BCS theory of superconductivity: a pedagogic short review by mathematical descriptions

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Abstract

In this manuscript different important outcomes of the BCS theory have been revisited in a nutshell focusing on every mathematical details to explain superconducting properties.

Keywords: *Superconductivity, BCS theory*

1. Introduction

Superconductivity is one of the most fascinating subjects of modern physics. After the discovery of the phenomena of Superconductivity in 1911 by H. Kamerlingh Onnes. it has gained tremendous research interest for last few decades. He received the Nobel Prize in Physics in 1993, for this discovery, i.e., that at very low temperatures, certain metals become perfect conductors of electricity. In 1933, Meissner and Oschenfeld discovered that a superconductor has diamagnetic properties, i.e., that the magnetic field inside the bulk superconductor becomes zero. This effect characterizes a superconductor and distinguishes it from a perfect conductor. Till then, many theories behind the superconductivity phenomena have been developed. The first theory to explain the occurrence of superconductivity in metallic superconductors was given by London *et. al.* in 1935 [2]. They formulated relation between current density and electromagnetic vector potential and using that explained the zero electric resistivity and Messiner effect subsequently. In addition to these, two contemporary physicists Cornelius Gorter and Hendrik Casimir provided first phenomenological two fluid model in 1934 and explained superconducting properties [3]. iI 1950, Vitaly Ginzburg and Lev Landau proposed Ginzburg - Landau (GL) theory introducing a complex wave function ($\Psi(\vec{r})$) as an order parameter ($n_s = |\Psi(\vec{r})|^2$) and this was one of the most successful phenomenological theories [4]. Interestingly, the eminence of GL theory was realized later on around 1959 by Gorkov and that is GL theory is analogus to the famous Bardeen, Cooper and Schrieffer (BCS) theory of 1957 [1] around the superconducting critical temperature (T_C), where GL order parameter $\Psi(\vec{r})$ is related to BCS energy gap parameter simply by a proportionality constant. Thus we reached the golden year of superconductivity when the complete theory microscopic theory of conventional superconductor was discovered by Bardeen, Cooper and Schrieffer which is till now one of the most succesful microscopic theories to explain conventional superconductivity. For the pioneering theory they were awared Nobel prize in 1972. Their theory was based on the famous "Cooper's one pair problem" [5] which states that, in a system of many electrons at low enough temperatures, a very weak attractive force, can bind two electrons together, forming the so called Cooper pair. The effective force between electrons can be attractive in a solid instead of becoming repulsive.

This arises due to the coupling between electrons and the phonons of the underlying crystal and this concept was suggested by Fröhlich in 1950 [6]. However, for some exotic and high temperature superconductors the BCS theory fails to explain the superconducting properties. And the underlying microscopic theory is matter of great interest of many researchers till date.

Thus to understand the pairing mechanism and different superconducting properties, BCS theory is the ideal platform to start with. Although this is now a welknown undergraduate topic in many unversitities during the discussion of superconductivity, the detailed mathematical desriptions starting from construction of the many particle wavefunction in which every electron is paired, should be a matter of interest and this will be very helpful for the novices. Although the detailed analysis has been discussed in many books [7-12], the different important outcomes of the BCS theory have been revisited in this manuscript in a nutshell focusing on every mathematical details due to its analytical complicacy. The BCS theory gives the following ideas which will be discussed in this manuscript.

I. Construction of many electron wavefunction.
II. Construction of Energy Gap equation and Energy Gap Parameter. They predicted an energy gap 2Δ, where 2Δ is the energy for breaking up a pair into two free electrons.
III. Temperature dependence of Δ .
IV. Estimation of Critical temperature (T_c).
V. Isotope effect: $T_c \propto M^{-\alpha}$, where the transition temperature varies with the mass of the crystal lattice ions, M. They predicted $\alpha = \frac{1}{2}$. Most common superconductors (Pb , Hg etc.) agree very well with this prediction.
VI. Evaluation of critical field H_C .
VII. Evaluation of Specific Heat.

2. Mathematical Formulations and Discussions

2.1 Construction of BCS wave-function:

We might examine a form like

$$\Psi_N = \psi(1,2)\psi(3,4)\psi(5,6) \ldots . \psi(N-1,N), \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

where it is defined that the two-particle pair wavefunction

$$\psi(1,2) = \varphi(\vec{r}_1, \vec{r}_2)\chi(\vec{\sigma}_1, \vec{\sigma}_2) \ldots\ldots\ldots\ldots\ldots (2)$$

To insure (1) satisfies the Pauli principle we must operate on it with the antisymmetrization operator, Â

$$\Psi_N = \hat{A}\{\psi(1,2)\psi(3,4)\psi(5,6) \ldots . \psi(N-1,N)\} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Assuming translational invariance, it can be written as: $\varphi(\vec{r}_1, \vec{r}_2) = \varphi(\vec{r}_1 - \vec{r}_2)$ and after Fourier expansion:

$$\varphi(\vec{r}) = \sum_{\vec{k}} g_{\vec{k}}\, e^{i\vec{k}.\vec{r}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

On substituting (4) into (3) we obtain the most general N-electron wave-function expressed in terms of momentum eigen functions:

$$\Psi_N = \sum_{\vec{k}_1} \dots \sum_{\vec{k}_{N/2}} g_{\vec{k}_1} \dots g_{\vec{k}_{N/2}} \hat{\mathrm{A}} \left(e^{i\vec{k}_1.(\vec{r}_1-\vec{r}_2)} \dots e^{i\vec{k}_{N/2}.(\vec{r}_1-\vec{r}_2)} \right) (1\uparrow)(2\downarrow) \dots (N-1\uparrow)(N\downarrow)$$

According to Pauli exclusion principle, as the space part of the wave function is symmetric, spin part has to be antisymmetric. That is why pairing of spin up and spin down electrons (singlet pairing) has to be considered. The function $\left(e^{i\vec{k}_1.(\vec{r}_1-\vec{r}_2)} \dots e^{i\vec{k}_{N/2}.(\vec{r}_1-\vec{r}_2)} \right) (1\uparrow)(2\downarrow) \dots (N-1\uparrow)(N\downarrow)$ has a simple interpretation. It describes a state one electron occupies the state $\vec{k}_1\uparrow$, another the $-\vec{k}_1\downarrow$, a third $\vec{k}_2\uparrow$, and so on. This is what usually called Slater determinant formed with states $(\vec{k}_1\uparrow)(-\vec{k}_1\downarrow)(\vec{k}_2\uparrow)(-\vec{k}_2\downarrow)\dots..(\vec{k}_{N/2}\uparrow)(-\vec{k}_{N/2}\downarrow)$. Rather than writing in coordinate representation, it is usually easier to perform calculations in the occupation number (Wigner-Jordan) representation, i.e. , to use the language of second quantization.

Instead of writing $\hat{\mathrm{A}} e^{i\vec{k}_1.(\vec{r}_1-\vec{r}_2)} (1\uparrow)(2\downarrow)$, we write $\hat{c}^\dagger_{\vec{k}_1\uparrow} \hat{c}^\dagger_{-\vec{k}_1\downarrow} |0\rangle$, where $|0\rangle$ is the vacuum state and $\hat{c}^\dagger_{\vec{k}_1\vec{\sigma}_1}$ is the Fermi creation operator for an electron 1 having momentum $\vec{k}$ and spin $\sigma(\uparrow \text{or} \downarrow)$.

