

QUASIPARTICLES IN THE SUPERCONDUCTING STATE OF METALS

By

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To:

-Tewodros the second of Ethiopia and those who are right but born at the wrong time like him

and

- To my Father

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Abstract

The microscopic theory of the low temperature superconductivity is reviewed along with the mechanism of electron-electron interaction. We have investigated the electrical and magnetic properties of superconductors. Our current research, which is fully theoretical and analytical, is targeted in illustrating and explaining the quasiparticles in the superconducting states of a metal. In this work, a comparatively simple mathematical procedure is developed in finding the energy of the ground state of a superconductor, the energy gap and dispersion relation of the energy of the elementary excitations. We have shown that as the quasiparticles (electron like and hole like) have a fractional charge, depending on their energy.

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Addis Ababa, Ethiopia Abebe Fentie

Introduction

The history of low temperature physics as we understand it today may be said to have started with the successful liquefaction of helium at Leiden by H.Kamerlingh Onnes, in 1908. Then in 1911 H.Kamerlingh Onnes discovered the new phenomena of superconductivity while studying the resistivity of a metal at low temperature. Thus, Onnes observed that the electrical resistivity of pure mercury dropped abruptly up on cooling to below 4.2K.

Superconductors are characterized by many unique features, one of which is that when an external magnetic field is applied on it, there is no possibility of the magnetic field to penetrate the sample. This clearly shows that a superconductor behaves as diamagnetic. A sufficiently strong magnetic field destroys superconducting state of a metal. Furthermore, the critical temperature of superconductors varies with the isotopic mass of the constituent ions of the crystal lattice.

In 1957 Bardeen, Cooper and Schrieffer (BCS) theory achieved in explaining the microscopic means of superconductors. The central feature of this mechanism involves the electron-electron interaction via phonon exchange. Thus, two electrons attract each other with equal and opposite momentum and spins. The superconducting state is obtained when the electron-electron attraction via phonons dominate the coulomb repulsion.

Because of their unique characteristics, superconductors are widely used in many scientific areas such as in low-loss electron power transmission, magnetic levitation, biomagnetism, weak magnetic field measurements, and high magnetic field production for nuclear fusion reactor and acceleration of charged particles.

Even though superconductors are widely applied in many areas of science, there are some inconvenience to use them since they require low transition temperature. To put such materials into use, it is necessary to have liquid helium which is expensive to produce and to liquefy.

But these short comings are overcome by the discovery of high temperature superconductivity in 1986 by Bednorz and *Müller*, at 35K in "LBCO" (a mixed oxide of lanthanum, barium, and copper).

The main objectives of this work are, in the first place, the description of quasi particles in the superconducting state of metals while explaining the basic features of superconducting state by developing a comparatively simple procedure. Secondly, the review of the fundamental experimental facts of a superconductor and showing the relevant consequences of the electron-phonon interaction and the BCS theory.

The over all approach of this thesis is begun in Chapter 1 with a short summary of the experimental facts of superconductors and the expressions for some thermodynamic quantities such as entropy and specific heat are formulated with graphical demonstration.

In Chapter 2 the electron-phonon interaction is introduced using deformation potential method. While treating these interactions, the adiabatic approximation is taken in to account so as it enables us to simplify our task of calculating the interaction Hamiltonian by separating the electronic and ionic motions.

Chapter 3 is devoted to the microscopic theory of superconductivity, the BCS theory, which provided the first quantum theoretical understanding of superconductivity, 46 years after the experimental discovery of the phenomena. In this chapter, the effective electron-electron interaction Hamiltonian and the cooper pairing with the binding energy for the formation of these pairs are treated thoroughly. Further more, the superconducting ground state wave function formation and the energy it possesses are calculated then the fact in which the superconducting ground state energy is less than that of the normal state of a metal is mathematically verified. Finally, the gap that exists between the ground state and spectrum of excitations is estimated.

In Chapter 4, the main part of this work, which is about the quasi particles in superconducting states with their basic characteristics are introduced.

In the last chapter, conclusion of the work is presented. Appendices and references are given at the end.

Chapter 1

Survey of the experimental facts

Low temperature physics as we understand it today may be said to have started with the successful liquefaction of helium at Leiden by H.Kamerlingh Onnes, 1908. Onnes promptly used liquid helium in a variety of studies of metals at low temperatures and observed in 1911 that the electrical resistivity of a pure mercury dropped abruptly up on cooling to below 4.2K [1].

Onnes concluded that Mercury has passed into a new state with an account of its remarkable electrical properties, that may be called Superconductive state.

The temperature at which an abrupt transition from normal to superconducting state takes place is known as the critical temperature T_c of phase transition. The transitions to the superconducting state is a sharp one in bulk specimen. Above the critical temperature, T_c, the properties of the metal are completely normal. Below T_c, superconducting states are displayed as shown in Fig.1.1. Furthermore, the transition temperatures of the superconducting elements are different for different elements as given in Table.6.1 (Appendix C).

The most outstanding property of a superconductor is, of course, at least the complete disappearance of the electrical resistivity at some critical temperature T_c.

Thus, the resistance of the superconductors is absent at the level $10^{-24}\ \Omega/cm$. For instance, resistance of a pure copper at $T = 4.2K$ is of the order of $10^{-9}\ \Omega/cm$.

Superconductivity is a phenomena in which the second-order phase transition occurs for which a new state is formed. Which must be described in a very different fashion from that used in a normal metal [2].

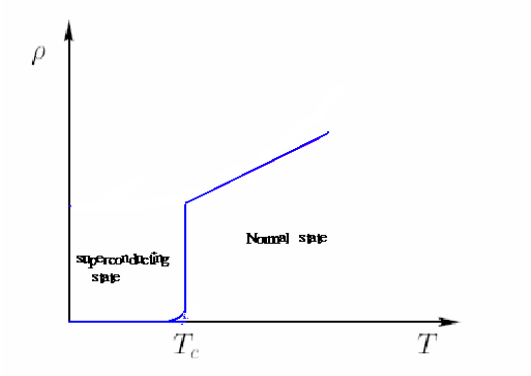


Figure 1.1: Resistance of a specimen versus absolute temperature.

1.1 Magnetic field and superconductivity

1.1.1 The critical magnetic field

Superconductivity can be destroyed by heating a sample to $T > T_c$ and a sufficiently strong magnetic field destroys it too. Therefore, the threshold or critical value of the applied magnetic field, $H_c(T)$, above which superconductivity is not observed, depends on temperature as experimentally verified and its dependence is given by a relation:

$$H_c(T) = H_c(0)[1 - (T/T_c)^2] \ , \tag{1.1.1}$$

where $H_c(0)$ is the critical magnetic field at absolute zero temperature. It is different for different elements and compounds as shown in Table.6.1 (Appendix C).

1.1.2 The Meissner-Ochsenfeld effect

As Meissner and Ochsenfeld discovered in 1933, superconductors are characterized by a property called diamagnetism. They discovered that if an external magnetic field B_a which is less than H_c is applied to a superconductor, a persistent current will be introduced in a direction which will oppose the effect of the applied field B_a (Lenz's Law) [3]. The field generated by this current will exactly cancel B_a and since it does not die away, the effective magnetic field within the superconductor, remains zero. This is a fundamental property called Meissner effect. It may be also demonstrated by cooling a superconductor which is initially in the field B_a above T_c until it is at a temperature T for which B_a is equal to H_c. At that point the field will be expelled so that $B = 0$. The demonstration of the above physical phenomena is shown below in Fig.1.2 [2].

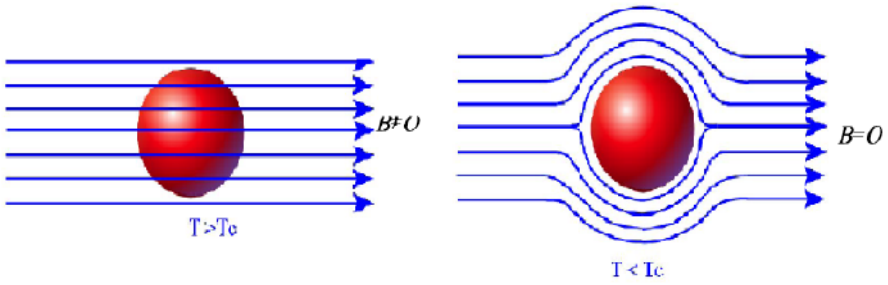


Figure 1.2: Meissner effect in a superconducting sphere cooled in a constant applied magnetic field. On passing below the transition temperature, the lines of induction B are ejected from the sphere.

1.1.3 Magnetic flux quantization

One of the remarkable phenomena associated with the superconducting state is the quantization of the magnetic flux through the superconducting ring. Experiments by Doll and Nabauer, and By Deaver and Faibanks (1961) [2,4], have shown that the flux Φ, which passes trough the ring, is quantized and can only take certain values [1,3]:

$$\Phi = n\Phi_0, \qquad n = 0, 1, 2... \tag{1.1.2}$$

$$\Phi_0 = \frac{\pi\hbar}{e} = 2.07 \times 10^{-7}\ Gauss\ cm^2\ , \tag{1.1.3}$$

where Φ_0 is the quantum of magnetic flux.

1.2 Thermodynamics of superconductors

Now we come to the thermodynamics treatment of superconductivity from which we can examine the type of transition and derive expressions which relate the entropy and the specific heat difference between the normal and superconducting states with the temperature variation of H_c. In a reversible change the transition from one phase to another occurs when the Gibbs free energy is the same in each phase. The free energy of the system has the form:

$$F_s(H_c) = F_s(0) + \frac{H_c^2}{8\pi}\ ,$$

where $F_s(0)$ is the free energy of the superconducting phase in zero magnetic field.

$F_s(H_c)$ is the free energy at transition and so it is the same for both the normal and superconducting states at H_c [2,4].

Thus, the free energy difference between two states at a temperature T is given by

$$F_n(T) - F_s(T) = \frac{H_c^2}{8\pi} \tag{1.2.1}$$

Therefore, the internal energy difference between two states is $\frac{H_c^2}{8\pi}$.

