Lecture notes on topological insulators

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CONTENTS

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*. 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 lectures we study the topology of such an "insulator". Two recommended references for the theory of superconductor are de Gennes, 1989 and Tinkham, 1996.

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**, also known as the **order parameter**. 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), $\Delta_{-k} = \Delta_k$. 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.

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.

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 $-E_k$,

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

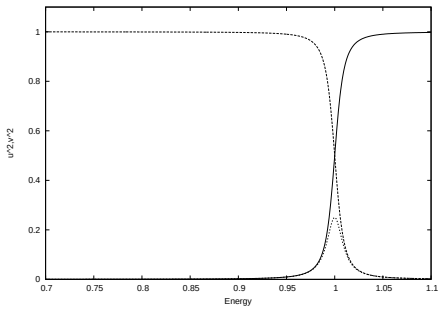

FIG. 1 The functions $|u_k|^2$ (solid line), $|v_k|^2$ (dotted line), and $|u_k|^2|v_k|^2$. The energy is in units of the Fermi energy, and $\Delta/\varepsilon_F = 0.01$.

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_-),

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

Note that both u_k and v_k are even functions of $\mathbf{k}$ since $\Delta_{-k} = \Delta_k$ for s-wave superconductor. Fig. 1 shows a plot of $|u_k|^2$ and $|v_k|^2$ as functions of energy ε_k.

1. Bogoliubov transformation

Define

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

$$\text{or,} \quad \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} = U \begin{pmatrix} \gamma_{k1} \\ \gamma^\dagger_{-k2} \end{pmatrix} = \begin{pmatrix} u_k & -v_k^* \\ v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_{k1} \\ \gamma^\dagger_{-k2} \end{pmatrix}.$$

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

$$\{\gamma_{ks}, \gamma^\dagger_{k's'}\} = \delta_{kk'}\delta_{ss'}, \tag{1.13}$$

$$\{\gamma_{ks}, \gamma_{k's'}\} = 0. \tag{1.14}$$

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

When written in new basis,

$$\begin{aligned} & H_{MF} \\ &= \sum_k (\gamma^\dagger_{k1} \gamma_{-k2}) \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \gamma_{k1} \\ \gamma^\dagger_{-k2} \end{pmatrix} + \sum_k \varepsilon_k \\ &= \sum_k E_k \left(\gamma^\dagger_{k1}\gamma_{k1} + \gamma^\dagger_{-k2}\gamma_{-k2} \right) + \text{const.} \end{aligned} \tag{1.15}$$

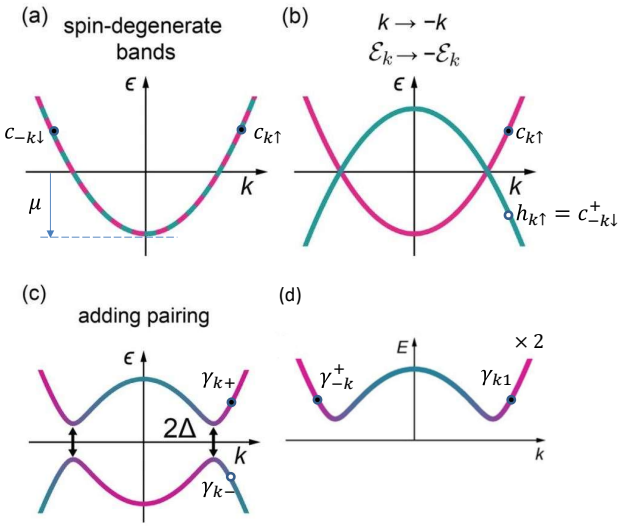

FIG. 2 Different representations of the superconducting energies using bases (a) $(c_{k\uparrow}, c_{-k\downarrow})^T$, (b) $(c_{k\uparrow}, c^\dagger_{-k\downarrow})^T$, (c) $(\gamma_{k+}, \gamma_{k-})^T$, and (d) $(\gamma_{k1}, \gamma^\dagger_{-k2})^T$. Red curves are electron-like; green curves are hole-like. The curve in d is two-fold degenerate. Figs. from M. Hays' 2021 thesis.