The commutation relation for these operators:

$$\hat{c}^\dagger_{\vec{k}\alpha}\hat{c}^\dagger_{\vec{l}\beta} + \hat{c}^\dagger_{\vec{l}\beta}\hat{c}^\dagger_{\vec{k}\alpha} = 0 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (5a)$$

$$\hat{c}_{\vec{k}\alpha}\hat{c}_{\vec{l}\beta} + \hat{c}_{\vec{l}\beta}\hat{c}_{\vec{k}\alpha} = 0 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (5b)$$

and

$$\hat{c}^\dagger_{\vec{k}\alpha}\hat{c}_{\vec{l}\beta} + \hat{c}_{\vec{l}\beta}\hat{c}^\dagger_{\vec{k}\alpha} = \delta_{\vec{k}\vec{l}}\delta_{\alpha\beta} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (5c)$$

where $\vec{k}$ and $\vec{l}$ denote wave vectors and α and β spin projections.

In the second quantized notation the many-body pair wavefunction can then be written

$$\Psi_N = \sum_{\vec{k}_1} \dots \sum_{\vec{k}_{N/2}} g_{\vec{k}_1} \dots g_{\vec{k}_{N/2}} \hat{c}^\dagger_{\vec{k}_1\uparrow}\hat{c}^\dagger_{-\vec{k}_1\downarrow} \dots \hat{c}^\dagger_{\vec{k}_{N/2}\uparrow}\hat{c}^\dagger_{-\vec{k}_{N/2}\downarrow}|0\rangle \dots\dots\dots\dots\dots (6)$$

It is quite difficult to perform calculations with (6) and Bardeen, Cooper and Schrieffer proposed an alternative wavefunction

$$\Psi_{BCS} = \prod_{\vec{k}} (1 + g_{\vec{k}}\hat{c}^\dagger_{\vec{k}\uparrow}\hat{c}^\dagger_{-\vec{k}\downarrow})|0\rangle \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (7)$$

BCS introduced pairing operators defined as:

$$\hat{b}^\dagger_{\vec{k}} = \hat{c}^\dagger_{\vec{k}\uparrow}\hat{c}^\dagger_{-\vec{k}\downarrow} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (8a)$$

$$\hat{b}_{\vec{k}} = \hat{c}_{-\vec{k}\downarrow}\hat{c}_{\vec{k}\uparrow} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (8b)$$

According to Schrieffer these operators are called “pairon operators”. The Cooper pair has total spin s=0. Therefore, according to the Pauli principle, the wave functions describing the cooper pair system have the

boson permutation symmetry, i.e., they are symmetric under permutations of pairs. But the cooper pair operators do not obey the boson commutation relations.

$$\left[\hat{b}_{\vec{k}}, \hat{b}^{\dagger}_{\vec{k'}}\right] = \left[\hat{b}^{\dagger}_{\vec{k}}, \hat{b}^{\dagger}_{\vec{k'}}\right] = \left[\hat{b}_{\vec{k}}, \hat{b}_{\vec{k'}}\right] = 0 \text{ for } \vec{k} \neq \vec{k}' \quad \text{.....(9a)}$$

$$\left[\hat{b}_{\vec{k}}, \hat{b}^{\dagger}_{\vec{k}}\right] = 1 - \hat{n}_{\vec{k}\uparrow} - \hat{n}_{-\vec{k}\downarrow} \text{ for } \vec{k} = \vec{k}' \quad \text{.....(9b)}$$

where $\hat{n}_{\vec{k}\vec{\sigma}} = \hat{c}^{\dagger}_{\vec{k}\vec{\sigma}}\hat{c}_{\vec{k}\vec{\sigma}}$ is the electron number operator. $\hat{n}_{\vec{k}\uparrow}$ and $\hat{n}_{\vec{k}\downarrow}$ are the number operators for spin-up and spin-down electrons, respectively. In dilute fermionic density limit, $\left[\hat{b}_{\vec{k}}, \hat{b}^{\dagger}_{\vec{k}}\right] = 1$, then cooper pairs behave like bosons.

From equ.(7) we can write $\Psi_{BCS} = \prod_{\vec{k}}(1 + g_{\vec{k}}\,\hat{b}^{\dagger}_{\vec{k}})|0\rangle$

Let us first normalize Ψ_{BCS}.

$$\langle\Psi_{BCS}|\,\Psi_{BCS}\rangle = \prod_{\vec{k}\vec{k}'}\langle 0|(1 + g^{*}_{\vec{k}}\,\hat{b}_{\vec{k}})\left(1 + g_{\vec{k'}}\hat{b}^{\dagger}_{\vec{k'}}\right)|0\rangle$$

$$= \prod_{\vec{k}\vec{k}'}\langle 0|(1 + g^{*}_{\vec{k}}\,\hat{b}_{\vec{k}} + g_{\vec{k'}}\hat{b}^{\dagger}_{\vec{k'}} + g^{*}_{\vec{k}}g_{\vec{k'}}\hat{b}_{\vec{k}}\hat{b}^{\dagger}_{\vec{k'}})|0\rangle$$

[Now we know that for fermionic operator

$$\hat{c}_k|0\rangle = 0$$

And $$\hat{c}^{\dagger}_k|1\rangle = 0 \;\&\; \hat{c}^{\dagger}_k|0\rangle = |1\rangle$$

So, $$\hat{b}_{\vec{k}}|0\rangle = \hat{c}_{-\vec{k}\downarrow}\hat{c}_{\vec{k}\uparrow}|0\rangle = 0, \hat{b}^{\dagger}_{\vec{k}}|0\rangle = \hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}^{\dagger}_{-\vec{k}\downarrow}|0\rangle = |\ldots 1{,}1 \ldots\rangle.$$

And $$\hat{n}_k|0\rangle = \hat{c}^{\dagger}_k\hat{c}_k|0\rangle = 0]$$

The term with an odd number operators vanish; using condition (9b) in the last term gives

$$\langle\Psi_{BCS}|\,\Psi_{BCS}\rangle = \prod_{\vec{k}\vec{k'}}\langle 0|1 + g^{*}_{\vec{k}}\,g_{\vec{k'}}(1 - \hat{c}^{\dagger}_{-\vec{k'}\downarrow}\hat{c}_{-\vec{k}\downarrow} - \hat{c}^{\dagger}_{\vec{k'}\uparrow}\hat{c}_{\vec{k}\uparrow})\delta_{\vec{k}\vec{k'}} + g^{*}_{\vec{k}}g_{\vec{k'}}\hat{b}^{\dagger}_{\vec{k}}\hat{b}_{\vec{k'}}|0\rangle$$

$$\langle\Psi_{BCS}|\,\Psi_{BCS}\rangle = \prod_{\vec{k}}(1 + g^{*}_{\vec{k}}g_{\vec{k}})$$