Since the entropy, S, is obtained from the free energy as

$$S_n = -\frac{\partial F_n}{\partial T}$$

$$S_s = -\frac{\partial F_s}{\partial T}$$

$$\triangle S = S_s - S_n = \frac{\partial}{\partial T}(\frac{H_c^2}{8\pi}) \tag{1.2.2}$$

$$\triangle S = \frac{H_c}{4\pi}\frac{dH_c}{dT} \tag{1.2.3}$$

As we know from statistical physics, entropy is defined as the degree of disorder of the system. After substituting (1.1.1) into (1.2.3), we observe that $\triangle S$ is negative. This implies that the entropy of the superconducting state is less than that of the normal states, i.e. the superconducting state is one of greater order. It is useful to note that the difference in entropy vanishes at two extreme temperatures, namely at zero temperature(third law of thermodynamics) and at the critical temperature. The transition from normal to superconducting state is shown clearly by discontinuity in the specific heat. The specific heat is defined as :

$$C = T\frac{\partial S}{\partial T} \tag{1.2.4}$$

in account of $S_n = -(\frac{\partial F_n}{\partial T})$ and $S_s = -(\frac{\partial F_s}{\partial T})$ the change in specific heat of the superconducting state with respect to the normal state is

$$C_s - C_n = \frac{T}{4\pi}[(\frac{dH_c(T)}{dT})^2 + H_c(T)\frac{d^2H_c(T)}{dT^2}] \tag{1.2.5}$$

Hence H_c vanishes at the critical temperature, we have

$$C_s - C_n = [\frac{T}{4\pi}[(\frac{dH_c(T)}{dT})^2]]_{T=T_c} \tag{1.2.6}$$

Thus, there is a discontinuity in the specific heat and which is called Specific heat jump and shown in Fig.1.3. Below T_c experiments predict an exponential dependence of C_s on T but above T_c it is linear and the over all picture is plotted here.

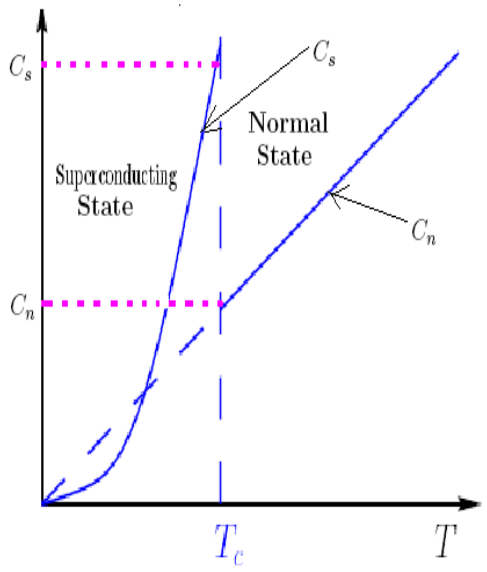


Figure 1.3: Schematic behavior of the specific heat. It shows a sudden jump at T_c.

1.3 Isotopic effect

The various phenomenological treatments based on their empirical characteristics of a superconductor provides an astonishingly complete macroscopic description of the superconducting phase. However, they do not give any clear indications as to the microscopic nature of the phenomenon [5].

One of the first such clues arose through the simultaneous and independent discovery in 1950 by Maxwell and by Ronalds et al [6]. It was shown that the critical temperature of superconductors varies with the isotopic mass of constituent atoms by the relation:

$$T_c M^{\alpha} = Constant \ , \tag{1.3.1}$$

where M is the isotopic mass and α is close to 0.5.

This is a hint that the lattice takes part in forming of the superconducting state with phonon frequency $\omega_k \sim 1/M^{1/2}$ [7,8].

Chapter 2

Electron-Phonon Interactions

In this section, we shall discuss the mutual interaction of the phonons and electrons. The theory of electrical conductivity of metals first developed by the Bloch electrons are considered to move freely through the lattice except for occasional scattering by the lattice vibration. This scattering is connected with vibrational quantum [9,10]. The word polaron is used to describe a single electron which is coupled to phonons [11,12,13].

The electron and phonon coupling has the chief effects on the properties of solids : It causes electrons to scatter from one state k to another $k^{'}$ leading to electrical resistivity. The basic interaction responsible for superconductivity appears to be that of the pair of electrons by means of an interchange of virtual phonons [14]. In other words this is to mean that the lattice is distorted by a moving electron, this distortion giving rise to a phonon. A second electron some distance away is in turn affected when it is reached by the propagating fluctuation in the lattice charge distribution. That is an electron of wave vector k emits a virtual phonon of wave vector, q, that is absorbed by an electron of wave vector $k^{'}$. Thus, the scattering phenomena in which k into k-q and $k^{'}$ into $k^{'} + q$ will happen as displayed in Fig. 3.1 [6].

2.1 The interaction Hamiltonian

In this subsection, we are going to derive the electron-phonon interaction Hamiltonian by considering the full Hamiltonian of the system and taking the adiabatic approximation in to account. This approximation principle is important because it allows us to separate ionic from electronic motion by leaving only a residual interaction between the electrons and the phonons [15,16].

Thus, the total Hamiltonian of the crystal can be separated into H_p , H_e , H_{e-p} and it has assumed to have the form

$$H = H_p + H_e + H_{e-p} \ , \tag{2.1.1}$$

where H_p describes the normal modes of vibration of the lattice that is the phonon Hamiltonian,

$$H_p = \sum_q \hbar\omega_q [a_q^+ a_q + \frac{1}{2}] \tag{2.1.2}$$

The second term in (2.1.1) involves electrons only and is given by :

$$H_e = \sum_k \epsilon_k c_k^+ c_k \ , \tag{2.1.3}$$

where (a_q^+, a_q) and (c_q^+, c_q) are the creation and annihilation operators of phonons and electrons, respectively.

The last term in (2.1.1) is due to the interaction between the electrons and phonons and written as

$$H_{e-p} = \sum \tilde{V}_{e-p}(r) \tag{2.1.4}$$

Now let us express H_{e-p} explicitly in the coming steps. If the interaction potential between the electrons at r_i and the ion at R_n be

$$V_{e-i} = V_{e-i}(r_i - R_n) \tag{2.1.5}$$

The total potential energy of the interaction of the electron at r_i and the lattice becomes:

$$V(\vec{r_i}) = \sum_n V_{e-i}(r_i - R_n) \tag{2.1.6}$$

If we now allow the α^{th} atoms to move from the equilibrium position by a displacement of an amount, $\vec{u}_{\alpha n}$, the new position of the ion will be

$$R_n = R_n^{(0)} + \vec{u}_{\alpha n} \ , \tag{2.1.7}$$

where $R_n^{(0)}$ is the equilibrium position of the ion in the crystal.

Moreover, from the relation between creation and annihilation operators of phonons and the displacement fields, we can obtain the following relationships:

$$\vec{u}_{\alpha n}(k) = \sum_{jk} [\frac{\hbar}{2M_\alpha N\omega_j(k)}]^{\frac{1}{2}} \vec{e}_\alpha(k)\{\hat{a}_j(k)e^{\ ik.R_n^{(0)}} + \hat{a}_j^+(k)e^{\ -ik.R_n^{(0)}}\} \ , \tag{2.1.8}$$

where $a_j(k)$ and $a_j^+(-k)$ are the annihilation and creation operators of the phonon respectively, $\omega_j(k)$ is the phonon frequency, j is the number of vibrational branches, M_α is the mass of the α^{th} atom, N is the number of primitive cells in the crystal, $e_\alpha(k)$ is the polarization vector of the vibration that determines the direction of the vibration of the α^{th} atom and $R_n = n_1\vec{a_1} + n_2\vec{a_2} + n_3\vec{a_3}$ is the lattice site.

Therefore, after some mathematical manipulation, the electron-phonon interaction Hamiltonian becomes:

$$H_{e-p} = \sum_{q,p,G} c_{p+q+G}^+ c_p V_{e-i}(q+G)[\frac{\hbar}{2M_\alpha N\omega_j(q)}]^{\frac{1}{2}} \vec{e}_\alpha.(q+G)[a_j(q+G) + a_j^+(-q-G)] \tag{2.1.9}$$

However, it is difficult and complicated to determine the interaction potential between the electrons and the ions in the crystal, V_{e-i}, in (2.1.9). Below we replace the original physical situation by some model, to obtain the interaction potential interms of physically measurable and experimentally determined parameters. One of the methods is the deformation potential and we shall discuss it in the next section [15].

2.2 The method of the deformation potential

Deformation potential method has been first justified by Bardeen and Schockley. While applying this method, the limit that only phonons whose wave length is long compared to the lattice spacing is considered and accurate results can be obtained. In this situation, the system of solid vibrations is treated as an elastic continuum and their effects can be described by applying the theory of deformation of an elastic media. The basic idea is that if the solid is subjected to a (tensor) strain, $U_{\alpha\beta}$, which is a function of position, there will be a change in energy of each electronic state which is proportional to the strain [11,15,17].

Thus, the elastic continuum can be described with the help of the deformation tensor as:

$$U_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right) , \tag{2.2.1}$$

where $u_{\alpha(\alpha=x,y,z)}$ is the displacement of the elastic media under the deformation.