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. In thermal equilibrium, they follow the Fermi-Dirac distribution,

$$f(E_k) = \frac{1}{e^{E_k/kT} + 1}. \tag{1.16}$$

Since $E_k \geq \Delta_k$, when the temperature $kT \ll \Delta_k$, there is nearly no quasiparticles.

Each QP is a superposition of an electron and a hole. For example,

$$\gamma^\dagger_{k1} = u_k c^\dagger_{k\uparrow} + v_k c_{-k\downarrow}. \tag{1.17}$$

It creates an electron in the state $(\mathbf{k}, \uparrow)$ and annihilates an electron in the state $(-\mathbf{k}, \downarrow)$ (or creates a hole with momentum $\mathbf{k}$ and up-spin.) Hence, each QP has a definite energy, momentum, and spin, but has no definite charge. Furthermore, from Fig. 1, we see that $\gamma^\dagger_{k1}$ is more like an electron when its energy is above the energy gap. On the other hand, $\gamma^\dagger_{-k2}$ is more like a hole when its energy is below the energy gap.

Fig. 2 is a summary of the different bases we have used so far, plus a basis in (c) that has not been used: $(\gamma_{k+}, \gamma_{k-})^T = (\gamma_{k1}, \gamma^\dagger_{-k2})^T$. In the $\gamma_{k\pm}$ basis, the diagonalized Hamiltonian would be

$$H_{MF} = \sum_k E_k \left(\gamma^\dagger_{k+}\gamma_{k+} - \gamma^\dagger_{k-}\gamma_{k-} \right). \tag{1.18}$$

B. BCS ground state

1. Boson coherent state

The BCS ground state can be understood as a coherent state of Cooper pairs. First, a short review of boson coherent state:

$$\begin{aligned} |\lambda\rangle &= e^{-|\lambda|^2/2} e^{\lambda a^\dagger} |0\rangle \\ &= e^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} |n\rangle. \end{aligned} \tag{1.19}$$

With the help of the identity (which is valid when $[A, B]$ commutes with both A and B),

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}, \tag{1.20}$$

one can show that the state is normalized, $\langle\lambda|\lambda\rangle = 1$. It is an eigenstate of the annihilation operator,

$$a|\lambda\rangle = \lambda|\lambda\rangle, \quad \text{and} \quad \bar{n} = \langle\lambda|\hat{n}|\lambda\rangle = |\lambda|^2. \tag{1.21}$$

In general,

$$\lambda = |\lambda| e^{i\theta} = \sqrt{\bar{n}} e^{i\theta}. \tag{1.22}$$

It's not difficult to see from Eq. (1.20) that

$$\frac{1}{i}\frac{\partial}{\partial\theta}|\lambda\rangle = \hat{n}|\lambda\rangle. \tag{1.23}$$

Therefore $\hat{n} \simeq \frac{1}{i}\frac{\partial}{\partial\theta}$, and just like the uncertainty relation, we have

$$\Delta n \Delta\theta \geq \frac{1}{2}. \tag{1.24}$$

That is, one cannot fix the values of n and θ simultaneously. What happens here is that in order to have a well-defined phase of a field (say, electromagnetic field), $\Delta\theta \ll 1$, the field strength (number of photons) cannot be too weak.

Note: The relation $\hat{n} \simeq \frac{1}{i}\frac{\partial}{\partial\theta}$ cannot be exact. If it is, then

$$[\hat{n}, \hat{\theta}] = \frac{1}{i}, \tag{1.25}$$

which leads to

$$(n - n')\langle n|\hat{\theta}|n'\rangle = \frac{1}{i}\delta_{nn'}. \tag{1.26}$$

This leads to contradiction when $n = n'$. That is why there can be no angle (or phase) operator in quantum mechanics. However, for a system with large n, when the fluctuation (uncertainty) is of little significance, the angle operator can be used in an approximate manner.