So, the normalized ground state BCS wave function is

$$|\,\boldsymbol{\Psi_{BCS}}\rangle = \prod_{\vec{\mathbf{k}}}\frac{(\mathbf{1}+g_{\vec{k}}\hat{b}^{\dagger}_{\vec{k}})|\mathbf{0}\rangle}{(\mathbf{1}+\boldsymbol{g}^{*}_{\vec{k}}\boldsymbol{g}_{\vec{k}})^{1/2}} \quad \text{.....(10)}$$

Now we can introduce the quantities

$$u_{\vec{k}} = \frac{1}{(\mathbf{1}+\boldsymbol{g}^{*}_{\vec{k}}\boldsymbol{g}_{\vec{k}})^{1/2}} \quad \text{.....(11a)}$$

And $$v_{\vec{k}} = \frac{g_{\vec{k}}}{(1+g^*_{\vec{k}}g_{\vec{k}})^{1/2}} \text{.....(11b)}$$

Using (11a),(11b) from (10) we get

$$|\Psi_{BCS}\rangle = \prod_{\vec{k}}\left(u_{\vec{k}} + v_{\vec{k}}\hat{b}^{\dagger}_{\vec{k}}\right)|0\rangle \text{.....(12)}$$

So, $g_{\vec{k}} = \frac{v_{\vec{k}}}{u_{\vec{k}}}$ and $u_{\vec{k}}$ & $v_{\vec{k}}$ satisfy $|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1$. The implication of this form is that the probability of the pair $(\vec{k}\uparrow, -\vec{k}\downarrow)$ being occupied is $|v_k|^2$, and the probability that it is unoccupied is $|u_k|^2 = 1 - |v_k|^2$.

The wavefunction (6) for the special case

$$g_{\vec{k}} = 1, |\vec{k}| < k_F,$$

$$g_{\vec{k}} = 0, |\vec{k}| > k_F,$$

describes the Fermi sphere; all states with $|\vec{k}| < k_F$ are filled and those with $|\vec{k}| > k_F$ are empty. The corresponding form for equ.(12) is

$$u_{\vec{k}} = 0, \quad v_{\vec{k}} = 1, |\vec{k}| < k_F,$$

$$u_{\vec{k}} = 1, \quad v_{\vec{k}} = 0, |\vec{k}| > k_F,$$

The difference between equ.(6) and equ.(12) for the general case is that the first defines a state with precisely N/2 pairs (N electrons) while the second is a superposition of pair states containing 2,4,6,….N,….. ∞ electrons, i.e., it does not describe a state with a fixed number of particles. By superposition we may relate the two wavefunctions as

$$\Psi_{BCS} = \sum_N \lambda_N \Psi_N \text{.....(13)}$$

with the normalization condition $\sum_N |\lambda_N|^2 = 1$. The average number of particles, $\bar{N}$, associated with BCS wavefunction is

$$\bar{N} = \langle\Psi_{BCS}|\hat{N}|\Psi_{BCS}\rangle \text{ .....(14)}$$

where $\hat{N} = \sum_{\vec{k},\vec{\sigma}} \hat{c}^{\dagger}_{\vec{k}\vec{\sigma}}\hat{c}_{\vec{k}\vec{\sigma}}$ is the total number operator.

So, $$\bar{N} = \langle\Psi_{BCS}|\sum_{\vec{k}}(\hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}_{\vec{k}\uparrow} + \hat{c}^{\dagger}_{\vec{k}\downarrow}\hat{c}_{\vec{k}\downarrow})|\Psi_{BCS}\rangle$$

$$= 2\sum_{\vec{k}}\langle\Psi_{BCS}|\hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}_{\vec{k}\uparrow}|\Psi_{BCS}\rangle$$

Since the electrons all occur in pairs with antiparallel spin. Putting form of $|\Psi_{BCS}\rangle$ from equ.(12) we get

$$\bar{N} = 2\sum_{\vec{k}}\langle 0|\left(u^*_{\vec{k}} + v^*_{\vec{k}}\hat{c}_{-\vec{k}\downarrow}\hat{c}_{\vec{k}\uparrow}\right)\hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}_{\vec{k}\uparrow}\left(u_{\vec{k}} + v_{\vec{k}}\hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}^{\dagger}_{-\vec{k}\downarrow}\right)$$

$$\times\prod_{\vec{l}\neq\vec{k}}\left(u^*_{\vec{l}} + v^*_{\vec{l}}\hat{c}_{-\vec{l}\downarrow}\hat{c}_{\vec{l}\uparrow}\right)\left(u_{\vec{l}} + v_{\vec{l}}\hat{c}^{\dagger}_{\vec{l}\uparrow}\hat{c}^{\dagger}_{-\vec{l}\downarrow}\right)|0\rangle$$

$= \quad 2 \quad \sum_{\vec{k}} \langle 0| \left(\left|u_{\vec{k}}\right|^2 \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} + v^{*}_{\vec{k}} u_{\vec{k}} \hat{c}_{-\vec{k}\downarrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} + u^{*}_{\vec{k}} v_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{-\vec{k}\downarrow} + |v_{\vec{k}}|^2 \hat{c}_{-\vec{k}\downarrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{-\vec{k}\downarrow} \right) \times \prod_{\vec{l}\neq\vec{k}} \left(|u_{\vec{l}}|^2 + v^{*}_{\vec{l}} u_{\vec{l}} \hat{c}_{-\vec{l}\downarrow} \hat{c}_{\vec{l}\uparrow} + u^{*}_{\vec{l}} v_{\vec{l}} \hat{c}^{\dagger}_{\vec{l}\uparrow} \hat{c}^{\dagger}_{-\vec{l}\downarrow} + |v_{\vec{l}}|^2 \hat{c}_{-\vec{l}\downarrow} \hat{c}_{\vec{l}\uparrow} \hat{c}^{\dagger}_{\vec{l}\uparrow} \hat{c}^{\dagger}_{-\vec{l}\downarrow} \right) |0\rangle$

[In the last part of the expression the middle two terms give zero, since they change the occupancy of the ***l*** th pair. The operators in the last term can be transformed to $\left(1 - \hat{c}^{\dagger}_{\vec{l}\uparrow} \hat{c}_{\vec{l}\uparrow}\right)\left(1 - \hat{c}^{\dagger}_{-\vec{l}\downarrow} \hat{c}_{-\vec{l}\downarrow}\right)$, both factors of which give unity when operating on $|0\rangle$.]

$\bar{N} = \quad 2 \quad \sum_{\vec{k}} \langle 0| \left(\left|u_{\vec{k}}\right|^2 \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} + v^{*}_{\vec{k}} u_{\vec{k}} \hat{c}_{-\vec{k}\downarrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} + u^{*}_{\vec{k}} v_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{-\vec{k}\downarrow} + |v_{\vec{k}}|^2 \hat{c}_{-\vec{k}\downarrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{-\vec{k}\downarrow} \right) \times \prod_{\vec{l}\neq\vec{k}} \left(|u_{\vec{l}}|^2 + |v_{\vec{l}}|^2\right) |0\rangle$.