The deformation potential method implies, the position of the conduction band

shift under strain. For small deformation, we can assume the energy shift :

$$E_c(U_{\alpha\beta}) = E_c(0) + \sum_{\alpha\beta} C_{\alpha\beta} U_{\alpha\beta} \ , \tag{2.2.2}$$

where $C_{\alpha\beta}$ is coefficient of the crystal and if we take a cubic crystal the coefficient becomes $\epsilon_1 \delta_{\alpha\beta}$. Thus equation (2.2.2) becomes:

$$E_c(U_{\alpha\beta}) = E_c(0) + \epsilon_1(\nabla.u) \ , \tag{2.2.3}$$

where $u_{\alpha\beta}$ is the displacement of an atom in the lattice vibration as given by (2.1.8). After combining (2.1.8) and (2.2.3) we have that

$$E_c(u_{\alpha\beta}) = E_c(0) + i\epsilon_1\{\sum_{jq}[\frac{\hbar}{2M_\alpha N\omega_j(q)}]^{\frac{1}{2}} \vec{e}_\alpha.\vec{q}[\hat{a}_j(q)e^{\ iq.R_n^0} - a_j^+(q)e^{\ -iq.R_n^0}]\} \tag{2.2.4}$$

Hence $\epsilon_1(\nabla.u)$ acts as a deformation field, it possess the form:

$$\vec{U}(r) = \epsilon_1(\nabla.u)$$

$$= i\epsilon_1 \sum_{jq}[\frac{\hbar}{2M_\alpha N\omega_j(q)}]^{\frac{1}{2}} \vec{e}_\alpha.\vec{q}[a_j(q)e^{\ iq.R_n^0} - a_j^+(q)e^{\ -iq.R_n^0}] \tag{2.2.5}$$

If we assume only one particle per unit cell and consider the long wave length approximation, we take the lattice as a continuum and the longitudinal vibration. so that

$$\vec{U}(\vec{r}) = i\epsilon_1 \sum_{q}[\frac{\hbar}{2M_\alpha N\omega(q)}]^{\frac{1}{2}} q[\hat{a}_q e^{\ iq.r} - \hat{a}_{-q}^+ e^{\ -iq.r}] \tag{2.2.6}$$

Furthermore, this deformation field will interact with electrons in the lattice then

$$\vec{U}(\vec{r_1}, \vec{r_2}, ...\vec{r}_N) = \sum_{i=1}^{N} \vec{U}(\vec{r_i}) \ , \tag{2.2.7}$$

where $\vec{U}(\vec{r_i})$ is the one particle operator.

Now let us expand the field operators $\Psi(r)$ and its conjugate $\Psi^+(r)$ interms of the

basis set as :

$$\Psi(r) = \sum_k c_k \Phi_k(r)$$
$$\Psi^+(r) = \sum_k c_k^+ \Phi_k^*(r) \ ,$$

where c_k^+ and c_k are the creation and annihilation operators of electrons respectively. Moreover, let us consider $\Phi_k(r)$ be the plane wave of a free electron in a box of volume V such that

$$\Phi_k(r) = \frac{1}{\sqrt{V}} \exp(ik.r)$$
$$\Phi_k^+(r) = \frac{1}{\sqrt{V}} \exp(-ik.r)$$

Then the Hamiltonian of the electron-phonon interaction in second quantized form becomes :

$$H_{e-p} = \int \Psi^+(r) U(r) \Psi(r) d^3r$$
$$= i\epsilon_1 \sum_{k,k',q} \frac{q}{V} [\frac{\hbar}{2M_\alpha N\omega(q)}]^{\frac{1}{2}} \int d^3r c_{k'}^+ e^{\ -ik'.r} [\hat{a}_q e^{\ iq.r} - \hat{a}_{-q}^+ e^{\ -iq.r}] c_k e^{\ ik.r}$$
$$= i\epsilon_1 \sum_{k,k',q} \frac{q}{V} [\frac{\hbar}{2M_\alpha N\omega(q)}]^{\frac{1}{2}} \int d^3r [c_{k'}^+ \hat{a}_q c_k e^{\ i(k-k'+q).r} - c_{k'}^+ \hat{a}_{-q}^+ c_k e^{\ i(k-k'-q).r}] \quad (2.2.8)$$

Remark : $\hat{a}_q^+$ refers to the longitudinal phonons of wave vector q and the integral in (2.2.8) vanishes unless

$$k - k' \pm q = \begin{cases} 0, \\ \text{vector in the reciprocal lattice}, otherwise \ , \end{cases}$$

where vector in the reciprocal lattice is to mean that a vector connecting two lattice points of the reciprocal lattice. But for plane waves the only possibility exists if $k - k' \pm q$ is zero (i.e $k' = k \pm q$) [11]. Thus,

$$H_{e-p} = i\epsilon_1 \sum_{k,q} \frac{q}{V} [\frac{\hbar}{2M_\alpha N\omega(q)}]^{\frac{1}{2}} \int d^3r [c_{k+q}^+ c_k \hat{a}_q - c_{k-q}^+ c_k \hat{a}_{-q}^+]$$

$$= i\epsilon_1 \sum_{k,q} \mid q \mid [\frac{\hbar}{2M_\alpha N\omega(q)}]^{\frac{1}{2}}[c^+_{k+q}c_k\hat{a}_q - c^+_{k-q}c_k\hat{a}^+_{-q}]$$

$$= i\epsilon_1 \sum_{k,q} \mid q \mid [\frac{\hbar}{2M_\alpha N\omega(q)}]^{\frac{1}{2}}[\hat{a}_q - \hat{a}^+_{-q}]c^+_{k+q}c_k \tag{2.2.9}$$

This can be equivalently written as

$$H_{e-p} = i\sum_{k,q} Dc^+_{k+q}c_k[\hat{a}_q - \hat{a}^+_{-q}] \ , \tag{2.2.10}$$

where, $D = \epsilon_1 \mid q \mid [\frac{\hbar}{2M_\alpha N\omega(q)}]^{\frac{1}{2}}$

The electron-phonon interaction (2.2.10) will be used further to show the possibility of the electrons to attract each other as we shall discuss in chapter three.

Chapter 3

Microscopic Theory of Superconductivity

After the discovery of an isotopic effect, it became clear that superconductivity is not only an electronic phenomenon but the lattice vibration has its own significant impact in explaining superconductivity [9]. Consequently, the theory of superconductivity is presented on the basis of which the interaction between electrons through the exchange of virtual phonons is attractive [18].

The microscopic theory of superconductivity was developed and formulated by Bardeen, Cooper and Schrieffer and presented by their classic paper in 1957. Then it is entitled as BCS theory, after its founders [5,19,20]. The theory allows for a calculation of several features related to the transition to superconductivity like isotopic effect and also features related to the ground-state like the opening of the gap in the one particle excitation spectrum.

In the next sections, we shall have a brief review of some fundamentals that enables one to explain the BCS theory, such as effective electron-electron interaction, cooper pairing, the superconducting ground state and its energy, and elementary excitations with the energy gap,density of states and coherence length.

3.1 Effective electron-electron interaction

In this subsection, we shall see the possibility of obtaining the effective electron-electron interaction from the electron-phonon interaction. The full Hamiltonian of the system of the lattice is

$$H = H_0 + H_{e-p} \ , \tag{3.1.1}$$

where H_0 is the Hamiltonian of the free electrons and phonons.
H_{e-p} represents the Hamiltonian of the electron-phonon interaction as calculated by deformation potential method. That is given by

$$H_{e-p} = i \sum_{k,q} D c^{+}_{k+q} c_k [\hat{a}_q - \hat{a}^{+}_{-q}] \tag{3.1.2}$$

In the first order H_{e-p} leads scattering and electrical resistivity. But the coupling of the two electrons is resulted from the second order H_{e-p}. In this case a phonon is created or annihilated in a scattering process with an electron. However, after a phonon is, e.g, created, it can be annihilated by another scattering process with an electron. The corresponding diagram is shown in Fig.3.1. Thus, a phonon is exchanged by the two electrons giving rise to an effective interactions [6,9,11,16,21].

Since our objective here is to obtain the effective electron-electron interaction from the electron-phonon interaction, we need to eliminate the first order term from the Hamiltonian and for doing this, we shall make a canonical transformation in which the canonical commutation relations of operators is preserved [11,22,23].

Then after some mathematical formulation (Appendix A), the electron-electron

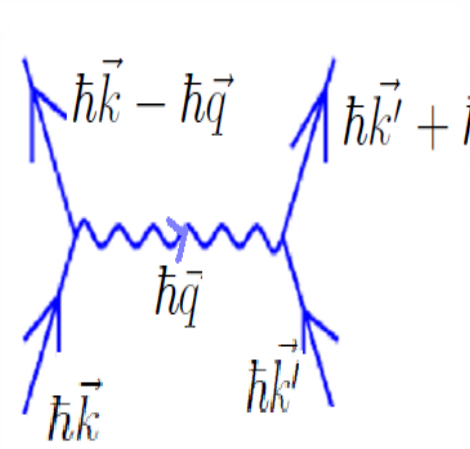


Figure 3.1: Effective electron-electron interaction through the exchange of phonons. Solid lines correspond to electrons and wave lines to phonons with momenta $\hbar\vec{k}$, $\hbar\vec{k} - \hbar\vec{q}$ and $\hbar\vec{k'}$, $\hbar\vec{k'} + \hbar\vec{q}$, where $\hbar\vec{q}$ is phonon momentum.

interaction through the exchange of phonons can be written as:

$$H_{e-e} = D^2 \sum_{k,k',q} c^+_{k'+q} c_{k'} c^+_{k-q} c_k [\frac{\hbar\omega_q}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2}] \tag{3.1.3}$$

From equation (3.1.3) we can observe that the electron-electron interaction is attractive for energies $|\epsilon_{k\pm q} - \epsilon_k| \leq \hbar\omega_q$ and repulsive otherwise. This energy must be compared with the energy of Coulomb repulsion at large D and it can be dominate over the Columbic repulsion and electrons with opposite spins and momentum can create the so called cooper pairs (see section 3.2).

However, in superconductors the attraction is dominant when $E_F - \hbar\omega_D < \epsilon_k$ and $\epsilon_{k\pm q} < E_F + \hbar\omega_D$. Therefore, the repulsive region of (3.1.3) is of little interest in the attraction process. So we can drop the repulsive parts from the Hamiltonian and

(3.1.3) have the form:

$$H_{e-e} = -V \sum_{k,k',q} c^{+}_{k'+q} c_{k'} c^{+}_{k-q} c_k \ , \tag{3.1.4}$$

where, $-V = D^2 \sum_q \frac{\hbar\omega_q}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2}$.

Finally, the reduced (or pairing) Hamiltonian of the system becomes:

$$\tilde{H}_{BCS} = \sum_{k\sigma} \epsilon_k n_{k\sigma} - V \sum_{k,k'} c^{+}_{k\uparrow} c^{+}_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow} \ , \tag{3.1.5}$$

where $n_{k\sigma}$ is occupation number operator and V is the coupling potential.

The first term is the kinetic energy of the electrons that are assumed to lie above the Fermi surface ($\epsilon_k = \frac{\hbar^2 k^2}{2m} - \epsilon_F$) and the second is the interaction term.