2. BCS coherent state

If we consider the Cooper pair as a single entity and define

$$b_k^\dagger = c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger. \tag{1.27}$$

With the help of the identities,

$$[A, BC] = [A, B]C + B[A, C], \tag{1.28}$$

$$\text{and} \quad [A, BC] = \{A, B\}C - B\{A, C\}, \tag{1.29}$$

one can show that

$$[b_k, b_{k'}^\dagger] = (1 - \hat{n}_{k\uparrow} - \hat{n}_{-k\downarrow})\,\delta_{kk'}. \tag{1.30}$$

Therefore, the new entity is not exactly a boson with the usual commutation relation. Also, $\left(b_k^\dagger\right)^2 = 0$, so it still has the fermion character.

How did Schrieffer arrive at the BCS wave function? He pictured the BCS state as a coherent state of Cooper pairs and wrote

$$\begin{aligned} |\Psi_{BCS}\rangle &= e^{\sum_k \alpha_k b_k^\dagger}|\mathbf{0}\rangle \\ &= \prod_k e^{\alpha_k b_k^\dagger}|\mathbf{0}\rangle \quad \text{due to Eq. (1.30)} \\ &= \prod_k \left(1 + \alpha_k b_k^\dagger\right)|\mathbf{0}\rangle, \end{aligned} \tag{1.31}$$

in which $|\mathbf{0}\rangle$ is the vacuum of the manybody system. After normalization, we have

$$|\Psi_{BCS}\rangle = \prod_k \left(\tilde{u}_k + \tilde{v}_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger\right)|\mathbf{0}\rangle, \tag{1.32}$$

in which $|\tilde{u}_k|^2 + |\tilde{v}_k|^2 = 1$ for all k, and $|\tilde{v}_k|^2$ is the probability that the states $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ are occupied by a Cooper pair. One can choose $\tilde{u}_k$ as real numbers, and $\tilde{v}_k$ are in general complex numbers.

When expanded with states having n Cooper pairs, we have

$$|\Psi_{BCS}(\phi)\rangle = \sum_{n=0}^{M} a_n e^{in\phi}|n\rangle, \tag{1.33}$$

where M is the number of k-states. This is peaked around $\bar{n}$. Similar to Eq. (1.23), one has

$$\frac{1}{i}\frac{\partial}{\partial\phi}|\Psi_{BCS}\rangle = \hat{n}|\Psi_{BCS}\rangle. \tag{1.34}$$

Also,

$$\langle\Psi_{BCS}(\phi')|\Psi_{BCS}(\phi)\rangle = \sum_{n=0}^{M} e^{in(\phi-\phi')}|a_n|^2. \tag{1.35}$$

For a macroscopic system, due to the rapid oscillation of $e^{i\bar{n}(\phi-\phi')}$, this product drops rapidly to zero as soon as $\phi \neq \phi'$. That is, the BCS state has a definite phase ϕ, but because of the number-phase uncertainty relation, the number of Cooper pairs n would be uncertain.

C. Excited states

The SC ground state can be defined as the vacuum of bogolons,

$$\gamma_{k1}|\Psi_G\rangle = \gamma_{-k2}|\Psi_G\rangle = 0. \tag{1.36}$$

This definition is consistent with the BCS ground state $|\Psi_{BCS}\rangle$ in Eq. (1.32). One can check that,

$$\begin{aligned}\gamma_{k1}|\Psi_G\rangle &= \left(u_k c_{k\uparrow} + v_k^* c_{-k\downarrow}^\dagger\right)\prod_{k'}\left(\tilde{u}_{k'} + \tilde{v}_{k'} c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger\right)|\mathbf{0}\rangle \\ &= 0 \ \text{ if } (\tilde{u}_k, \tilde{v}_k) = (u_k, -v_k^*).\end{aligned} \tag{1.37}$$

The two sets of coefficients can be made identical if in Eq. (1.11), instead of (u_k, v_k), we wrote the components of the first eigenvector as $(u_k, -v_k^*)$ (which is a common practice). Note that the phase of $\tilde{v}_k$ is the same as that of the order parameter $\Delta_k = e^{i\phi}|\Delta_k|$, which is the phase of the macroscopic condensate.