Using the condition $|u_{\vec{l}}|^2 + |v_{\vec{l}}|^2 = 1$, we get

$$\bar{N} = 2 \sum_{\vec{k}} \langle 0| \left(\left|u_{\vec{k}}\right|^2 \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} + v^{*}_{\vec{k}} u_{\vec{k}} \hat{c}_{-\vec{k}\downarrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} + u^{*}_{\vec{k}} v_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{-\vec{k}\downarrow} + \left|v_{\vec{k}}\right|^2 \hat{c}_{-\vec{k}\downarrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{-\vec{k}\downarrow} \right) |0\rangle$$

In the upper expression only last part contributes.

$$\bar{N} = 2 \sum_{\vec{k}} \left|v_{\vec{k}}\right|^2 \quad \text{.....(15)}$$

The mean square fluctuation of the number of particles is defined as

$$\overline{\Delta N^2} = \overline{N^2} - \overline{N}^2 = \langle \Psi_{BCS} | \hat{N}\hat{N} | \Psi_{BCS} \rangle - \langle \Psi_{BCS} | \hat{N} | \Psi_{BCS} \rangle^2$$

Similar to the above calculation, we can get:

$$= 4 \sum_{\vec{k}} \left|u_{\vec{k}}\right|^2 \left|v_{\vec{k}}\right|^2 + 4 \sum_{\vec{k}} \left|v_{\vec{k}}\right|^2 \left|v_{\vec{l}}\right|^2 - 4 \sum_{\vec{k}} \left|v_{\vec{k}}\right|^2 \left|v_{\vec{l}}\right|^2$$

In a similar manner, we get

$$\overline{\Delta N^2} = \sum_{\vec{k}} 4 |v_{\vec{k}}|^2 \, |u_{\vec{k}}|^2 \quad \text{.....(16)}$$

So, $$\frac{\left(\overline{\Delta N^2}\right)^{1/2}}{\bar{N}} \sim \bar{N}^{-1/2}$$

For a metal $\bar{N} \sim 10^{22}$ and therefore $\bar{N}^{-1/2}$ is of the order of 10^{-11}. This says that the coefficients in the expansion (13) will be highly peaked around $\bar{N}$.

Important conclusion is that calculations performed using (6) or (12) should differ by amounts of order10^{-11}. Since it is far easier to calculate using (12), this form was adopted by BCS.

2.2 Calculation of Gap-equation:

The appropriate ground state energy is obtained by equ.(12) as a trial wave function and evaluating the expectation value of the Hamiltonian of the system of electrons; this is followed by minimization of the resultant energy with respect to the free parameter, $v_{\vec{k}}$, subject to the condition that the average number of particles is $\bar{N}$.

We can write the Hamiltonian of the system of electrons as:

$$\hat{H} = \sum_{\vec{k},\vec{\sigma}} \frac{\hbar^2 k^2}{2m} \hat{c}^{\dagger}_{\vec{k}\vec{\sigma}} \hat{c}_{\vec{k}\vec{\sigma}} + \sum_{\vec{k},\vec{k}',\vec{q},\vec{\sigma},\vec{\sigma}'} V_{\vec{k},\vec{k}',\vec{q},\vec{\sigma},\vec{\sigma}'} \hat{c}^{\dagger}_{\vec{k}+\vec{q},\vec{\sigma}} \hat{c}^{\dagger}_{\vec{k'}-\vec{q},\vec{\sigma}'} \hat{c}_{\vec{k}',\vec{\sigma}'} \hat{c}_{\vec{k},\vec{\sigma}}$$

Where the second term accounts for all electron-electron interactions and momentum conservation (and transfer by an amount $\vec{q}$) has been built into the scattering potential, V. Since the BCS wavefunction does not fix the number of electrons we must introduce a constraint that the average number of particles is $\bar{N}$,i.e., $\bar{N} = \langle \Psi_{BCS} | \sum_{\vec{k},\vec{\sigma}} \hat{c}^{\dagger}_{\vec{k}\vec{\sigma}} \hat{c}_{\vec{k}\vec{\sigma}} \mid \Psi_{BCS} \rangle$. This constraint is introduced through a Lagrange multiplierμ, which is actually chemical potential. Incorporating these considerations we write the Hamiltonian as

$$\hat{H}' = \hat{H} - \mu\hat{N} = \sum_{\vec{k},\vec{\sigma}} \xi_{\vec{k}} \, \hat{c}^{\dagger}_{\vec{k}\vec{\sigma}} \hat{c}_{\vec{k}\vec{\sigma}} + \sum_{\vec{k},\vec{k}',\vec{q},\vec{\sigma},\vec{\sigma}'} V_{\vec{k},\vec{k}',\vec{q},\vec{\sigma},\vec{\sigma}'} \hat{c}^{\dagger}_{\vec{k}+\vec{q},\vec{\sigma}} \hat{c}^{\dagger}_{\vec{k'}-\vec{q},\vec{\sigma}'} \hat{c}_{\vec{k}',\vec{\sigma}'} \hat{c}_{\vec{k},\vec{\sigma}}$$

$$= \hat{H}'_0 + \hat{H}_1$$

Where $\xi_{\vec{k}} = \frac{\hbar^2 k^2}{2m} - \mu$.

We now restrict ourselves to that part of the interaction Hamiltonian which contributes to superconductivity; i.e., we retain only the attractive part leading to the formation of pairs with opposite momenta and opposite spins. Replacing $\vec{k} + \vec{q}$ by $\vec{l}$ and $\vec{k'} - \vec{q}$ by $-\vec{l}$, and $\vec{k'}$ by $-\vec{k}$, the 'reduced' Hamiltonian becomes:

$$\hat{H}'_R = \sum_{\vec{k},\vec{\sigma}} \xi_{\vec{k}} \, \hat{c}^{\dagger}_{\vec{k}\vec{\sigma}} \hat{c}_{\vec{k}\vec{\sigma}} + \sum_{\vec{k},\vec{l}} V_{\vec{k},\vec{l}} \hat{c}^{\dagger}_{\vec{l}\uparrow} \hat{c}^{\dagger}_{-\vec{l}\downarrow} \hat{c}_{-\vec{k}\downarrow} \hat{c}_{\vec{k}\uparrow}$$

$$= \sum_{\vec{k},\vec{\sigma}} \xi_{\vec{k}} \, \hat{c}^{\dagger}_{\vec{k}\vec{\sigma}} \hat{c}_{\vec{k}\vec{\sigma}} + \sum_{\vec{k},\vec{l}} V_{\vec{k},\vec{l}} \hat{b}^{\dagger}_{\vec{l}} \hat{b}_{\vec{k}}$$

$$= \hat{H}'_0 + \hat{H}_{IR}$$

The ground state energy is:

$$E' = E - \mu\bar{N} = \langle \Psi_{BCS} | \hat{H}'_R | \Psi_{BCS} \rangle \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (17)$$

$$= \langle \Psi_{BCS} | \hat{H}'_0 | \Psi_{BCS} \rangle + \langle \Psi_{BCS} | \hat{H}'_{IR} | \Psi_{BCS} \rangle$$