3.2 Cooper pairing

The most important process in the theory of superconductivity is the formation of cooper pairs. Which was first suggested by cooper who showed that fermions, interacting above the closed Fermi sea, will shown an instability towards the formation of the bound state despite the weakness of the attractive interaction as long as the interaction is attractive [6,24].

The possibility of electrons to attract each other is unusual physical phenomena. So, to understand this, let us switch on the attractive interaction energy between the pair of electrons just above the Fermi surface. Since this energy is associated with the effective attraction between electrons, its contribution will be negative and the total energy of the system will be reduced. While the interaction energy is switched on the scattering of electron from the state (k_1, k_2) to the state (k_1', k_2') with an account of the momentum conservation law defined by

$$k_1 + k_2 = k_1' + k_2' \tag{3.2.1}$$

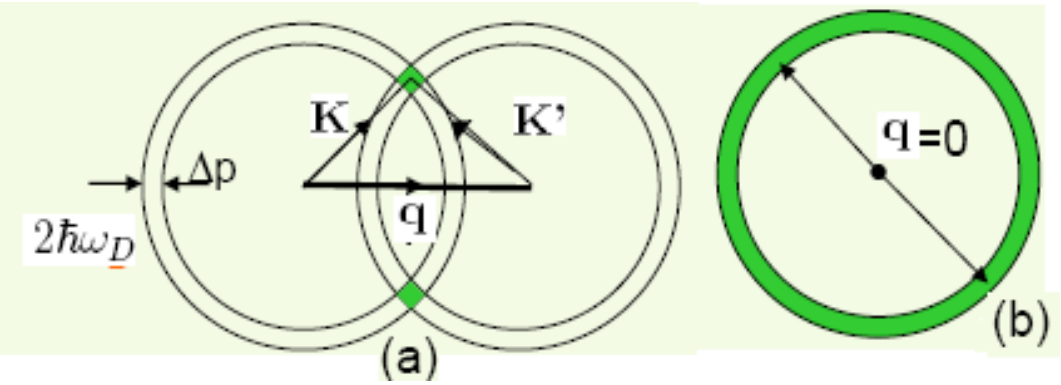


Figure 3.2: (a) The shaded part is the region in which the paired electrons satisfy the conservation of momentum relation, (b)Region of attraction around the Fermi surface due to the electron-phonon coupling.

Having made such a transition, we need to specify possible values of (k_1, k_2) which satisfy equation (3.2.1) and to restrict these values, let us construct a concentric circles of radii $k_F + \delta$ and $k_F - \delta$ and consider that $k_1 + k_2 = q$ as shown in Fig.3.2a. Thus, only electrons occupying the k state in the shaded region of the momentum space are allowed to participate in the transitions.

At $q \rightarrow 0$ the shaded area considerably increases and a maximum electrons are paired. Consequently all states with a band width $\sim 2\hbar\omega_D$ near the Fermi surface will contribute to the reduction of the average energy (Fig.3.2b), that is the electrons that participate in the transition form the bound state with binding energy less than the Fermi energy. To verify this let us consider a complete set of two electrons system that satisfy the periodic boundary condition in a cube of unit volume, then the plane-wave product function of the pair (where electrons are assumed to have opposite spin)

has the form [6,9,15,21]:

$$\Psi(k_1, k_2, r_1, r_2) \propto e^{\,i(k_1.r_1+k_2.r_2)} \tag{3.2.2}$$

Introduce the center of mass and relative coordinates $R = \frac{1}{2}(r_1 + r_2), r = r_1 - r_2, K = k_1 + k_2, k = \frac{k_1 - k_2}{2}$ and letting the kinetic energy of the two electron system be

$$\epsilon_{k_1} + \epsilon_{k_2} \Rightarrow \epsilon_k + \epsilon_K = \frac{\hbar^2}{2m}(K^2/4 + k^2) \tag{3.2.3}$$

Since the largest number of possible transitions yielding the most appreciable lowering of energy is obtained by pairing all possible states such that their total momentum vanishes (i.e., $q \to 0$) this implies $k_1 = -k_2$ [6]. Thus, if the pairing electrons are subjected to an interaction, they will posses a binding energy (Appendix B) of the form:

$$\Delta = \frac{2\hbar\omega_D}{\exp(\frac{1}{N(0)V}) - 1}\ , \tag{3.2.4}$$

where ω_D is the Debye frequency. Following the result (3.2.4), we need to see the two possibilities:

- When $V \to 0$, we obtain $2E_F = \epsilon$ that is the energy of the electrons at the Fermi surface.

- When $V \neq 0$, we have that $\epsilon < 2E_F$, that is the energy of the electrons is lower by the formation of a bound pair state.

Therefore, we can conclude that electrons lower the energy of the system by forming the so called cooper pairs and the binding energy for these pairs is given by equation (3.2.4). Cooper pairs condense to form a macroscopic quantum state. The reason for this is that cooper pairs, being formed of two fermions with opposite momenta and spins, behave like bosons having zero spin. They form a single coherent quantum

state called superconducting Condensate that is responsible for all superconducting phenomenon in elements and compounds exhibiting isotopic effect.

3.3 The superconducting ground state

In normal metals, the ground state at $T = 0K$ is characterized by lowest energy of states in k-space. In these states all electron states inside the Fermi surface are completely occupied while others out side it are empty. Since there is no attractive interaction (i.e. zero potential), the kinetic energy of such a state ($\epsilon_k = \frac{\hbar^2 k_F^2}{2m}$) is minimum.

However, as we have discussed in section 3.2, after the interaction potential is switched on, the Fermi sphere with all states below the Fermi level occupied and empty out side it, no longer represents a state of minimum energy at $T = 0K$. Hence, the superconducting ground states are formed following the formation of the pairs.

So far, we have discussed that the Fermi sea is unstable against the formation of cooper pairs having zero spin. The pairs condense on the lowest energy level. The ground state wave function as proposed by BCS theory takes the form:

$$|\Phi_0\rangle = \prod_k (u_k + v_k b_k^+)|0\rangle \ , \tag{3.3.1}$$

where $b_k^+ = c_{k\uparrow}^+ c_{-k\downarrow}^+$ is the creation operator of cooper pairs, $|0\rangle$ is the vacuum state with no particle present, u_k and v_k are some variational parameters [21].

In this work, we use a comparatively simple procedure for obtaining the ground state energy of a superconductor without using the wave function given by equation (3.3.1).

From quantum mechanics, we know that any function can be presented as

$$\Psi = \sum_n a_n \psi_n \ , \tag{3.3.2}$$

where a_n is the amplitude of the state ψ_n, $|a_n^2|$ is the probability to find the system in the state ψ_n.

The average energy of the system is

$$\bar{E} = \int \Psi^* \hat{H} \Psi d\tau = \bar{E}_{kin} + \bar{V} \ , \tag{3.3.3}$$

where

$$\bar{V} = \int \Psi^* V \Psi d\tau = \sum_{nm} a_n^* a_m V_{nm} \tag{3.3.4}$$

Here V_{nm} is the matrix element for the transition from state Ψ_m to state Ψ_n :

$$V_{nm} = \int \psi_n^* V \psi_m d\tau \tag{3.3.5}$$

We assume that all possible states depicted in Fig.3.3, are a complete set of functions. The wave function of the ground state of a superconductor can be expanded over these functions. Consider the scattering of a pair of electrons with $(\vec{k} \uparrow, -\vec{k} \downarrow)$ into state $(\vec{k'} \uparrow, -\vec{k'} \downarrow)$. Below, we omit arrows denoting spins. The scattering process is possible if in the state Ψ_n, the cell $(\vec{k}, -\vec{k})$ is occupied and the cell $(\vec{k'}, -\vec{k'})$ is free. At the same time in the state Ψ_m the cells $(\vec{k}, -\vec{k})$ is empty and $(\vec{k'}, -\vec{k'})$ is occupied.

Now if we introduce the probability v_k^2 that the cell $(\vec{k}, -\vec{k})$ is occupied, the amplitude of the state, ψ_n corresponding to this probability will be

$$a_n = [v_k^2(1 - v_{k'}^2)]^{1/2} = v_k u_{k'} \ , \tag{3.3.6}$$

where $u_{k'}^2 = 1 - v_{k'}^2$ is the probability that the cell $(\vec{k'}, -\vec{k'})$ is empty.

By analogy, the amplitude of the state, ψ_m, corresponding to the probability, u_k^2

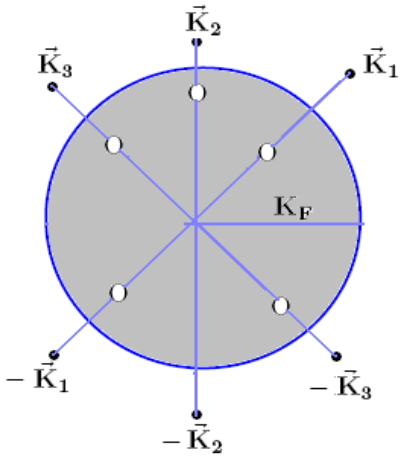


Figure 3.3: The state with total energy smaller than the state with cells $k < k_F$ are occupied and $k > k_F$ are empty.

becomes:

$$a_m = [v_{k'}^2(1 - u_k^2)]^{1/2} = v_{k'}u_k \tag{3.3.7}$$

Thus, the total energy of the superconducting state will be

$$E_s = 2\sum_k \xi_k v_k^2 - V\sum_{kk'}{}' v_{k'}u_k v_k u_{k'} \tag{3.3.8}$$

Provided that $\xi_k = \epsilon_k - E_F$, the coefficient 2 appears in (3.3.8) because the sum is over pair of states $(\vec{k}, -\vec{k})$ and V is the coupling potential.

The first term in (3.3.8) is the kinetic energy of the system, the second term is the potential energy with account of attraction between electrons in the layer $[-\hbar\omega_D, \hbar\omega_D]$ on the Fermi surface.

Now the problem is to minimize the energy E_s as a function of the variational parameters u_k and v_k.

