CHAPTER 2. THEORIES OF SUPERCONDUCTIVITY

§2.1. Bardin-Cooper-Schrieffer (BCS) theory

2.1.1. Main ideas and results.

As it was told in chapter 1, the microscopic theory explaining the nature of the phenomenon of superconductivity was created only in 1957, in 46 years after discovery of superconductivity.

The main result on which this theory was based - the effect of grouping of electrons in pairs - was opened by L. Cooper in 1956.

Cooper considered a behavior of two electrons at existence of an attraction between them when other electrons form the main state, i.e. like in normal metal, according to Pauli principle fill all sphere of Fermi.

Calculation showed that in this case the behavior of two interacting electrons sharply differs from behavior of these electrons if they are isolated from the others. In the presence of the filled Fermi sphere at any, as much as small, attraction these two electrons form the connected state which has smaller energy and is separated from the main state of normal metal by an energy gap. The connected pair possesses the smallest energy (i.e. a gap is maximum) when the electrons have anti-parallel spins and the equal, but oppositely directed momenta.

Bardin, Cooper and Schrieffer generalized Cooper's results on a case when all electrons are connected in pairs. Then each electron plays a double role. On the one hand, owing to Pauli principle it creates restrictions on possible values of wave vectors of other electrons that gives them the chance to be grouped in pairs. On the other hand, this electron itself is a part of one of pairs.

Thus, for an explanation of grouping of electrons in pairs it is necessary to find the possible reason of an attraction between electrons. The theoretical analysis showed that this attraction can be realized due to an exchange of phonons, i.e. due to the interaction of electrons with a crystal lattice. Such interaction can be presented as follows. In knots of a lattice there are positively charged ions. The electron attracts them to itself. Thus, in the area surrounding an electron there is a polarization of a lattice which is expressed in a congestion of the positive charges. The second electron which is nearby is attracted to this congestion, i.e. to the first electron. Considering a picture in dynamics, it is possible to tell that one electron in the process of its movement creates a flute on which it is favorable to second electron to move. It explains why most obviously the effect is shown for oppositely moving electrons - each of them moves in the track left by another one.

At first sight, there can be doubts in what the polarization can do. It is possible to understand that it reduces a force of repulsion, but whether it can replace repulsion with an attraction? For an assessment of its opportunities we consider interaction of a charged dot with a not charged sphere. It is clear that the polarization connected with redistribution of charges on a sphere will lead to an attraction. For compensation of this force it is necessary to place on a sphere some charge, of the same sign with the dot's one. Since the charge of a sphere is less than this value, the attraction of like electric charges takes place!

According to the theory of BCS, half-width of an energy gap at a zero temperature is defined by expression

$$\Delta(0) = 2\hbar\omega_D \exp\left(-\frac{1}{U \cdot N(E_F)}\right), \qquad (2.1)$$

where $U>0$ – the potential of electron-lattice interaction, $N(E_F)$ - the density of electronic states at the level of Fermi, ω_D - the Debye frequency of a crystal.

From expression (2.1) it is clear, why the theory of superconductivity has been creating so long. This expression can't expand in power series on small interaction of U. Therefore the perturbation theory which is usually used at calculation of changes in an electronic energy spectrum couldn't lead to the correct result, i.e. to the emergence of a gap.

From (2.1) an interesting conclusion can be made. In normal metals the stronger the interaction of electrons of conductivity with a lattice the higher is the resistance, i.e. the higher is U. In superconductors, the more U, the higher is the critical temperature. Thus, the more is a metal resistance in a normal state, the easier it passes into the superconducting state. However this regularity takes place only for metals with comparable concentration of electrons.

From detailed calculations it follows that the critical temperature is connected with half-width of an energy gap by the formula

$$3{,}5k_BT_C = 2\Delta, \qquad (2.2)$$

where k_B is the Boltzmann constant. Formula (2.2.) confirms the experimentally received communication (1.3).

The BCS theory shows that in order to create in a superconductor two unconnected electrons, i.e. two excited states, it is necessary to break off a Cooper pair, i.e. to spend a minimum energy 2Δ. It means that the minimum energy of one excitement (quasi-particle) is equal to Δ. Detailed calculation gives an expression for an energy of a quasi-particle with a momentum p

$$\varepsilon_p = \sqrt{\left(\frac{p^2}{2m} - \varepsilon_F\right)^2 + \Delta^2}, \qquad (2.3)$$

where ε_F - Fermi energy.