We have calculated $\bar{N} = 2 \sum_{\vec{k}} \langle \Psi_{BCS} | \, \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} | \Psi_{BCS} \rangle = 2 \sum_{\vec{k}} |v_{\vec{k}}|^2$

So, $$\boldsymbol{\langle \Psi_{BCS} | \hat{H}'_0 | \Psi_{BCS} \rangle = 2 \sum_{\vec{k}} \xi_{\vec{k}} |v_{\vec{k}}|^2} \ldots\ldots\ldots\ldots (18a)$$

Now, $\langle\Psi_{BCS}|\hat{H}_{IR}|\Psi_{BCS}\rangle = \sum_{\vec{k},\vec{l}}\langle 0|\left(u_{\vec{l}}^{*}+v_{\vec{l}}^{*}\hat{b}_{\vec{l}}\right)\left(u_{\vec{k}}^{*}+v_{\vec{k}}^{*}\hat{b}_{\vec{k}}\right)V_{\vec{k},\vec{l}}\hat{b}_{\vec{l}}^{\dagger}\,\hat{b}_{\vec{k}}\left(u_{\vec{k}}+v_{\vec{k}}\hat{b}_{\vec{k}}^{\dagger}\right)\left(u_{\vec{l}}+v_{\vec{l}}\hat{b}_{\vec{l}}^{\dagger}\right)\times \prod_{\vec{n}\neq\vec{k},\vec{l}}\left(u_{\vec{n}}^{*}+v_{\vec{n}}^{*}\hat{b}_{\vec{n}}\right)\left(u_{\vec{n}}+v_{\vec{n}}\hat{b}_{\vec{n}}^{\dagger}\right)|0\rangle$

Only contributing term is $u_{\vec{l}}^{*}v_{\vec{l}}u_{\vec{k}}v_{\vec{k}}^{*}\hat{b}_{\vec{l}}\hat{b}_{\vec{l}}^{\dagger}\hat{b}_{\vec{k}}\hat{b}_{\vec{k}}^{\dagger}$.

So, $$\boldsymbol{\langle\Psi_{BCS}|\hat{H}_{IR}|\Psi_{BCS}\rangle = \sum_{\vec{k},\vec{l}} u_{\vec{k}}^{*}v_{\vec{k}}u_{\vec{l}}v_{\vec{l}}^{*}V_{\vec{k},\vec{l}}}\ldots\ldots\ldots\ldots\ldots(18b)$$

$$\langle\Psi_{BCS}|\hat{H}_{R}'|\Psi_{BCS}\rangle = 2\sum_{\vec{k}}\ \xi_{\vec{k}}|v_{\vec{k}}|^{2} + \sum_{\vec{k},\vec{l}}u_{\vec{k}}^{*}v_{\vec{k}}u_{\vec{l}}v_{\vec{l}}^{*}V_{\vec{k},\vec{l}}\ldots\ldots\ldots\ldots(19)$$

Now to evaluate the ground-state energy using the BCS variational wavefunction we must minimize the (17) subject to the condition $|u_{\vec{k}}|^{2}+|v_{\vec{k}}|^{2}=1$. This constraint is conventionally imposed by letting

$$|u_{\vec{k}}| = \cos\theta_{\vec{k}} \qquad |v_{\vec{k}}| = \sin\theta_{\vec{k}}$$

Thus $\langle\Psi_{BCS}|\hat{H}_{R}'|\Psi_{BCS}\rangle = 2\sum_{\vec{k}}\ \xi_{\vec{k}}\sin^{2}\theta_{\vec{k}} + \frac{1}{4}\sum_{\vec{k},\vec{l}}\sin 2\theta_{\vec{k}}\sin 2\theta_{\vec{l}}\,V_{\vec{k},\vec{l}}$

And minimizing with respect to the parameter $\theta_{\vec{k}}$ yields

$$2\xi_{\vec{k}}\sin 2\theta_{\vec{k}} + \cos 2\theta_{\vec{k}}\sum_{\vec{l}}V_{\vec{k},\vec{l}}\sin 2\theta_{\vec{l}} = 0$$

$$\xi_{\vec{k}}\tan 2\theta_{\vec{k}} = -\frac{1}{2}\sum_{\vec{l}}V_{\vec{k},\vec{l}}\sin 2\theta_{\vec{l}}\ldots\ldots\ldots\ldots\ldots\ldots\ldots(20)$$

We define the function

$$\Delta_{\vec{k}} = -\frac{1}{2}\sum_{\vec{l}}V_{\vec{k},\vec{l}}\sin 2\theta_{\vec{l}}\ldots\ldots\ldots\ldots\ldots\ldots\ldots(21)$$

which is called "Gap function" and equ. (20) becomes

$$\tan 2\theta_{\vec{k}} = \frac{\Delta_{\vec{k}}}{\xi_{\vec{k}}}$$

Or, $$\sin 2\theta_{\vec{k}} = 2|u_{\vec{k}}|\,|v_{\vec{k}}| = \frac{\Delta_{\vec{k}}}{E_{\vec{k}}}\ldots\ldots\ldots\ldots(22)$$

Where $E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^{2}+\Delta_{\vec{k}}^{2}}$

$$\cos 2\theta_{\vec{k}} = |u_{\vec{k}}|^{2} - |v_{\vec{k}}|^{2} = \frac{\xi_{\vec{k}}}{E_{\vec{k}}}\ldots\ldots\ldots\ldots\ldots(23)$$

Solving equ. (23) and the relation $|u_{\vec{k}}|^{2}+|v_{\vec{k}}|^{2}=1$, we get,

$$|u_{\vec{k}}|^{2} = \frac{1}{2}\left[1+\frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right]\ldots\ldots\ldots\ldots\ldots\ldots(24a)$$

$$|v_{\vec{k}}|^2 = \frac{1}{2}\left[1 - \frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right] \text{.....(24b)}$$

These two are called “Bogolibov co-efficients”.

Actually $E_{\vec{k}}$ is the excitation energy of a quasi-particle of momentum $\hbar\vec{k}$, while $\Delta_{\vec{k}}$ is independent of $\vec{k}$ and is the minimum excitation energy, or energy gap.

We can now substitute equ. (22) into equ. (21) to evaluate $\Delta_{\vec{k}}$, leading to the condition for self-consistency

$$\Delta_{\vec{k}} = -\frac{1}{2}\sum_{\vec{l}} V_{\vec{k},\vec{l}} \frac{\Delta_{\vec{l}}}{E_{\vec{l}}} \text{ .....(25)}$$

Equ. (25) has the trivial solution $\Delta_{\vec{k}} = 0$ and using equ. (24a) and equ. (24b) we have

$$|v_{\vec{k}}| = 1, \ \ |u_{\vec{k}}| = 0, \ \text{for } \xi_{\vec{k}} > 0.$$

And

$$|u_{\vec{k}}| = 1, \ \ |v_{\vec{k}}| = 0, \ \text{for } \xi_{\vec{k}} < 0.$$

Hence the BCS wavefunction is then

$$|\Psi_{BCS}\rangle = \sum_{\vec{k}<\vec{k}_F} \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}^{\dagger}_{-\vec{k}\downarrow} |0\rangle \text{.....(26)}$$

It is the usual ground-state wavefunction of a filled Fermi sea.