The minimum of (3.3.8), we find from the condition $\frac{\partial E_s}{\partial v_k^2} = 0$:

$$\frac{\partial E_s}{\partial v_k^2} = 2\xi_k - V\frac{1-2v_k^2}{u_k v_k}\sum_{k'}{}' v_{k'}u_{k'} = 0 \tag{3.3.9}$$

Define the quantity,

$$\Delta_0 = V\sum_{k'}{}' v_{k'}u_{k'} \tag{3.3.10}$$

Then we obtain,

$$\frac{u_k v_k}{1-2v_k^2} = \frac{\Delta_0}{2\xi_k} \tag{3.3.11}$$

That gives a quadratic equation

$$v_k^4 - v_k^2 + \frac{\Delta_0^2}{4E_k^2} = 0 \tag{3.3.12}$$

with

$$E_k = \sqrt{\Delta_0^2 + \xi_k^2} \tag{3.3.13}$$

Finally, its solution is

$$v_k^2 = \frac{1}{2}(1 - \frac{\xi_k}{E_k}) \tag{3.3.14}$$

From the relation $u_k^2 + v_k^2 = 1$, we have that

$$u_k^2 = \frac{1}{2}(1 + \frac{\xi_k}{E_k}) \tag{3.3.15}$$

Thus, the dependence of v_k^2 on k is plotted in Fig.3.4.

From the relations (3.3.14) and (3.3.15), we observe that for electronic energies $\xi_k << \Delta_0$, the occupation probability $v_k^2 \approx 1$ where as $u_k^2 \approx 0$. This implies that electrons of energies which is less than the Fermi energy are the same as that of normal metal electrons. On the other hand for $\xi_k >> \Delta_0$, the occupation probability

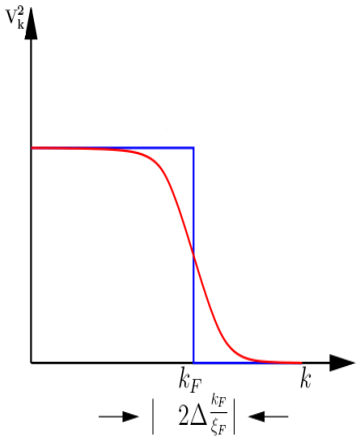


Figure 3.4: The probability distribution function v_k^2 and its dependence on k. The large variation in momentum space occurs in the interval $\triangle k$.

$v_k^2 \approx 0$ where as $u_k^2 \approx 1$. Which implies that electrons characterized by energies above the Fermi energy do not contribute for the superconducting ground state wave function formation [3,21,25].

Once we obtained u_k and v_k , we can go back to express Δ_0 as

$$\Delta_0 = V \sum_k [\frac{1}{4}(1 - \frac{\xi_k}{E_K})(1 - \frac{\xi_k}{E_K})]^{1/2}$$

$$\Delta_0 = \frac{V}{2} \sum_k \frac{\Delta_0}{E_k}$$

It follows that

$$1 = \frac{V}{2} \sum_k \frac{1}{E_k} \tag{3.3.16}$$

Thus, the integral equivalent of (3.3.16) over ε with the density of states at the energy, $N(\varepsilon)$ is

$$1 = \frac{V}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} N(\varepsilon) \frac{d\varepsilon}{\sqrt{\Delta_0^2 + \varepsilon^2}} \tag{3.3.17}$$

Because $\hbar\omega_D << \xi_F$, we can replace $N(\varepsilon)$ by N (0) which is the density of states at the Fermi level. Then (3.3.17) takes the form:

$$1 = VN(0)\int_0^{\hbar\omega_D} \frac{d\varepsilon}{\sqrt{\Delta_0^2 + \varepsilon^2}} \tag{3.3.18}$$

Evaluating the integral

$$\frac{\hbar\omega_D}{\Delta_0} = \sinh(1\backslash N(0)V)$$
$$= \frac{1}{2}[e^{\ 1/N(0)V} - e^{\ -1/N(0)V}]$$

Then for weak coupling limit $N(0)V << 1$ (the typical value of N(0)V for most superconductors is ≤ 0.3),the above expresssion becomes:

$$\frac{2\hbar\omega_D}{\triangle_0} \approx e^{\ -1/N(0)V} \tag{3.3.19}$$

Thus, the approximate expression for Δ_0 becomes

$$\Delta_0 = 2\hbar\omega_D \exp[\frac{-1}{VN(0)}] \tag{3.3.20}$$

After substituting (3.3.10), (3.3.14), and (3.3.15) into (3.3.8), the total superconducting ground state energy becomes:

$$E_s = \sum_k \xi_k(1 - \frac{\xi_k}{E_k}) - \frac{\Delta_0^2}{V} \tag{3.3.21}$$

In the normal state, the ground state of the metal when all states below the Fermi level are filled and the interaction potential is switched off is characterized by an energy, E_n as

$$E_n = \sum_{k<k_F} 2\xi_k \tag{3.3.22}$$

Since the sum is taken over pairs of states $(\vec{k}, -\vec{k})$, the coefficient 2 appears in (3.3.22) above.

Hence the ground state energy of the superconductor is measured in relative to the ground state energy of the normal metal, let us define the quantity W as

$$W = E_s - E_n = \sum_k \xi_k(1 - \frac{\xi_k}{E_k}) - \frac{\Delta_0^2}{V} - \sum_{k<k_F} 2\xi_k$$

This implies

$$W = 2\sum_{k>k_F} \xi_k(1 - \frac{\xi_k}{E_k}) - \frac{\Delta_0^2}{V} \tag{3.3.23}$$

The summation in (3.3.23) can be changed into integration over ε as

$$W = 2N(0)\int_0^{\hbar\omega_D} \varepsilon(1 - \frac{\varepsilon}{\sqrt{\varepsilon^2 + \Delta_0^2}}) \ - \frac{\Delta_0^2}{V}$$

Evaluating the integral and applying the weak coupling limit approximation, we obtained

$$W = -\frac{1}{2}N(0)\Delta_0^2 \tag{3.3.24}$$

This energy difference is the condensation energy at $T = 0K$ and we observe that as the superconducting state has lower energy than that of the normal state of a metal.

3.4 The spectrum of elementary excitations

So far, we have discussed the ground state energy of a superconducting state characterized by formation of cooper pairs and if the pairs are broken by a certain means the two electrons will occupy higher states other than the ground state. Thus, the spectrum of these excitations shall be studied in the coming subsections by explaining certain parameters such as the energy gap, density of states, coherence length.

3.4.1 The energy gap

The existence of the energy gap between the ground state and the elementary excitations spectrum of a superconductor is an important parameter for the description of the fundamental properties of a superconductor.

To obtain an expression of the energy gap, let us consider an arbitrary pair of states $(\vec{q}\uparrow, -\vec{q}\downarrow)$ to estimate its contribution, w_q, to the total energy of a superconductor. That is given by

$$w_q = 2\xi_q v_q^2 - 2V v_q u_q \sum_k v_k u_k \tag{3.4.1}$$

in account of Cooper's assumption in which $V_{kk'} = -V$

Now putting (3.3.10), (3.3.13), and (3.3.14) into (3.4.1) gives

$$w_q = \xi_q - (\frac{\xi_q^2}{E_q} + \frac{\Delta_0^2}{E_q})$$

$$w_q = \xi_q - E_q \tag{3.4.2}$$

Once we obtain the pairs' energy contribution, let us assume that the pair of the states $(\vec{q}\uparrow, -\vec{q}\downarrow)$ is not occupied and if we allow the system to introduce one extra electron with, $\vec{q}$, of kinetic energy, ξ_q, the energy of the superconductor becomes:

$$W_q = W - w_q + \xi_q \ , \tag{3.4.3}$$

with $W_q = W + E_q$. Where W is the ground state energy of a superconductor and $E_q = \sqrt{\xi_q^2 + \Delta_0^2}$ is the additional energy.

From the above analysis, we can observe that adding one electron results increasing of the energy where Δ_0 is the minimum possible value of E_q. This implies that the spectrum of the elementary excitations of the superconductor is separated from the

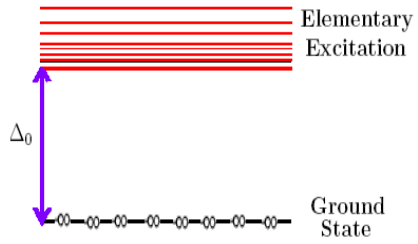


Figure 3.5: The energy gap Δ_0 separates the energy levels of the elementary excitations from the ground state levels [22].

ground state energy level by an energy gap, Δ_0, as sketched in Fig.3.5.

Meanwhile, for destroying one cooper pair consisting of two electrons, the system energy needs to be raised by $2E_q$. Thus, the minimum energy required to form an excitation is $2\Delta_0$. The excitation energy defined by equation (3.3.13) is the one that shows how much the system of the energy is increased when an extra electron with momentum k is added and takes the form:

$$E_k = \sqrt{\xi_k^2 + \Delta_0^2} = \sqrt{\frac{\hbar^2}{2m}(k^2 - k_F^2) + \Delta_0^2} \tag{3.4.4}$$

And its dependence on k is schematically represented by Fig.3.6. The energy gap $\Delta(T)$ depends on temperature and the variation along with temperature is approximated by a relation, [8] :

$$\Delta(T) \approx 1.76 k_B T_c [1 - T/T_c]^{1/2} \tag{3.4.5}$$

in account of $\Delta_0 = \Delta(T = 0)$ and $\Delta(T_c) = 0$.

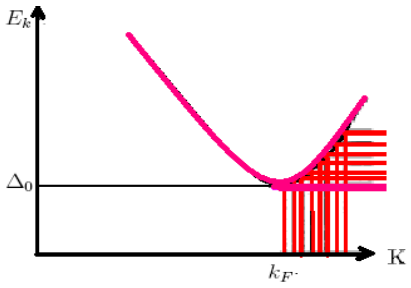


Figure 3.6: The dependence of E_k on k [22].

3.4.2 The density of state of elementary excitations

Density of states of elementary excitations is the number of energy levels per unit energy interval, and defined as

$$\rho(E) = \frac{d\nu}{dE} = \frac{d\nu}{d\xi}\frac{d\xi}{dE} = N(0)\frac{E}{\sqrt{E^2 - \Delta_0^2}}\ , \tag{3.4.6}$$

where $d\nu$ is the number of energy levels in the energy interval dE, $N(0) = d\nu/d\xi$ is the density of state on the Fermi level and its dependence on E is shown in Fig.3.7.