The excited states with one bogolon are

$$\begin{aligned}\gamma_{k1}^\dagger|\Psi_G\rangle &= c_{k\uparrow}^\dagger \prod_{k'\neq k}\left(u_{k'} - v_{k'}^* c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger\right)|\mathbf{0}\rangle, \\ \gamma_{-k2}^\dagger|\Psi_G\rangle &= c_{-k\downarrow}^\dagger \prod_{k'\neq k}\left(u_{k'} - v_{k'}^* c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger\right)|\mathbf{0}\rangle.\end{aligned} \tag{1.38}$$

For $\gamma_{k1}^\dagger$, it adds an electron to one of the states of $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$, which raises the energy (for the lack of Cooper binding energy). Similarly for the other operator $\gamma_{-k2}^\dagger$.

The number of electrons in state-k of the BCS ground state is

$$\begin{aligned}\langle\Psi_G|\sum_s c_{ks}^\dagger c_{ks}|\Psi_G\rangle &= 2|v_k|^2 \\ &= 2 \ \to \ 0 \text{ as energy increases.}\end{aligned} \tag{1.39}$$

On the other hand, the number of electrons in state-k of the 1-bogolon state is

$$\langle\Psi_G|\gamma_{k1}\sum_{s'} c_{ks'}^\dagger c_{ks'}\gamma_{k1}^\dagger|\Psi_G\rangle = 1. \tag{1.40}$$

Compared to the ground state, the 1-bogolon state has one less electron below the Fermi energy, but one more electron above the Fermi energy. Therefore, the excited state moves one electron from below the Fermi energy to above.

D. Particle-hole symmetry

The eigenstates in Eqs. (1.11),(1.12) are electron-like states and hole-like states (above the Fermi energy). They can be related by particle-hole (PH) transformation P. In next lecture, 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 $(c_{k\uparrow}, c_{-k\downarrow}^\dagger)$ with $(c_k, c_{-k}^\dagger)$. 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 momentum and the sign of a charge, $P(\mathbf{p} + e\mathbf{A})P^{-1} = -(\mathbf{p} - e\mathbf{A})$, $PiP^{-1} = -i$ is required. Second, because of Eq. (1.9), if $\Delta_{-k} = \Delta_k$, then one has

$$u_{-k} = u_k, \ v_{-k} = v_k. \tag{1.41}$$

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

$$u_{-k} = u_k, \ v_{-k} = -v_k. \tag{1.42}$$

For a s-wave SC,

$$\begin{aligned}&\text{if } \psi_k = \begin{pmatrix} u_k \\ v_k \end{pmatrix} \text{ has energy } E_k, \\ &\text{then } P\psi_k = \begin{pmatrix} -v_{-k}^* \\ u_{-k} \end{pmatrix} = \begin{pmatrix} -v_k^* \\ u_k \end{pmatrix} \text{ has energy } -E_{-k}.\end{aligned}$$

Therefore, we choose

$$P = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K = -i\tau_y K, \tag{1.43}$$

where K is the operation of complex conjugation.

For a spinless p-wave SC,

$$\begin{aligned}&\text{if } \psi_k = \begin{pmatrix} u_k \\ v_k \end{pmatrix} \text{ has energy } E_k, \\ &\text{then } P\psi_k = \begin{pmatrix} -v_{-k}^* \\ u_{-k} \end{pmatrix} = \begin{pmatrix} v_k^* \\ u_k \end{pmatrix} \text{ has energy } -E_{-k}.\end{aligned}$$

Therefore, we choose

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} K = \tau_x K. \tag{1.44}$$