The simplest example of non-trivial solution to eq. (25) is using the Cooper model potential,

$$V_{\vec{k},\vec{l}} = \begin{cases} -V, & |\xi_{\vec{k}}| \text{ and } |\xi_{\vec{l}}| \leq \hbar\omega_c \text{ where } V > 0. \\ 0, & |\xi_{\vec{k}}| \geq \hbar\omega_c \text{ or } |\xi_{\vec{l}}| \geq \hbar\omega_c. \end{cases}$$

The function will then have the form

$$\Delta_{\vec{k}} = \begin{cases} 0, & |\xi_{\vec{k}}| > \hbar\omega_c. \\ \Delta, & \left(\text{independent of } \vec{k}\right) \text{ for } |\xi_{\vec{k}}| < \hbar\omega_c. \end{cases}$$

So, the equ. (25) becomes

$$1 = \frac{V}{2}\sum_{\vec{k}} \frac{1}{E_{\vec{k}}} \text{.....(27)}$$

Upon replacing the summation by an integration from $-\hbar\omega_c$ to $\hbar\omega_c$, and using the symmetry of $\pm\xi$ values, this becomes

$$\frac{1}{N(0)V} = \int_0^{\hbar\omega_c} \frac{d\xi}{(\Delta^2+\xi^2)^{1/2}} = \sinh^{-1}\frac{\hbar\omega_c}{\Delta} \text{.....(28)}$$

$$\therefore \Delta = \frac{\hbar\omega_c}{\sinh\left[1/N(0)V\right]} \text{.....(29)}$$

Where $N(0)$ is the density of states per unit volume at the Fermi energy. The fluctuation of density of states within the range $\hbar\omega_c$around Fermi surface is small. So, we can take the density of states per unit volume as constant at the Fermi energy.

In the weak coupling limit, $N(0)V \ll 1$, for which

$$\Delta = 2\hbar\omega_c e^{-1/N(0)V} \text{ .....(30).}$$

Let us estimate Δ: Taking $\hbar\omega_c$ as corresponding to the Debye temperature~ 100 K and $N(0)V$~0.3, we obtain Δ~4 K.

2.3 Evaluation of Ground-State energy:

From eq. (19), using eq. (25), eq. (22), eqs. (24a) and (24b), we have in the superconducting state,

$$\langle \Psi_{BCS} | \hat{H}'_R | \Psi_{BCS} \rangle_s = 2\sum_{\vec{k}} \frac{\xi_{\vec{k}}}{2}\left[1 - \frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right] + \frac{1}{4}\sum_{\vec{k},\vec{l}} V_{\vec{k},\vec{l}} \frac{\Delta_{\vec{k}}\Delta_{\vec{l}}}{E_{\vec{k}}E_{\vec{l}}}$$

$$= \sum_{\vec{k}}\left[\xi_{\vec{k}} - \frac{{\xi_{\vec{k}}}^2}{E_{\vec{k}}}\right] - \frac{\Delta^2}{V} \text{.....(31)}$$

[Using eq. (25) twice to evaluate the second (interaction) term in eq. (31) we obtain $-\frac{\Delta^2}{V}$.]

In the normal state there is no gap, i.e. , $\Delta = 0$ and in this case $E_{\vec{k}} = |\xi_{\vec{k}}|$. Thus

$$\langle \Psi_{BCS} | \hat{H}'_R | \Psi_{BCS} \rangle_n = \sum_{|\vec{k}|<k_F} 2\,\xi_{\vec{k}} \text{ .....(32)}$$

the terms for $|\vec{k}| > k_F$, gives zero, since $E_{\vec{k}} = \xi_{\vec{k}}$.

The ground-state energy of the superconductor is measured from the ground-state energy of the normal state. The difference in these energies is

$$\langle E \rangle_s - \langle E \rangle_n = \sum_{|\vec{k}|>k_F}\left[\xi_{\vec{k}} - \frac{{\xi_{\vec{k}}}^2}{E_{\vec{k}}}\right] + \sum_{|\vec{k}|<k_F}\left[-\xi_{\vec{k}} - \frac{{\xi_{\vec{k}}}^2}{E_{\vec{k}}}\right] - \frac{\Delta^2}{V}$$

$$= 2\sum_{|\vec{k}|>k_F}\left[\xi_{\vec{k}} - \frac{{\xi_{\vec{k}}}^2}{E_{\vec{k}}}\right] - \frac{\Delta^2}{V}$$

by symmetry about the Fermi energy.

Going over to the continuum approximation, we have to carry out the integration on ξ from 0 to $\hbar\omega_c$.

$$\langle E\rangle_s - \langle E\rangle_n = 2\,N(0)\int_0^{\hbar\omega_c} \xi\, d\xi - 2\,N(0)\int_0^{\hbar\omega_c} \frac{\xi^2}{(\Delta^2+\xi^2)^{1/2}} d\xi - \frac{\Delta^2}{V}$$

Where $N(0)$ is the density of states per unit volume at the Fermi surface.

$$\langle E\rangle_s - \langle E\rangle_n = N(0)\hbar^2{\omega_c}^2 - N(0)\Delta^2\left[\frac{\hbar\omega_c}{\Delta}\left(1+\frac{\hbar^2{\omega_c}^2}{\Delta^2}\right)^{1/2} - \sinh^{-1}\left(\frac{\hbar\omega_c}{\Delta}\right)\right] - \frac{\Delta^2}{V}$$

In the weak coupling limit, using the eq. (28) we get

$$\langle E\rangle_s - \langle E\rangle_n = \left[\frac{\Delta^2}{V} - \frac{1}{2}N(0)\Delta^2\right] - \frac{\Delta^2}{V} = -\frac{1}{2}N(0)\Delta^2 \text{ .....(33)}$$

Introducing the thermodynamic symbol $U(T)$ for the internal energy of the system, and anticipating that $\Delta(T)$ is temperature dependent, we have

$$U_s(0) - U_n(0) = -\frac{1}{2}N(0)\Delta^2(0) \text{ .....(34)}$$

This is the "condensation energy" at T= 0 K. The difference in energy between the superconducting and normal state is negative, that is the superconducting state is more favorable energetically. From thermodynamic calculation, the condensation energy is equal to $-\frac{H_c^2(0)}{8\pi}$. Where $H_c(T)$ is the thermodynamic critical field.

So, $$\frac{1}{2}N(0)\Delta^2(0) = \frac{H_c^2(0)}{8\pi}.$$

$$\Longrightarrow H_c = \Delta(0)\sqrt{4\pi N(0)} \text{.....(35)}$$

Thus we have expressed the thermodynamic critical field in terms of characteristic parameters of the superconductor, i.e., the energy gap.

Let us check whether eq. (35) gives reasonable orders of magnitude for relevant physical quantities.1 cm^3 of metal contains~10^{22} electrons and the width of the electron band is~10 eV. Then the density of states per unit volume is $N(0)$~10^{33}erg^{-1}cm^{-3}. According to the previous estimation $\Delta\sim 10\,K\sim 10^{-15}$ erg. This leads to $H_c\sim$ 100 Oe, which is reasonable value of thermodynamic critical field.