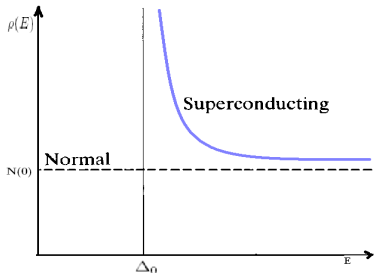


Figure 3.7: The dependence of $\rho(E)$ on E [22].

3.4.3 Evaluation of the coherence length

From the Ginzburg-Landau theory of superconductivity, the coherence length is defined as a measure of the minimum spatial extent of a transition layer between the normal and the superconducting state of a metal. The intrinsic coherence length ξ is defined as

$$\xi = \frac{\hbar^2 k_F}{2mE_g} = \frac{\hbar^2 V_F}{2E_g} \ , \tag{3.4.7}$$

where E_g is the energy gap.

Now let us evaluate the coherence length from the microscopic theory of superconductivity approach. As we have seen in section 3.3.1 the ground state wave function of a superconductor is given by distribution of paired electrons with a distribution probability v_k^2.

Even if v_k^2 is dependent on k, its variation with k is dominant in the region where $k \rightarrow k_F$. In the momentum space large variation will occur in the interval $\triangle k$, given by

$$\triangle k \ \sim \ 2\Delta_0 \frac{k_F}{\xi_F} \tag{3.4.8}$$

Whereas, if we consider the real space the large variation is expected to occur in the interval, $\triangle x$, given by

$$\triangle x \triangle k \ \sim \ 1$$

This implies that

$$\triangle x \ \sim \ \frac{\xi_F}{2\Delta_0 k_F} = \frac{\hbar^2 k_F}{4m\Delta_0} = \frac{\hbar p_F}{4m\Delta_0} = \frac{\hbar V_F}{4\Delta_0} \ , \tag{3.4.9}$$

where, V_F is the velocity of electrons on the Fermi surface. $\triangle x$ is the quantity which is equivalent to the so called coherence length, ξ. Then the coherence length of the

superconductor at $T = 0K$ in the microscopic theory can be estimated as

$$\xi \sim \frac{\hbar V_F}{4\Delta_0} \tag{3.4.10}$$

For a given superconductor $\Delta_0 \sim k_B T_C$, where k_B is the Boltzmann constant. Thus, the approximate value of ξ will be

$$\xi \approx 0.18 \frac{10^{-27} \times 10^8}{1.38 \times 10^{-10} \times 1} \sim 10^{-4}\ cm\ , \tag{3.4.11}$$

where $V_F \sim 10^8\ cm\ s^{-1}$ and $T_c \sim 1K$.

Equation (3.4.11) is the estimated value of the coherence length in a superconductor. This parameter appears in the phenomenological theory of Ginzburg-Landau (GL) [2,8,25].

Chapter 4

Quasiparticles in the Superconducting State of Metals

The ground state of a superconductor at $T = 0$ is a condensate consisting of the cooper pairs [1,8,15]. At $T \neq 0$ the excited state can be presented as a set of elementary excitations. They are fermions and obey the Fermi distribution that takes the form:

$$f_k = \frac{1}{e^{\beta E_k} + 1} , \tag{4.0.1}$$

where $\beta = 1/k_B T$ and $E_k = \sqrt{\xi_k^2 + \Delta^2(T)}$.

We note that in (4.0.1) the chemical potential, $\mu = 0$. The point is that the number of elementary excitations is not conserved and depends on T.

4.1 Quasiparticles: Electrons and Holes

Consider the normal state of a metal to have a more accurate definition of quasiparticles. In the ground state of a normal metal (at $T = 0K$) : all the states inside the Fermi sphere ($k < k_F$) are occupied by the free electrons whereas the states out side ($k > k_F$) are free. By following the same thing that we have implemented in

section 3.4.1, let us introduce one extra electron to the metal. This electron will occupy one of the states that are free. Consequently, the total energy of the system will be increased by an amount $\frac{\hbar^2}{2m}(k_F^2 - k^2)$ [18].

Therefore, such type of excitation (quasiparticles) is said to be electron like that possess energy of the form:

$$\xi_k^- = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}(k^2 - k_F^2) \tag{4.1.1}$$

On the contrary, if we remove one electron from the filled state ($k < k_F$) of a ground state of the normal metal. After the electron removed, its state inside the Fermi sphere is empty, such a state is considered as a quasiparticle of another type that behaves as holes with momentum -k and excitation energies of the form:

$$\xi_k^+ = \frac{\hbar^2 k_F^2}{2m} - \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}(k_F^2 - k^2) \tag{4.1.2}$$

Up to now, we have seen excitations in normal metals but now let us discuss them in superconducting states of the metal.

From section 3.3.1, we know that the ground state energy of a superconductor is determined by v_k^2, the probability of occupation of pairs of states (k, -k) by a pair of electrons.

Now if we introduce one extra electron to a superconductor, it takes one free state in the $\vec{K}$ space and the $-\vec{K}$ state will be kept free. Since some of the $\vec{K}$ states in the ground state of a superconductor are unoccupied, the state $\vec{K}$ can be inside or out of the Fermi sphere [25].

Therefore, unlike normal metals, the electron like excitation in superconductors can be characterized with momentum of $k < k_F$ and $k > k_F$.

On the other hand, if one electron is removed from the state $-\vec{k}$ of the ground

state of a superconductor, we will have unpaired electron in the state k and it behaves as holes of momentum $\vec{k}$ such that $k < k_F$ and $k > k_F$.

In the superconductor, it is clear that the excitation for the state $\vec{k}$ (occupied) and $-\vec{k}$ (empty) can be electron like and hole like as schematically represented by Fig. 4.1.

Thus, the probability for the hole like excitation is proportional to v_k^2, which is the probability of the state $\vec{k}$ that is occupied by a superconducting electron. Whereas the formation of the electron like excitation is proportional to the probability that one of the state $\vec{k}$ is empty, that is $u_k^2 = 1 - v_k^2$.

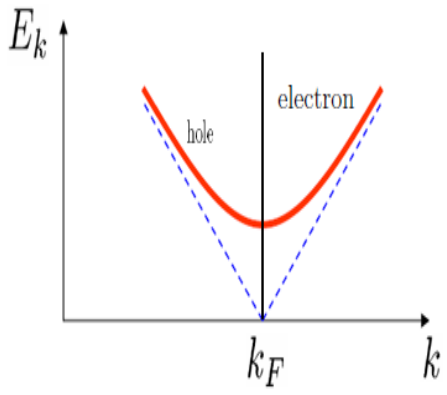


Figure 4.1: The energy spectrum of quasiparticles in the superconductors. Dashed lines show the spectrum of the normal metal [22].

Thus, the electron type excitation in the superconductor is defined as a quasiparticle with a momentum $\vec{k}$ if $|k - k_F|/k_F >> \Delta/\xi_F$, with $k > k_F$. A quasiparticle is a hole like if $|k_F - k|/k_F >> \Delta/\xi_F$, with $k < k_F$. Quasiparticles propagate with group

velocity, V_g, defined as

$$V_g = \frac{dE_k}{dp_k} = \frac{1}{\hbar}\frac{dE_k}{dk} = \frac{\xi_k^{\pm} k\hbar/m}{E_k} \tag{4.1.3}$$

Equation (4.1.3) implies that the holes move to the left and the electrons move to the right for $k > 0$ as shown in Fig. 4.1.

4.2 Properties of quasiparticles in superconducting states of a metal

4.2.1 Charge of quasiparticles in superconductors

From Fig.4.1, it is seen that as we move along the curve of the spectrum of the elementary excitations, the transitions from the electron to hole is continuous this gives an idea that the quasi particles have a fractional electric charge as first proposed by Pethick and Smith before discovering the fractional quantum hall effect [26].

Consider a superconductor at $T \neq 0$ where it possess a paired electrons (superconducting electrons) and elementary excitations. As we mentioned at the beginning of this chapter, excitations are distributed according to f_k. The probability to find electrons in the state $\vec{K}$ is $f_k u_k^2$ where u_k^2 is the probability that the state $\vec{K}$ is free from paired electrons [25,27].

But this state can be filled by a superconducting electron with there is no electrons forming an excitation (of probability $1 - f_k$) and there is superconducting electrons (of probability v_k^2). Then we can find a net superconducting electrons in the state $\vec{K}$ with a probability of $(1 - f_k)v_k^2$.

If we take the electrons charge equal to $\mathbf{e}$, the total charge of the electrons in the

state $\vec{K}$ in the superconductor is given by

$$Q_{total} = \sum_k \mathbf{e} f_k u_k^2 + \sum_k \mathbf{e}(1 - f_k) v_k^2 \tag{4.2.1}$$

If we allow the system to be disturbed, the distribution of quasiparticles and superconducting electrons have changed by δf_k and δv_k^2 respectively. Then the total charge will be changed by

$$\delta Q_{total} = \sum_k \mathbf{e}(u_k^2 - v_k^2)\delta f_k + \sum_k \mathbf{e}(1 - 2f_k)\delta v_k^2 \tag{4.2.2}$$

The first term in (4.2.2) represents the variation of the total charge of the quasi particles.

Now define the quantity

$$q_k = (u_k^2 - v_k^2)\mathbf{e} \tag{4.2.3}$$

After substituting (3.3.14), (3.3.15) into (4.2.3) we obtain

$$q_k = \frac{\mathbf{e}\xi_k}{(\xi_k^2 + \Delta^2(T))^{1/2}} \tag{4.2.4}$$

The quantity q_k is treated as a charge of the quasiparticles.

4.2.2 Andreev reflection

It is a type of particle scattering that occurs at the interface between the normal state (N) and the superconducting state (S) of a metal. It is named after the Russian physicist Alexander.F.Andreev [25,28].

Having defined Andreev reflection, let us see the interface between the normal (N) and the superconducting (S) states. Consider an electron incident on the interface

at energies less than the energy gap, $\Delta(T)$ from the normal state of the metal. The normal electron will be transformed into electron like quasiparticle when reached at position in the superconducting region which is characterized by momentum of $\vec{k}$ and small energy gap.