Theoretically received expression (2.3) coincides with a formula (1.6) on the basis of which the existence of not fading superconducting currents was proved in chapter 1. The same fact can be explained in a different way. Unlike electrons, which are fermions, i.e. having half-integer spins, a Cooper pair is a new particle having spin, equal to zero. Particles with integer spins are called bosons and submit to Bose-Einstein statistics. For them there is no Pauli ban. Moreover, all bosons seek to be in the same state. There is a so-called bose-condensation - all Cooper pairs drop out in "condensate", i.e. have all identical parameters. In particular, all Cooper pairs have an identical momentum. It would seem, there is nothing special in this fact, because every pair contains two electrons with oppositely directed momentums and therefore the momentum of each pair is equal to zero. However the situation changes if all set of pairs starts moving, for example, in an electric field. All pairs seek to have an identical momentum. It means that no one of them can be braked, transferring energy to a lattice, i.e. the transfer of a charge through a lattice goes without resistance.

The BCS theory explains the electronic spectrum of superconductors on the basis of what it is possible to predict practically all features of behavior of superconductors. It should be noted that in case of "low-temperature" superconductivity there is not only qualitative, but also quantitative consent of the theory and experiment. In the frame of this theory many properties of high-temperature superconductors can be explained as well, though the quantitative consent is not so good.

2.1.2. Cooper effect. Cooper pairs.

Let us consider the interaction of two electrons at completely filled Fermi sphere.

We will transfer the concept of quasi-particles used in normal metals to this case. Electronic states near Fermi level are similar to usual particles. Therefore it is natural to count energy from Fermi level. We have already spoken about it in §1.6.

We write down Schrödinger's equation for two interacting quasi-particles with the identical $|\vec{k}|$:

$$\left(H_0(\vec{r}_1)+H_0(\vec{r}_2)+U(\vec{r}_1;\vec{r}_2)\right)\Psi(\vec{r}_1;\vec{r}_2)=E\Psi(\vec{r}_1;\vec{r}_2) \qquad (2.4)$$

Here $H_0(\vec{r}_1)$ is a Hamiltonian of one free particle

$$H_0(\vec{r}_1)\psi_{\vec{k}}(\vec{r}_1)=|\xi_{\vec{k}}|\psi_{\vec{k}}(\vec{r}_1),$$

where the wave function for a free particle has an appearance

$$\psi_{\vec{k}}(\vec{r}_1)=V^{-1/2}\exp(i\vec{k}\vec{r}_1).$$

In the main state the total momentum and the spin have to equal to zero. Therefore we will construct a wave function in the form

$$\Psi(\vec{r}_1;\vec{r}_2)=V^{-1/2}\sum_{\vec{k}}c_{\vec{k}}\psi_{\vec{k}\uparrow}(\vec{r}_1)\psi_{-\vec{k}\downarrow}(\vec{r}_2) \qquad (2.5)$$

Substituting (2.5) in (2.4), we obtain

$$2|\xi_{\vec{k}}|c_{\vec{k}}+\sum_{\vec{k}'}U_{\vec{k}\vec{k}'}c_{\vec{k}'}=Ec_{\vec{k}} \qquad (2.6)$$

We consider the simple model:

$$U_{\vec{k}\vec{k}'}=\begin{cases}-\lambda & if \quad k_F-\omega_D/v_F<k,k'<k_F+\omega_D/v_F\\ 0 & beyond\ the\ diapazon\end{cases} \qquad (2.7)$$

Having introduced the notation:

$$I=\sum_{|\vec{k}'|=k_F-\omega_D/v_F}^{|\vec{k}'|=k_F-\omega_D/v_F}c_{\vec{k}'} \qquad (2.8)$$

we obtain

$$c_{\vec{k}}=\frac{\lambda I}{2|\xi_{\vec{k}}|-E}. \qquad (2.9)$$

Having substituted (2.9) in (2.8), we come to the equation of self-consistence

$$I=\sum_{|\vec{k}'|=k_F-\omega_D/v_F}^{|\vec{k}'|=k_F-\omega_D/v_F}\frac{\lambda I}{2|\xi_{\vec{k}}|-E} \qquad (2.10)$$

We are looking for the main state with <u>negative</u> energy. Having introduced the notation $E=-2\Delta$ and having transformed the sum to integral, we obtain

$$1=\lambda N(E_F)\ln\frac{\hbar\omega_D}{\Delta},$$

whence we come to the relation

$$\Delta=\hbar\omega_D\exp\left(-\frac{1}{\lambda N(E_F)}\right) \qquad (2.11)$$

We see that $\Delta\neq 0$ at any force of attraction.