2.4 How the energy gap comes?

Let us focus on an arbitrary pair of states $(\vec{k}, -\vec{k})$ in a superconductor, in momentum space. First we find contribution of this pair,$w_{\vec{k}}$, to the total energy of the superconductor. That is,

$$w_{\vec{k}} = 2\xi_{\vec{k}}\left|v_{\vec{k}}\right|^2 - 2V v_{\vec{k}} u_{\vec{k}}^* \sum_{\vec{l}} u_{\vec{l}} v_{\vec{l}}^*.$$

$$\Longrightarrow w_{\vec{k}} = 2\frac{\xi_{\vec{k}}}{2}\left[1 - \frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right] - 2\Delta(0)\left[\frac{1}{4}\left\{1 - \left(\frac{\xi_{\vec{k}}}{E_{\vec{k}}}\right)^2\right\}\right]^{\frac{1}{2}}$$

$$w_{\vec{k}} = \xi_{\vec{k}} - E_{\vec{k}} \text{.....(36)}$$

Suppose that the pair state $(\vec{k}, -\vec{k})$ in the ground state of a superconductor is empty. How will the energy of the system change if we add one more electron to it from outside and place it in the state$\vec{k}$? Since we then have a single electron in the state $\vec{k}$, the pair state $(\vec{k}, -\vec{k})$ is not allowed to take part in the scattering events, i.e., it cannot contribute to the ground-state energy of the superconductor. Hence the energy of the superconductor with one ''extra'' electron in the state $\vec{k}$ will be

$$W_{\vec{k}} = W - w_{\vec{k}} + \xi_{\vec{k}} \text{ ....(37)}$$

We refer to this "extra" uncoupled electron as an elementary excitation of our system, or quasiparticle. W is the ground-state energy of the superconductor and $\xi_{\vec{k}}$ accounts for the kinetic energy of the "extra" electron.

$$\Longrightarrow W_{\vec{k}} = W + E_{\vec{k}}.$$

We know that, $E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + \Delta^2(0)}$.

So, by adding one extra electron to a superconductor in the ground state, we increase the energy of the system by at least the value of $\Delta(0)$ (the minimum increase corresponds to $\xi_{\vec{k}} = 0$, i.e., to the state $\vec{k}$ being on the Fermi surface).

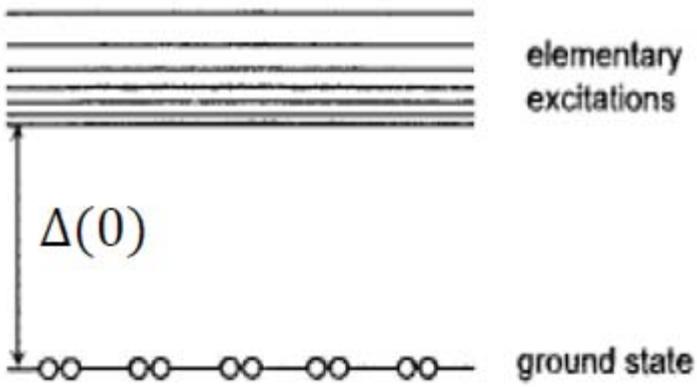

FIG 1: Schematic representation of energy gap in superconducting phase

This means that the spectrum of elementary excitations of the superconductor is separated from the ground-state energy level by an energy gap.

Suppose that, as a result of an external effect, one of the electrons from the pair $(\vec{k}, -\vec{k})$ is moved to a neighboring state in momentum space. Initially all states were either occupied in pairs or empty in pairs. Then the transfer of one electron from the pair $(\vec{k}, -\vec{k})$ to the neighboring state implies that two uncoupled (excited) electrons have appeared. One of them stays in one of the states $(\vec{k}, -\vec{k})$ while the other turns up in the neighboring $\vec{k}$ state.

But from the diagram, it is found that in order to break a pair, one needs at least the energy $2\Delta(0)$. All pair states belong to the condensate occupying the ground-state energy level. A single extra electron is not allowed to be at this level and must therefore occupy the first empty level available in the elementary excitation spectrum. If a pair is broken, both electrons must go up to the elementary excitation levels which requires an energy larger than $2\Delta(0)$.

2.5 Wavefunctions associated with excitations:

We next examine the wavefunctions associated with various excitations. We may write the wavefunction of a particle (electron)-like state with spin ↑ and wave vector $\vec{k}$ as

$$\hat{c}^{\dagger}_{\vec{k}\uparrow}|\Psi_{BCS}\rangle = (u_{\vec{k}}\hat{c}^{\dagger}_{\vec{k}\uparrow} + v_{\vec{k}}\hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}^{\dagger}_{-\vec{k}\downarrow})\prod_{\vec{k}'\neq\vec{k}}(u_{\vec{k}'} + v_{\vec{k}'}\hat{c}^{\dagger}_{\vec{k}'\uparrow}\hat{c}^{\dagger}_{-\vec{k}'\downarrow})\,|0\rangle.$$

$$= u_{\vec{k}}\hat{c}^{\dagger}_{\vec{k}\uparrow}\prod_{\vec{k}'\neq\vec{k}}\left(u_{\vec{k}'} + v_{\vec{k}'}\hat{c}^{\dagger}_{\vec{k}'\uparrow}\hat{c}^{\dagger}_{-\vec{k}'\downarrow}\right)|0\rangle.$$

$$= u_{\vec{k}}|\vec{k}\uparrow\rangle \quad \ldots\ldots(38)$$

Where $|\vec{k}\vec{\sigma}\rangle = \hat{c}^{\dagger}_{\vec{k}\vec{\sigma}}\prod_{\vec{k}'\neq\vec{k}}\left(u_{\vec{k}'} + v_{\vec{k}'}\hat{c}^{\dagger}_{\vec{k}'\uparrow}\hat{c}^{\dagger}_{-\vec{k}'\downarrow}\right)|0\rangle$ ……(39)

We may write a hole state with spin ↓ and wave-vector $-\vec{k}$.

$$\hat{c}_{-\vec{k}\downarrow}|\Psi_{BCS}\rangle = (u_{\vec{k}}\hat{c}_{-\vec{k}\downarrow} + v_{\vec{k}}\hat{c}_{-\vec{k}\downarrow}\hat{c}^{\dagger}_{\vec{k}\uparrow}\hat{c}^{\dagger}_{-\vec{k}\downarrow})\prod_{\vec{k}'\neq\vec{k}}(u_{\vec{k}'} + v_{\vec{k}'}\hat{c}^{\dagger}_{\vec{k}'\uparrow}\hat{c}^{\dagger}_{-\vec{k}'\downarrow})\,|0\rangle.$$

$$= -v_{\vec{k}}|\vec{k}\uparrow\rangle \quad \ldots\ldots(40)$$

Note that, the same state has been generated by either adding an electron to $+\vec{k}\uparrow$ or removing it from $-\vec{k}\downarrow$. Similarly we have

$$\hat{c}_{\vec{k}\uparrow}|\Psi_{BCS}\rangle = v_{\vec{k}}|-\vec{k}\downarrow\rangle \quad \ldots\ldots(41)$$