Meanwhile, since the quasiparticle is continued to move forward and reached at an area with large energy gap and momentum $k \rightarrow k_F$, the group velocity and the charge of the quasiparticle become zero in account of (4.1.3) and (4.2.4).

Upon reaching the region with state defined by momentum $k \rightarrow k_F$, the quasiparticle is reflected back to the normal state as hole. Finally, the reflected quasiparticle forms a cooper pair with the incident normal electron of opposite spin and momentum in the superconductor as shown in Fig.4.2

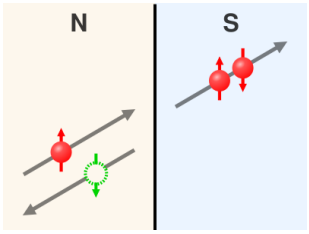


Figure 4.2: An electron (red) meeting the interface between a normal conductor (N) and a superconductor (S) produces a Cooper pair in the superconductor and a reflected hole (green) in the normal conductor. Vertical arrows indicate the spin band occupied by each particle [28].

Thus, from the above analysis of Andreev reflection, we observed that the transformation of the normal current (electrons in the normal state of a metal) into dissipative less current.

The over all physical processes observed in Andreev reflection are sketched below.

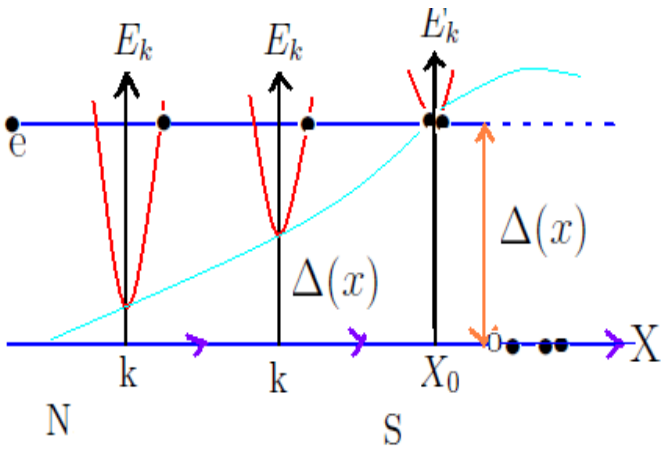


Figure 4.3: Schematic diagram of Andreev reflection [22].

4.3 The critical current and persistent current in superconductors

In this section, we shall demonstrate the possibility of a persistent current which is one of the properties of a superconductor. Consider a superconductor and allow a current to flow in it. If all cooper pairs have the same momentum k, the Fermi sphere is shifted by a vector $\vec{q}$ as a result of the current persistent inside the superconductor. Thus, this shifting process is accompanied by an energy decrease by an amount of

$$\frac{\hbar^2}{2m}([k+q]^2 - [k-q]^2) = \frac{\hbar^2}{m}k_F q \tag{4.3.1}$$

where m is the electron mass and k_F is the radius of the Fermi sphere.

, If $\frac{\hbar^2}{m}k_F q > 2\triangle$, then the pair can be broken. However, a break down of a current state begins when it becomes energetically favourable to break cooper pairs, that is, when

$$\frac{\hbar^2}{m}k_F q_c \simeq 2\triangle \tag{4.3.2}$$

Now let $P_c = \hbar q_c$ be the critical momentum of a pair. Hence

$$P_c = \hbar q_c \simeq \frac{2m\triangle}{P_F} = \frac{2\triangle}{v_F}$$

where V_F is the electron velocity on the Fermi surface . Thus, the current density corresponding to the critical momentum becomes:

$$j_c = n_s e v_c \tag{4.3.3}$$

where n_s is the density of superconducting electron. Then, equation(4.3.3) becomes:

$$j_c = n_s e\frac{P_c}{2m} = n_s e\frac{\Delta}{mv_F} \tag{4.3.4}$$

Therefore if the current is greater than j_c it is dissipative current whereas if the current is less than j_c it is a dissipative less one.

4.4 Relation between Ginzburg-Landau theory and the Microscopic theory

As we know the Ginzburg-Landau (GL) theory is a phenomenological one in which it is impossible to interprate coefficients on the microscopic level. But after the the microscopic theory came to the picture, Gorkov showed that the possibility of interpreting the coefficient at a microscopic level. The main idea of Gorkov's analysis

is that, the energy gap $\Delta(T)$ represents the order parameter in the superconductor, and therefore, at $T \to T_C$. must be proportional to the order parameterΨ of the GL theory. The after some mathematical manipulations the exact result is :

$$\Psi = [\frac{7\zeta(3)mv_F^2N(0)}{2\pi^2k_B^2T_c^2}]^{1/2}\Delta(T) \tag{4.4.1}$$

where $\zeta(3) \simeq 1.202$ is the Riman function

Chapter 5

Discussion and Conclusion

5.1 Discussion

The microscopic theory of low temperature superconductivity after the discovery of an isotopic effect is considered as a well developed theory in explaining fundamental facts of a superconductor. In this work, we studied low temperature superconductivity from microscopic point of view and we obtain different crucial results for the description of different parameters. Thus, in this section we enumerate and discuss a number of results:

The superconducting ground state

The electron-phonon interaction has a chief effect on the properties of solids. The significance of this interaction is that it results new ground state called superconducting state caused by attractive interaction between electrons through the exchange of phonons. At $T = 0$, the ground state of the superconducting state is characterized by a unique wave function proposed by BCS theory and possess lower energy than

the ground state of the normal metal and it takes the form:

$$W = -\frac{1}{2}N(0)\Delta_0^2 \tag{5.1.1}$$

Now if we introduce a thermodynamic quantity $U(T)$ for the internal energy of the system and assuming that $\Delta(T)$ is temperature dependent, we obtain the following relation

$$E_s - E_n = -\frac{1}{2}N(0)\Delta_0^2 \tag{5.1.2}$$

where, $U_s(0) = E_s$ and $U_n(0) = E_n$

And as we know that from equation (1.2.1) the energy difference between the two states should be equal to $\frac{H_c^2}{8\pi}$, where H_c is the critical magnetic field. Meanwhile, this energy difference should be equal to the one given by equation (5.1.2) if we are neglecting the entropy contribution in the superconducting state since it is the most ordered state. According to equation (3.3.20), $\Delta_0 \propto \hbar\omega_D$ and on the other hand from section (1.3), $\omega_D \propto M^{-1/2}$ where M is the atomic mass. Therefore, based on the BCS theory, $\Delta_0 \propto M^{-1/2}$.

Thus, we arrived at the conclusion that $H_c \propto \Delta_0 \propto \hbar\omega_D \propto M^{-1/2}$. That shows the strength of the BCS theory in explaining the experimentally observed isotopic effect.

The charge of quasiparticles

A quasiparticle possesses a fractional charge of the form:

$$q_k = \frac{\mathbf{e}\xi_k}{(\xi_k^2 + \Delta^2(T))^{1/2}} \ , \tag{5.1.3}$$

where the magnitude of the charge continuously changes between (-**e** for electrons) and (+**e** for holes). This value depends on the magnitude of k as demonstrated by the figure below:

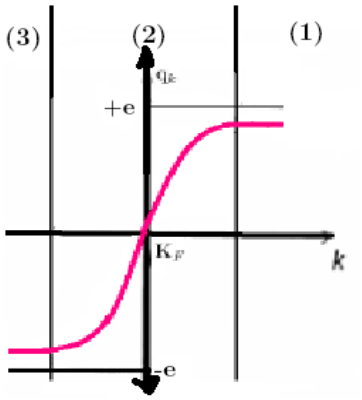


Figure 5.1: The schematic diagram of quasiparticle charge versus k.

As we see in Fig.5.1, in region (1), the quasiparticles charge is close to +**e**, in region (3) it is close to -**e** and in region (2) it may assume any value of +e or -e. Thus, the quasiparticle transitions between different k states are accompanied by change of those charges, q_k.

5.2 Conclusion

In this work, for the description of low temperature superconductivity we have used different branches of theoretical physics: quantum mechanics, statistical physics, and field theory etc. Besides that we have used a comparatively simple procedure for evaluating the ground state of a superconductor avoiding the second quantized Hamiltonian and u-v Bogoliubov transformation. Using this simplified procedure the fractional charge of the electron-like and hole-like elementary excitations is shown. Furthermore, we have applied the idea of variable charge of elementary excitations to analyze the super current between the normal and superconducting states. Mean while, the modern theory of the low temperature superconductivity is based on Londons', GL, and BCS theory; GL theory consists of order parameterΨ, α, β are the coefficients of expanding the Gibbs free energy in the powers of the order parameter. Gorkov using the Green's function method gave interpretation of the phenomenological parameters interms of the microscopic theory where the energy gap is the main property of the superconductor but With the help of the obtained u_k and v_k we Gorkov's assumption is verified.

