5 BCS theory of superconductivity

Refs: [Mar] Section 27.3, [LP] E.M.Lifshitz et L.P.Pitaevskii, "Statistical Physics, Part 2" (vol.9 of "Landau et Lifshitz"), Sections 39,40.

As we have seen, phonons mediate an attraction between electrons. In this section, we will see how superconductivity emerges in an electron gas with attraction (the theory of Bardeen–Cooper–Schriffer).

5.1 Superconductivity as spontaneous symmetry breaking

Superconductivity is associated with developing nonzero *anomalous averages*

$$\langle a_\alpha a_\beta \rangle \neq 0 \,, \tag{5.1.1}$$

where a_α and a_β are annihilation operators and α and β denote electron degrees of freedom (momentum/coordinate and spin). Such an average breaks the U(1) (electromagnetic) symmetry

$$a \mapsto e^{i\alpha} a \,, \qquad a^+ \mapsto e^{-i\alpha} a^+ \,. \tag{5.1.2}$$

The anomalous average (5.1.1) may only be nonzero in a superposition of states with different particle numbers. Physically, the number of electrons in an isolated piece of a superconductor is fixed, in which case (5.1.1) should be understood as a long-range order

$$\lim_{|x-y|\to\infty} \langle (a_\alpha a_\beta)_x \, (a_\beta^+ a_\alpha^+)_y \rangle \neq 0 \,, \tag{5.1.3}$$

and the phase of an individual average $\langle a_\alpha a_\beta \rangle$ remains undetermined.

A good analogy to think of is the ferromagnetic transition: in a ferromagnet, the average magnetization is non-zero and points in a spontaneously chosen direction, even though in an isolated system, formally, the ground state is a superposition of states with all equivalent orientations of magnetization.

The phase of the average $\langle a_\alpha a_\beta \rangle$ is the spontaneously broken symmetry. It is not observable directly, but only in comparison with other such phases (the *Josephson effect*). A spatial modulation of this phase corresponds to the *supercurrent* (an electric current which propagates without dissipation).

Superconductors may be classified by the symmetry of indices in the anomalous average (5.1.1). The most common symmetry (usually favored in superconductors with attraction due to phonons) is the *s-wave* superconductivity: the spin indices in (5.1.1) form a singlet, and the pairing is isotropic in space.

5.2 Model Hamiltonian and mean-field approximation

We consider a model Hamiltonian of the form

$$H = H_0 + H_{\text{int}} \,, \tag{5.2.1}$$

where

$$H_0 = \sum_{k,\alpha} (\varepsilon_k - \mu) a_{k,\alpha}^+ a_{k,\alpha} \tag{5.2.2}$$

is the free part, and

$$H_{\rm int} = -\frac{1}{2\mathcal{V}} \sum_{\tilde{k}_1,\tilde{k}_2,\tilde{k}_3} a^+_{\tilde{k}_1} a^+_{\tilde{k}_2} a_{\tilde{k}_3} a_{\tilde{k}_1+\tilde{k}_2-\tilde{k}_3} V_{\tilde{k}_1,\tilde{k}_2,\tilde{k}_3,\tilde{k}_1+\tilde{k}_2-\tilde{k}_3} \,, \tag{5.2.3}$$

where $\mathcal{V}$ is the system volume and $V_{\tilde{k}_1,\tilde{k}_2,\tilde{k}_3,\tilde{k}_4}$ are the interaction matrix elements (the spin indices are included in $\tilde{k}_i$ for simplicity). In this chapter, we use the "sum" notation (the sum over k instead of integration over $d^3k/(2\pi)^3$), with the electronic states normalized as $\{a_k, a^+_{k'}\} = \delta_{kk'}$ (instead of the delta function of the continuous variable $k - k'$).

We will use the *mean-field approximation*: first, replace the products $a_k a_{k'}$ by their nonzero averages and then solve the *self-consistency* equation for those averages.

The structure of the non-zero anomalous averages depends on the interaction $V_{\tilde{k}_1,\tilde{k}_2,\tilde{k}_3,\tilde{k}_4}$. We assume that the superconductor is s-wave, with $\langle a_{k\uparrow} a_{-k\downarrow}\rangle \neq 0$. Correspondingly, we only consider the terms of this type in the interaction and neglect the k dependence of the interaction matrix elements (since, as we will see below, only k values around the Fermi surface are relevant). As a result, we simplify the interaction term to

$$H_{\rm int} = -\frac{g_0}{\mathcal{V}} \sum_{k,k'} a^+_{k\uparrow} a^+_{-k\downarrow} a_{-k'\downarrow} a_{k'\uparrow} = -\frac{g_0}{\mathcal{V}} \left(\sum_k a^+_{k\uparrow} a^+_{-k\downarrow}\right) \left(\sum_{k'} a_{-k'\downarrow} a_{k'\uparrow}\right) \,, \tag{5.2.4}$$

where g_0 is some positive interaction constant.