2.1.3. Energy spectrum.

In the Cooper effect two interacting electrons differ from all others as they change the state and are grouped in pair. Other electrons remain in an initial state. Actually, it is necessary to consider reorganization of states of all electrons. Each of them, on the one hand, owing to Pauli principle, creates restrictions on possible values of wave vectors of other electrons that gives them the chance to be grouped in pairs. On the other hand, this electron itself is a part of one of pairs.

For calculation the energy spectrum we will use the method of secondary quantization, i.e. we will pass to the occupation-number representation. We should minimize free energy. We will calculate the energy of the main state for a case of an attraction of electrons. Not to add an additional condition of constancy of number of particles, we will count their energy from the chemical potential μ, i.e. $\xi_{\vec{k}} = \frac{\hbar^2 k^2}{2m} - \mu$.

As a model Hamiltonian of N electrons in a volume of V we will accept

$$H = \sum_{\vec{k},\sigma} \xi_{\vec{k}} a^+_{\vec{k},\sigma} a_{\vec{k},\sigma} - \frac{1}{2V} \sum_{\vec{k},\vec{k}',\sigma} U_{\vec{k}\vec{k}'} a^+_{\vec{k}',\sigma} a^+_{-\vec{k}',-\sigma} a_{-\vec{k},-\sigma} a_{\vec{k},\sigma}, \qquad (2.12)$$

where a^+ and a - operators of the creation and annihilation, $U_{\vec{k}\vec{k}'}$ - the matrix element of the energy of interaction of two electrons. The first member is the own energy of electrons. The second is the energy of interaction between electrons caused by an exchange of virtual phonons. In each member of the sum a pair of electrons with opposite spins (σ and $-\sigma$) and momentums ($\vec{k}$ and $-\vec{k}$) is destroyed and another pair is born with ($\vec{k}'$ and $-\vec{k}'$).

The members, differing only in values of spin, give an identical contribution in (2.12), therefore we can write down

$$H = 2\sum_{\vec{k}} \xi_{\vec{k}} a^+_{\vec{k},1/2} a_{\vec{k},1/2} - \frac{1}{V} \sum_{\vec{k},\vec{k}'} U_{\vec{k}\vec{k}'} a^+_{\vec{k}',1/2} a^+_{-\vec{k}',-1/2} a_{-\vec{k},-1/2} a_{\vec{k},1/2} \qquad (2.13)$$

The task of finding the ground state and the spectrum of excitations for the system with this Hamiltonian can be solved in the different ways: Bogolyubov transformation, summation of Feynman diagrams, method of spin analogy, etc. We will solve it by means of Bogolyubov canonical transformation - we will define quasi-particle operators $A_{\vec{k}0}, A_{\vec{k}1}$ by the following relations:

$$a_{\vec{k},1/2} = u_{\vec{k}} A_{\vec{k}0} + v_{\vec{k}} A^+_{\vec{k}1} \qquad a_{-\vec{k},-1/2} = u_{\vec{k}} A_{\vec{k}1} - v_{\vec{k}} A^+_{\vec{k}0} \qquad (2.14)$$

where $u_{\vec{k}}$ and $v_{\vec{k}}$ are the real functions symmetric with respect to the transformation $\vec{k} \to -\vec{k}$.

For all Fermi operators the commutation relations for anti-commutators have to be satisfied: $\{a_i^+ a_k\} = \delta_{ik}$, $\{a_i a_k\} = 0$, $\{a_i^+ a_k^+\} = 0$, and similarly for A. All of them are carried out, if the functions $u_{\vec{k}}$ and $v_{\vec{k}}$ meet the conditions:

$$u^2_{\vec{k}} + v^2_{\vec{k}} = 1 \qquad (2.15)$$

To check it, let us calculate, for example, the anti-commutator:

$$\left\{a_{\vec{k},1/2}a^{+}_{\vec{k},1/2}\right\}=u^2_{\vec{k}}\underbrace{\left\{A_{\vec{k}0}A^{+}_{\vec{k}0}\right\}}_{=1}+v^2_{\vec{k}}\underbrace{\left\{A^{+}_{\vec{k}1}A_{\vec{k}1}\right\}}_{=1}+u_{\vec{k}}v_{\vec{k}}\underbrace{\left\{A^{+}_{\vec{k}1}A^{+}_{\vec{k}0}\right\}}_{=0}+u_{\vec{k}}v_{\vec{k}}\underbrace{\left\{A_{\vec{k}1}A_{\vec{k}0}\right\}}_{=0}=u^2_{\vec{k}}+v^2_{\vec{k}}=1.$$