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

$$P\mathsf{H}(\mathbf{k})P^{-1} = -\mathsf{H}(-\mathbf{k}). \tag{1.45}$$

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

$$U_P\mathsf{H}^*(\mathbf{k})U_P^{-1} = -\mathsf{H}(-\mathbf{k}). \tag{1.46}$$

In comparison, under TR transformation,

$$T\mathsf{H}(\mathbf{k})T^{-1} = \mathsf{H}(-\mathbf{k}). \tag{1.47}$$

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

$$U_T \mathsf{H}^*(\mathbf{k}) U_T^{-1} = \mathsf{H}(-\mathbf{k}). \tag{1.48}$$

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,

$$\begin{aligned} zQ = Q^2 Q &= QQ^2 && (1.49)\\ &= Qz = \bar{z}Q, && (1.50)\\ \to z &= \bar{z} = \pm 1. && (1.51) \end{aligned}$$

E. 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

$$H_{eff} = \int d^3 r \left\{ \sum_{s=\uparrow,\downarrow} \psi_s^\dagger H_0 \psi_s + \Delta(\mathbf{r}) \psi_\uparrow^\dagger \psi_\downarrow^\dagger + \Delta^*(\mathbf{r}) \psi_\downarrow \psi_\uparrow \right\}, \tag{1.52}$$

where

$$H_0 = \frac{1}{2m} (\mathbf{p} + e\mathbf{A})^2 + V(\mathbf{r}) - \mu, \tag{1.53}$$

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

$$\begin{aligned} \{\psi_s(\mathbf{r}), \psi_{s'}(\mathbf{r}')^\dagger\} &= \delta(\mathbf{r} - \mathbf{r}')\delta_{ss'}, && (1.54)\\ \{\psi_s(\mathbf{r}), \psi_{s'}(\mathbf{r}')\} &= 0. && (1.55) \end{aligned}$$

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

$$\begin{aligned} \psi_\uparrow(\mathbf{r}) &= \sum_{n\geq 0} \left(u_n(\mathbf{r}) \gamma_{n\uparrow} - v_n^*(\mathbf{r}) \gamma_{n\downarrow}^\dagger \right), && (1.56)\\ \psi_\downarrow^\dagger(\mathbf{r}) &= \sum_{n\geq 0} \left(v_n(\mathbf{r}) \gamma_{n\uparrow} + u_n^*(\mathbf{r}) \gamma_{n\downarrow}^\dagger \right). && (1.57) \end{aligned}$$

The summation is over the index n of yet to be determined eigenstates. 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

$$H_{eff} = \sum_{n,s} E_n \gamma_{ns}^\dagger \gamma_{ns}, \tag{1.58}$$

and demand that

$$\begin{aligned} \{\gamma_{ns}, \gamma_{n's'}^\dagger\} &= \delta_{nn'}\delta_{ss'}, && (1.59)\\ \{\gamma_{ns}, \gamma_{n's'}\} &= 0. && (1.60) \end{aligned}$$

This leads to the equations of motion,

$$\begin{aligned} i\hbar\dot{\gamma}_{ns} &= [\gamma_{ns}, H_{eff}] = E_n \gamma_{ns}, && (1.61)\\ i\hbar\dot{\gamma}_{ns}^\dagger &= [\gamma_{ns}^\dagger, H_{eff}] = -E_n \gamma_{ns}^\dagger. && (1.62) \end{aligned}$$

Note that it is *commutators*, instead of anti-commutators in the equations of motion, so Eq. (1.29) helped.

On the other hand, one has

$$\begin{aligned} i\hbar\dot{\psi}_\uparrow(\mathbf{r}) &= [\psi_\uparrow(\mathbf{r}), H_{eff}] = H_0 \psi_\uparrow(\mathbf{r}) + \Delta(\mathbf{r}) \psi_\downarrow^\dagger(\mathbf{r}) && (1.63)\\ i\hbar\dot{\psi}_\downarrow(\mathbf{r}) &= [\psi_\downarrow(\mathbf{r}), H_{eff}] = H_0 \psi_\downarrow(\mathbf{r}) - \Delta(\mathbf{r}) \psi_\uparrow^\dagger(\mathbf{r}) && (1.64) \end{aligned}$$

Rewrite ψ's using γ's, and compare with Eqs. (1.61),(1.62), we get

$$\begin{aligned} H_0 u_n(\mathbf{r}) + \Delta(\mathbf{r}) v_n(\mathbf{r}) &= E_n u_n(\mathbf{r}), && (1.65)\\ H_0^* v_n(\mathbf{r}) - \Delta^*(\mathbf{r}) u_n(\mathbf{r}) &= -E_n v_n(\mathbf{r}). && (1.66) \end{aligned}$$

