52)\end{aligned}$$

Some remarks: First, the operators of particle-hole transformation are the same as those in Eqs. (1.21), and Eq. (1.23) becomes,

$$P\mathsf{H}(\mathbf{r},\mathbf{p})P^{-1} = -\mathsf{H}(\mathbf{r},-\mathbf{p}). \tag{1.53}$$

Second, similar to the uniform case, if (u_n, v_n) is a solution with energy E_n, then $(-v_n^*, u_n^*)$ is a solution with energy $-E_n$ (for s-wave SC). But we only keep the solution with positive excitation energy.

Exercise

1. Consider a homogeneous s-wave superconductor with $H_0 = p^2/2m - \mu$, and $\Delta(\mathbf{r})$ is a constant Δ_0. Show that, by postulating

$$\begin{aligned}u_n(\mathbf{r}) &= \frac{1}{\sqrt{V_0}}u_k e^{i\mathbf{k}\cdot\mathbf{r}}, &(1.54)\\ v_n(\mathbf{r}) &= \frac{1}{\sqrt{V_0}}v_k e^{i\mathbf{k}\cdot\mathbf{r}}, &(1.55)\end{aligned}$$

where V_0 is the volume of the SC, the BdG equation reduces to the momentum-space version in Sec. I.A.

2. Consider a s-wave superconductor with an uniform current. The center of mass of Cooper pairs move with momentum $2\hbar\mathbf{q}$, and the gap function is,

$$\Delta(\mathbf{r}) = |\Delta_0|e^{2i\mathbf{q}\cdot\mathbf{r}}. \tag{1.56}$$

The eigenstates in the BdG equation can be postulated as (see p.144 of de Gennes, 1989 for details),

$$\begin{aligned}u_n(\mathbf{r}) &= \frac{1}{\sqrt{V_0}}u_k e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}, &(1.57)\\ v_n(\mathbf{r}) &= \frac{1}{\sqrt{V_0}}v_k e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}}. &(1.58)\end{aligned}$$

Solve the BdG equation to get the excitation energy,

$$E_k = \frac{\varepsilon_{k+q} - \varepsilon_{k-q}}{2} + \left[\left(\frac{\varepsilon_{k+q} + \varepsilon_{k-q}}{2} \right)^2 + |\Delta_0|^2 \right]^{1/2} . \tag{1.59}$$

Assume $q \ll k$ (which is of order k_F), expand E_k to first order in $\mathbf{q}$, and based on this result, find out the critical velocity $\hbar \mathbf{q}_c/m$ (in terms of $|\Delta_0|$) that closes the SC gap. Note: in fact, $|\Delta_0|$ itself also depends on q, but this is not considered here.

3. Substitute Eqs. (1.49),(1.50) to Eqs. (1.37)(1.38), and confirm the orthogonality relations in Eqs. (1.47), (1.48).

4. Substitute Eqs. (1.34),(1.35) to Eqs. (1.32)(1.33), and confirm the completeness relations in Eqs. (1.51), (1.52).

References

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