Appendices

5.3 Appendix A

Evaluation of the effective electron-electron interaction Hamiltonian

The full Hamiltonian of the system of the lattice is defined as

$$H = H_0 + H_{e-p} \tag{5.3.1}$$

Consider an antiunitary operator S (i.e. $S^+ = -S$) such that $\exp(S)$ is unitary [11,29]. Hence all physical quantities remain unchanged under unitary transformation, let us transform the full Hamiltonian, H, in to a new Hamiltonian,$\tilde{H}$, as

$$\tilde{H} = \exp(-S) H \exp(S) \tag{5.3.2}$$

That is

$$\tilde{H} = H + [H, S] + \frac{1}{2!}[[[H, S], S] + \frac{1}{3!}[[[H, S], S, S] + ... \tag{5.3.3}$$

As we planned to eliminate the first order term, the canonical transformation should be chosen in such a way that the contributions from the electron-phonon interaction are canceled out in first order. Then H is supposed to be

$$H = H_0 + \lambda H_{e-p} \tag{5.3.4}$$

such that

$$\tilde{H} = H_0 + \lambda H_{e-p} + [H_0, S] + \lambda[H_{e-p}, S] + \frac{1}{2}[[H_0 + \lambda H_{e-p}, S], S] + ... \tag{5.3.5}$$

Now choose S in such a way that to satisfy

$$\lambda H_{e-p} + [H_0, S] = 0 \tag{5.3.6}$$

That is $S \sim O(\lambda)$, implying that $\tilde{H}$ has no term linear in λ, then (5.3.5) becomes

$$\tilde{H} = H_0 + \lambda[H_{e-p}, S] - \frac{1}{2}\lambda[H_{e-p}, S] + O(\lambda^3)$$

$$\tilde{H} = H_0 + \frac{1}{2}\lambda[H_{e-p}, S] + O(\lambda^3) \tag{5.3.7}$$

The matrix element of the condition (5.3.4) for states $|m\rangle$ and $|n\rangle$ of H_0 with eigne values E_m and E_n respectively becomes

$$\lambda\langle n|H_{e-p}|m\rangle = -\langle n|[H_0, S]|m\rangle$$

$$\langle n|SE_m|m\rangle - \langle n|E_nS|m\rangle = \lambda\langle n|H_{e-p}|m\rangle$$

$$(E_m - E_n)\langle n|S|m\rangle = \lambda\langle n|H_{e-p}|m\rangle$$

Thus,

$$\langle n|S|m\rangle = \frac{\lambda\langle n|H_{e-p}|m\rangle}{(E_m - E_n)} \tag{5.3.8}$$

Provided that $E_m \neq E_n$

Since the phenomena we are interested in occur at very low temperature, we consider the phonon at absolute zero, thus the eigne states, either $|m\rangle$ or $|n\rangle$ represents the vacuum phonon states. If $|0\rangle$ stands for ground state, then $|1_q\rangle$ is that of the

excited state. Now let us discuss the possible cases for the scattering of electrons in Fig.3.1.

Case 1. If an electron is scattered from state $|0\rangle$ to $|1_q\rangle$ by creating a phonon, then equation (5.3.8) can be written as

$$\langle 1_q|S|0\rangle = \frac{\langle 1_q|i\sum_{k,q} Dc^+_{k+q}c_k[\hat{a_q} - \hat{a_{-q}}^+]|0\rangle}{E_0 - E_{1_q}}$$

$$\langle 1_q|S|0\rangle = -iD\sum_k \frac{c^+_{k-q}c_k}{E_q - E_{k-q} - \hbar\omega_q} \tag{5.3.9}$$

Case 2. If an electron is scattered from state $|1_q\rangle$ to $|0\rangle$ by creating a phonon, then equation (5.3.8) can be written as

$$\langle 0|S|1_q\rangle = \frac{\langle 0|i\sum_{k,q} Dc^+_{k+q}c_k[\hat{a_q} - \hat{a_{-q}}^+]|1_q\rangle}{E_{1_q} - E_0}$$

$$\langle 0|S|1_q\rangle = -iD\sum_{k'} \frac{c^+_{k'+q}c_{k'}}{E_q - E_{k'+q} - \hbar\omega_q} \tag{5.3.10}$$

Neglect higher order terms in λ that are greater than the second order from (5.3.9)

$$\tilde{H} = H_0 + \frac{1}{2}\lambda[H_{e-p}, S] \tag{5.3.11}$$

Now let us again evaluate the matrix elements of $[H_{e-p}, S]$, thus if we tackle $H_{e-p}S$ and SH_{e-p} separately, we obtain the following expressions

$$\langle n|H_{e-p}S|m\rangle = D^2\sum_{k,k',q} c^+_{k'+q}c_{k'}c^+_{k-q}c_k\frac{1}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_q} \tag{5.3.12}$$

$$\langle n|SH_{e-p}|m\rangle = D^2\sum_{k,k',q} c^+_{k'-q}c_{k'}c^+_{k+q}c_k\frac{1}{\epsilon_{k'} - \epsilon_{k'-q} + \hbar\omega_q} \tag{5.3.13}$$

Thus, equation (5.3.11) can be written as

$$\tilde{H} = H_0 + \frac{1}{2}D^2\sum_{k,k',q} c^+_{k'+q}c_{k'}c^+_{k-q}c_k[\frac{1}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_q} - \frac{1}{\epsilon_{k'} - \epsilon_{k'-q} + \hbar\omega_q}] \tag{5.3.14}$$

While summing over q in equation (5.3.14) one must take the possible terms with phonons of wave vectors q and -q with $\omega_q = \omega_{-q}$ and by taking the energy conservation that is $\epsilon_k - \epsilon_{k'} = \epsilon_k - \hbar k + \epsilon_{k'} + \hbar k'$ into account, the total Hamiltonian of the system is

$$\tilde{H} = H_0 + D^2 \sum_{k,k',q} c^+_{k'+q} c_{k'} c^+_{k-q} c_k [\frac{\hbar\omega_q}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2}] \tag{5.3.15}$$

Thus, the electron-electron interaction through the exchange of phonons may be written as

$$H_{e-e} = D^2 \sum_{k,k',q} c^+_{k'+q} c_{k'} c^+_{k-q} c_k [\frac{\hbar\omega_q}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2}] \tag{5.3.16}$$

5.4 Appendix B

Evaluation of the binding energy Δ

The kinetic energy of the two electron system is

$$\epsilon_{k_1} + \epsilon_{k_2} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m}$$

$$= \frac{\hbar^2}{2m}(k_1^2 + k_2^2)$$

Then in the new coordinate transformations

$$\epsilon_K + \epsilon_k = \frac{\hbar^2}{m}(\frac{1}{4}K^2 + k^2) = H_0 \tag{5.4.1}$$

Since the largest number of possible transitions yielding the most appreciable lowering of energy is obtained by pairing all possible states such that their total momentum vanishes (i.e, $q = 0$) such that $k_1 = -k_2$ [6].

Suppose that the pairing electrons are subjected to an interaction H_1 then the total hamiltonian is

$$H = H_0 + H_1 \tag{5.4.2}$$

Let the eigne function of the pair electrons be

$$\Psi(r) = \sum_k g_k \exp(ik.r) = \sum_k g_k \exp(ik.(r_1 - r_2)) \tag{5.4.3}$$

Then the schrodinger eigne value equation can be written as

$$H\Psi(r) = \epsilon\Psi(r) \ , \tag{5.4.4}$$

where ϵ is the eigne value. Then

$$(H - \epsilon)\sum_k g_k \exp(ik.r) = 0 \tag{5.4.5}$$

Take the elements between the eigne states of the system as

$$\int dr \sum_k g_k \exp(-ik.r)(H - \epsilon)\sum_{k'} g_{k'} \exp(ik^{'}.r) = 0$$

$$\Rightarrow (E_k - \epsilon)g_k + \sum_{k'}\langle k|H_1|k^{'}\rangle = 0 \tag{5.4.6}$$

Now let us change the summation in (5.4.5) into integration, while doing this consider$D(E^{'})$ be the density of the two states with $q = 0$ per unit energy range, with energy $E^{'}$ then we have that

$$(E - \epsilon)g_E + \int dE^{'} N(E^{'})g(E^{'})\langle E|H_1|E^{'}\rangle = 0 \tag{5.4.7}$$

Consider the matrix elements $\langle E|H_1|E^{'}\rangle = \langle k|H_1|k^{'}\rangle$ of the effective electron-electron interaction via the lattice [12]. It appears that the matrix element can be approximated as

$$\langle E|H_1|E^{'}\rangle = \begin{cases} -|V|, for(E-E^{'}) \leq \pm\hbar\omega_D \\ 0, otherwise. \end{cases} \tag{5.4.8}$$

The possible states that for the two electrons are above the Fermi level that is between E_F and E_m. Thus, equation (5.4.6) becomes

$$(E-\epsilon)g(E) = |V| \int_{2E_F}^{2E_m} dE^{'} N(E^{'}) g(E^{'}) = C \ , \tag{5.4.9}$$

where $E_m = E_F + \hbar\omega_D$ and C is constant that is independent of E. Then

$$g(E) = \frac{C}{E-\epsilon} \Rightarrow 1 = V \int_{2E_F}^{2E_m} \frac{dE^{'} N(E^{'})}{E^{'}-\epsilon} \tag{5.4.10}$$

For the small energy range $E_F >> \hbar\omega_D, N(E^{'})$ is approximately constant and equal to $N(0)$ and we can take it out of the integral to obtain :

$$\begin{aligned} 1 &= N(O)V \int_{2E_F}^{2E_m} \frac{dE^{'}}{E^{'}-\epsilon} \\ &= N(O)V \ln[\frac{2E_m-\epsilon}{2E_F-\epsilon}] \end{aligned} \tag{5.4.11}$$

Let the eigne value ϵ of the system be written as

$$\epsilon = 2E_F - \Delta \ ,$$

where Δ is the binding energy of the electron pair, relative to the two free electrons of the Fermi level. Then equation (5.4.10) becomes

$$\begin{aligned} 1 &= N(0)V \ln[\frac{2\hbar\omega_D + \Delta}{\Delta}] \\ \triangle &= \frac{2\hbar\omega_D}{exp(1/N(0)V) - 1} \end{aligned} \tag{5.4.12}$$

5.5 Appendix C

Table 1.1 Critical temperature and magnetic field of some superconducting elements and compounds

ELEMETS	T_C(K)	H_C(T)	COMPOUNDS	T_C(K)
Technetium	11.2	1410	Nb_3Ge	23.2
Niobium	9.46	1980	Nb_3Ga	20.3
Lead	7.18	803	Nb_3Sn	18.05
Tantalum	4.48	830	NbN	16.0
Mercury	4.15	412	Mo_3Ir	8.80
Indium	3.41	293	NiBi	4.25
Aluminum	1.19	105	AuBe	2.64
Candium	0.56	30	$PdSb_2$	1.25
Titanium	0.40	171	TiCo	
Iridium	0.14	19	$AuSb_2$	
Tungsten	0.01	1.07	$ZrAl_2$	

Table 5.1: Superconducting transition temperatures and critical magnetic field at absolute zero in gauss (10^{-4} *tesla*) for selected elements and compounds [1, 2].

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Declaration

This thesis is my original work, has not been presented for a degree in any other University and that all the sources of material used for the thesis have been dully acknowledged.

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