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

$$\begin{pmatrix} H_0 & \Delta \\ \Delta^* & -H_0^* \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} = E_n \begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{1.67}$$

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. 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). Thus, they are orthonormal to each other,

$$\begin{aligned} \int d^3 r \, (u_n^*(\mathbf{r}), v_n^*(\mathbf{r})) \begin{pmatrix} u_{n'}(\mathbf{r}) \\ v_{n'}(\mathbf{r}) \end{pmatrix} &= \delta_{nn'}, && (1.68)\\ \int d^3 r \, (u_n^*(\mathbf{r}), v_n^*(\mathbf{r})) \begin{pmatrix} -v_{n'}^*(\mathbf{r}) \\ u_{n'}^*(\mathbf{r}) \end{pmatrix} &= 0. && (1.69) \end{aligned}$$

The first equation is for particle-state and particle-state; the second for particle-state and hole-state.

With the help of Eqs. (1.68),(1.69), we have (see Exercise 3)

$$\begin{aligned} \gamma_{n\uparrow} &= \int d^3 r \left(u_n^*(\mathbf{r}) \psi_\uparrow(\mathbf{r}) + v_n^*(\mathbf{r}) \psi_\downarrow^\dagger(\mathbf{r}) \right), && (1.70)\\ \gamma_{n\downarrow}^\dagger &= \int d^3 r \left(-v_n(\mathbf{r}) \psi_\uparrow(\mathbf{r}) + u_n(\mathbf{r}) \psi_\downarrow^\dagger(\mathbf{r}) \right). && (1.71) \end{aligned}$$

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

$$\begin{aligned} \sum_n [u_n(\mathbf{r}) u_n^*(\mathbf{r}') + v_n^*(\mathbf{r}) v_n(\mathbf{r}')] &= \delta(\mathbf{r} - \mathbf{r}'), && (1.72)\\ \sum_n [u_n(\mathbf{r}) v_n^*(\mathbf{r}') - v_n^*(\mathbf{r}) u_n(\mathbf{r}')] &= 0, && (1.73) \end{aligned}$$

The operators of particle-hole transformation are the same as those in Eqs. (1.43), and Eq. (1.45) becomes,

$$P\mathsf{H}(\mathbf{r}, \mathbf{p}) P^{-1} = -\mathsf{H}(\mathbf{r}, -\mathbf{p}). \tag{1.74}$$

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

$$u_n(\mathbf{r}) = \frac{1}{\sqrt{V_0}} u_k e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{1.75}$$

$$v_n(\mathbf{r}) = \frac{1}{\sqrt{V_0}} v_k e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{1.76}$$

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 a Cooper pair is moving with momentum $2\hbar\mathbf{q}$, and the gap function is,

$$\Delta(\mathbf{r}) = |\Delta_0| e^{2i\mathbf{q}\cdot\mathbf{r}}. \tag{1.77}$$

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

$$u_n(\mathbf{r}) = \frac{1}{\sqrt{V_0}} u_k e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}, \tag{1.78}$$

$$v_n(\mathbf{r}) = \frac{1}{\sqrt{V_0}} v_k e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}}. \tag{1.79}$$

Solve the BdG equation to get the excitation energy,

$$E_k = \frac{\varepsilon_{k+q} - \varepsilon_{k-q}}{2} + \left[\left(\frac{\varepsilon_{k+q} + \varepsilon_{k-q}}{2} \right)^2 + |\Delta_0|^2 \right]^{1/2}. \tag{1.80}$$

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. Derive Eqs. (1.70),(1.71) from Eqs. (1.56)(1.57) with the help of the orthogonality relations in Eqs. (1.68), (1.69).

4. Substitute Eqs. (1.56),(1.57) to Eqs. (1.54)(1.55), and confirm the completeness relations in Eqs. (1.72), (1.73).

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