Then (2.13) will be transformed to a form:

$$H=E_0+H^0_0+H_1+H_2$$

where $E_0=2\sum_{\vec{k}}\xi_{\vec{k}}v^2_{\vec{k}}-\frac{1}{V}\sum_{\vec{k},\vec{k}',\sigma}U_{\vec{k}\vec{k}'}u_{\vec{k}'}v_{\vec{k}'}u_{\vec{k}}v_{\vec{k}}$ - (2.16)

a constant, not depending on fermi-operators and corresponding to the energy of the ground state;

$$H^0_0=\sum_{\vec{k}}[\xi_{\vec{k}}(u^2_{\vec{k}}-v^2_{\vec{k}})+\frac{2u_{\vec{k}}v_{\vec{k}}}{V}\sum_{\vec{k}}U_{\vec{k}\vec{k}'}u_{\vec{k}'}v_{\vec{k}'}](A^{+}_{\vec{k}0}A_{\vec{k}0}+A^{+}_{\vec{k}1}A_{\vec{k}1}) \text{ -} \qquad (2.17)$$

the diagonal part of the Hamiltonian;

$$H_1=\sum_{\vec{k}}[2\xi_{\vec{k}}u_{\vec{k}}v_{\vec{k}}-\frac{1}{V}(u^2_{\vec{k}}-v^2_{\vec{k}})\sum_{\vec{k}'}U_{\vec{k}\vec{k}'}u_{\vec{k}'}v_{\vec{k}'}](A^{+}_{\vec{k}0}A^{+}_{\vec{k}1}+A_{\vec{k}1}A_{\vec{k}0}) \text{ -} \qquad (2.18)$$

the off-diagonal part of the Hamiltonian containing the product of two Fermi operators. The operator H_2 contains the product of four new Fermi operators. In the study of low-energy excited states it can be omitted.

So far the functions $u_{\vec{k}}$ and $v_{\vec{k}}$ were arbitrary, on condition of (2.15). We will choose them so that to turn into zero the operator (2.18). For this purpose it is sufficient to require the equality

$$2\xi_{\vec{k}}u_{\vec{k}}v_{\vec{k}}=\frac{1}{V}(u^2_{\vec{k}}-v^2_{\vec{k}})\sum_{\vec{k}'}U_{\vec{k}\vec{k}'}u_{\vec{k}'}v_{\vec{k}'} \qquad (2.19)$$

It is possible to be convinced that this equality when performing (2.15) is at the same time a condition of a minimum of energy of the main state (2.16). One can ensure that this equality, when (2.15), is at the same time minimizing the energy of the ground state (2.16).

We introduce the notation: $\Delta_{\vec{k}}\equiv\frac{1}{V}\sum_{\vec{k}'}U_{\vec{k}\vec{k}'}u_{\vec{k}'}v_{\vec{k}'}.$ (2.20)

Then from (2.15) and (2.19) it is possible to express required $u_{\vec{k}}$ and $v_{\vec{k}}$ through $\xi_{\vec{k}}$ and $\Delta_{\vec{k}}$:

$$u^2_{\vec{k}}=\frac{1}{2}\left[1+\frac{\xi_{\vec{k}}}{\sqrt{\Delta^2_{\vec{k}}+\xi^2_{\vec{k}}}}\right];\qquad v^2_{\vec{k}}=\frac{1}{2}\left[1-\frac{\xi_{\vec{k}}}{\sqrt{\Delta^2_{\vec{k}}+\xi^2_{\vec{k}}}}\right] \qquad (2.21)$$

Having substituted (2.21) in (2.19), we will find the nonlinear equation defining $\Delta_{\vec{k}}$:

$$\Delta_{\vec{k}}=\frac{1}{2V}\sum_{\vec{k}'}\frac{U_{\vec{k}\vec{k}'}\Delta_{\vec{k}'}}{\sqrt{\Delta^2_{\vec{k}'}+\xi^2_{\vec{k}'}}} \qquad (2.22)$$

Substituting (2.20) and (2.21) in (2.17), it is possible to transform diagonal part of a Hamiltonian to the form

$$H^0_0=\sum_{\vec{k}}\sqrt{\xi^2_{\vec{k}}+\Delta^2_{\vec{k}}}\,(A^{+}_{\vec{k}0}A_{\vec{k}0}+A^{+}_{\vec{k}1}A_{\vec{k}1}) \qquad (2.23)$$

Thus, owing to interaction of electrons with each other the spectrum of elementary excitations has a form:

$$\varepsilon_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2} \qquad (2.24)$$

Each value of the quasi-momentum $\vec{k}$ corresponds to two types of excitations relating to the operators of creation $A_{\vec{k}0}^{+}$ and $A_{\vec{k}1}^{+}$.