We further define the complex numbers

$$d_k = \langle a_{-k\downarrow} a_{k\uparrow}\rangle \qquad d^*_k = \langle a^+_{k\uparrow} a^+_{-k\downarrow}\rangle \,. \tag{5.2.5}$$

These numbers will be later determined from the self-consistency conditions.

By replacing the products in the four-fermion operator by their averages, we get the quadratic Hamiltonian

$$H_{\rm BCS} = \sum_k \left[(\varepsilon_k - \mu)(a^+_{k\uparrow} a_{k\uparrow} + a^+_{-k\downarrow} a_{-k\downarrow}) + \Delta^* a_{-k\downarrow} a_{k\uparrow} + \Delta a^+_{k\uparrow} a^+_{-k\downarrow}\right] \,, \tag{5.2.6}$$

where

$$\Delta = -\frac{g_0}{\mathcal{V}} \sum_k d_k \,. \tag{5.2.7}$$

5.3 Bogoliubov quasiparticles and the BCS ground state

This quadratic Hamiltonian may be diagonalized by a rotation in the particle-hole space:

$$\gamma^+_{k\uparrow} = u_k a^+_{k\uparrow} + v_k a_{-k\downarrow} \,. \tag{5.3.1}$$

The coefficients u_k and v_k can be found, e.g., from the commutation relation

$$[H_{\rm BCS}, \gamma^+_{k\uparrow}] = \tilde{\varepsilon}_k \gamma^+_{k\uparrow} \,. \tag{5.3.2}$$

We find the equation on the coefficients:

$$\begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta^* & -(\varepsilon_k - \mu) \end{pmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \tilde{\varepsilon}_k \begin{pmatrix} u_k \\ v_k \end{pmatrix} \,. \tag{5.3.3}$$

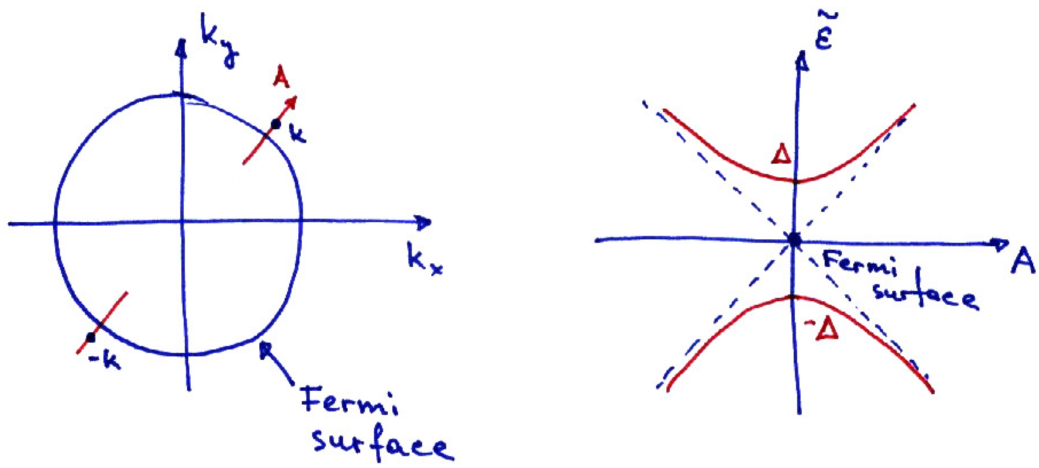

Figure 18: Left: The two sections across the Fermi surface contributing to the spectrum in the right panel. Each quasiparticle in the right panel corresponds to a linear combination of an electron with momentum k and a hole with momentum $-k$ and opposite spin. Right: The BCS spectrum (5.3.4).

The eigenvalues give the spectrum:

$$\tilde{\varepsilon}_k = \pm\sqrt{(\varepsilon_k - \mu)^2 + |\Delta|^2}\,. \tag{5.3.4}$$

Thus $|\Delta|$ plays the role of the *gap* in the spectrum (see Fig. 18).

The fermionic Fock space may be now represented in terms of the occupation numbers for (Bogoliubov) quasiparticles $\gamma^+_{k\uparrow}$. There are two ways to label quasiparticles:

- We can consider only *spin-up* operators, as in (5.3.2). In this case, we get two solutions for each k vector: one with positive, and one with negative energy.

- Alternatively, we can re-label the negative-energy solutions (5.3.4) as annihilation operators $\gamma_{-k\downarrow}$. Then, for each k vector, we will have two quasiparticles $\gamma^+_{k\uparrow}$ and $\gamma^+_{k\downarrow}$, both with positive energies.

In any of these notations, the total number of quasiparticle states (the dimension of the Hilbert space) is the same as for original electrons: two single-particle states per k vector. We will use the second notation (with positive-energy quasiparticles).

It will also be convenient to normalize the coefficients so that

$$|u_k|^2 + |v_k|^2 = 1\,. \tag{5.3.5}$$

This would produce the canonical anticommutation relations for the quasiparticles:

$$\{\gamma_{k\alpha}, \gamma^+_{k'\beta}\} = \delta_{kk'}\delta_{\alpha\beta}\,. \tag{5.3.6}$$

The Hamiltonian (5.2.6) can now be written in terms of quasiparticles as

$$H_{\rm BCS} = \sum_k \tilde{\epsilon}_k \left(\gamma^+_{k\uparrow}\gamma_{k\uparrow} + \gamma^+_{k\downarrow}\gamma_{k\downarrow}\right) + E_0\,, \tag{5.3.7}$$

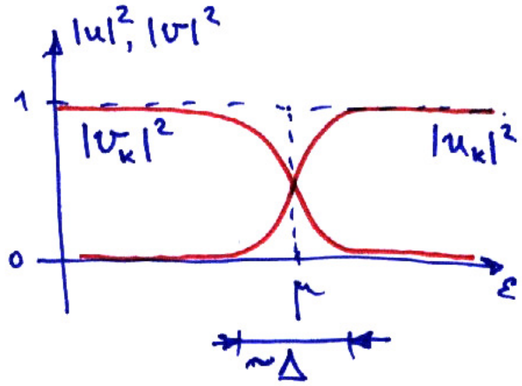

Figure 19: The coherence factors (5.3.11) as a function of energy.

The ground state of the superconductor $|\mathrm{GS}\rangle$ may be found from the condition that it contains no quasiparticles:

$$\gamma_{k\alpha}|\mathrm{GS}\rangle = 0\,. \tag{5.3.8}$$

Since sectors with different k vectors are decoupled in the Hamiltonian, this equation can be solved independently for each k vector:

$$|\mathrm{GS}\rangle_k = (u_k^* - v_k^* a_{k\uparrow}^+ a_{-k\downarrow}^+)|\star\rangle_k\,, \tag{5.3.9}$$

where $|\star\rangle$ is the state without electrons and the subscript k denotes that only states with a given k vector are considered. Combining all the k vectors together, we find the expression for the ground state of the superconductor:

$$|\mathrm{GS}\rangle = \prod_k (u_k^* - v_k^* a_{k\uparrow}^+ a_{-k\downarrow}^+)|\star\rangle\,. \tag{5.3.10}$$

Note that this state is a superposition of states with different numbers of particles.

If we calculate u_k and v_k explicitly from diagonalizing the matrix (5.3.3), we find

$$\begin{aligned} u_k &= e^{i\varphi}\sqrt{\frac{1}{2}\left(1+\frac{\epsilon_k-\mu}{\tilde{\epsilon}_k}\right)}\,, \\ v_k &= \sqrt{\frac{1}{2}\left(1-\frac{\epsilon_k-\mu}{\tilde{\epsilon}_k}\right)}\,, \end{aligned} \tag{5.3.11}$$

where φ is the phase of Δ. The absolute values of u_k and v_k are plotted in Fig. 19. We see that superconductivity changes the structure of the ground state only in the window of energies of the order Δ around the Fermi level (we usually have $\Delta \ll \mu$ in superconductors).

Problem Set 11

Problem 11.1

By diagonalizing the matrix in (5.3.3), derive the spectrum (5.3.4) and the eigenvectors (5.3.11).

Problem 11.2

(a) In superconductors, there is a characteristic length scale ξ called the *coherence length*. One of its possible definitions is the extent of the pair correlations. Consider the anomalous correlations in real space

$$\Delta(x-y) = \langle a_\downarrow(x) a_\uparrow(y) \rangle$$

It decays at a certain length scale ξ. Calculate this length in the BCS ground state.

Hint 1: In the BCS ground state, different wave vectors k are decoupled, so it is convenient to do a calculation at a given k vector, and then Fourier transform.

Hint 2: Only a vicinity of the Fermi surface contributes to this anomalous correlator, so you may linearize the electron spectrum near the Fermi surface.

Hint 3: You will find $\xi = v_F/\Delta$.

(b) For Aluminum, find in the literature the value of the gap Δ and estimate the superconducting coherence length ξ.