And

$$\hat{c}^{\dagger}_{-\vec{k}\downarrow}|\Psi_{BCS}\rangle = u_{\vec{k}}|-\vec{k}\downarrow\rangle \quad \ldots\ldots(42)$$

If we multiply eq. (38) by $v_{\vec{k}}$ and eq. (40) by $u_{\vec{k}}$ and add we obtain

$$\left(u_{\vec{k}}\hat{c}_{-\vec{k}\downarrow} + v_{\vec{k}}\hat{c}^{\dagger}_{\vec{k}\uparrow}\right)|\Psi_{BCS}\rangle = 0 \quad \ldots\ldots(43)$$

Or,

$$\hat{\gamma}_{-\vec{k},\downarrow}|\Psi_{BCS}\rangle = 0 \quad \ldots\ldots(44)$$

Where $\hat{\gamma}_{-\vec{k},\downarrow} = u_{\vec{k}}\hat{c}_{-\vec{k}\downarrow} + v_{\vec{k}}\hat{c}^{\dagger}_{\vec{k}\uparrow}$ ……(45)

Multiplying eq. (41) by $v_{\vec{k}}$ and eq. (42) by $u_{\vec{k}}$, adding and applying normalization condition yields

$$\hat{\gamma}^{\dagger}_{-\vec{k},\downarrow}|\Psi_{BCS}\rangle = |-\vec{k}\downarrow\rangle \quad \text{....................................(46)}$$

Similarly using equ. (39) and (41), yields

$$\left(u_{\vec{k}}\hat{c}^{\dagger}_{\vec{k}\uparrow} - v_{\vec{k}}\hat{c}_{-\vec{k}\downarrow}\right)|\Psi_{BCS}\rangle = |\vec{k}\uparrow\rangle.$$

Or,

$$\hat{\gamma}^{\dagger}_{\vec{k},\uparrow}|\Psi_{BCS}\rangle = |\vec{k}\uparrow\rangle \quad \text{..................................(47)}$$

Where $\hat{\gamma}^{\dagger}_{\vec{k},\uparrow} = u_{\vec{k}}\hat{c}^{\dagger}_{\vec{k}\uparrow} - v_{\vec{k}}\hat{c}_{-\vec{k}\downarrow}$ ....(48)

Using (41) and (42) we obtain

$$\hat{\gamma}_{\vec{k},\uparrow}|\Psi_{BCS}\rangle = 0 \quad \text{...................................(49)}$$

The two pairs of operators $\hat{\gamma}_{\vec{k},\uparrow}, \hat{\gamma}_{-\vec{k},\downarrow}, \hat{\gamma}^{\dagger}_{\vec{k},\uparrow}, \hat{\gamma}^{\dagger}_{-\vec{k},\downarrow}$ play the role of quasiparticle destruction and creation operators. Since the ground state contains no quasiparticle excitations, we must have $\hat{\gamma}|\Psi_{BCS}\rangle = 0$; on the other hand $\hat{\gamma}^{\dagger}|\Psi_{BCS}\rangle = |\vec{k}\rangle$, an excited state with one quasiparticle. The operators $\hat{\gamma}, \hat{\gamma}^{\dagger}$ are called Bogoliubov-Valitin operators. They follow the Fermi anticommution rules:

$$\left[\hat{\gamma}_{\vec{k},\vec{\sigma}}, \hat{\gamma}_{\vec{k}',\vec{\sigma}'}\right]_{+} = 0, \quad \text{...(50a)}$$

$$\left[\hat{\gamma}^{\dagger}_{\vec{k},\vec{\sigma}}, \hat{\gamma}^{\dagger}_{\vec{k}',\vec{\sigma}'}\right]_{+} = 0, \quad \text{...(50b)}$$

And

$$\left[\hat{\gamma}_{\vec{k},\vec{\sigma}}, \hat{\gamma}^{\dagger}_{\vec{k}',\vec{\sigma}'}\right]_{+} = \delta_{\vec{k},\vec{k}'}\delta_{\vec{\sigma},\vec{\sigma}'} \quad \text{............................(50c)}$$

And using eq. (45) and (48) we get

$$\hat{c}_{-\vec{k}\downarrow} = u_{\vec{k}}\hat{\gamma}_{-\vec{k},\downarrow} - v_{\vec{k}}\,\hat{\gamma}^{\dagger}_{\vec{k},\uparrow} \quad \text{..............................(51a)}$$

$$\hat{c}^{\dagger}_{\vec{k}\uparrow} = u_{\vec{k}}\hat{\gamma}^{\dagger}_{\vec{k},\uparrow} + v_{\vec{k}}\hat{\gamma}_{-\vec{k},\downarrow} \quad \text{.................................(51b)}$$

2.6 Temperature Dependence of the Energy Gap:

As the temperature increases, the energy gap Δ decreases (where $\Delta(0)$ will be kept for T=0 K). As we already know, in order to break a Cooper pair and create two elementary excitations, the energy gap 2Δ is needed. If the temperature T is such that $k_B T \sim 2\Delta$, it is evident that many Cooper pairs will be broken through thermal processes. Accordingly, a large number of states in momentum space will be filled by elementary excitations (single electrons).

The elementary excitations obey the Fermi-Dirac statistics, the probability that the state $\vec{k}$ is occupied by a single electron is

$$f_{\vec{k}} = \frac{1}{\exp\left(E_{\vec{k}}/k_B T\right)+1} \quad \text{.....(52)}$$

Where $E_{\vec{k}}$ is the energy of an elementary excitation. So, $f_{\vec{k}} \ll 1$ at $k_B T \ll E_{\vec{k}}$, and $f_{\vec{k}} \approx 0.5$ at $k_B T \gg E_{\vec{k}}$. If at least one of the states, $(\vec{k})$ or $(-\vec{k})$, is occupied, the pair state $(\vec{k}, -\vec{k})$ cannot take part in creating the superconducting state. The probability of this is $2f_{\vec{k}}$. Therefore, the probability that the pair state $(\vec{k}, -\vec{k})$ can participate in the scattering processes, i.e., they can take part in creating the superconducting state, is $1 - 2f_{\vec{k}}$.

Let us suppose that we are dealing with the state$|f_{\vec{k}}\rangle$, in which the average number of quassi-particles in the $\vec{k}$ th state is given by eq. (52). And

$$\langle \hat{\gamma}^{\dagger}_{\vec{k},\vec{\sigma}} \hat{\gamma}_{\vec{k},\vec{\sigma}} \rangle = f_{\vec{k},\vec{\sigma}} \text{.....(53a)}$$

And

$$\langle \hat{\gamma}_{\vec{k},\vec{\sigma}} \hat{\gamma}^{\dagger}_{\vec{k},\vec{\sigma}} \rangle = 1 - f_{\vec{k},\vec{\sigma}} \text{.....(53b)}$$

Inserting equation (51a) and (51b) into the reduced Hamiltonian

$\hat{H}'_R = \hat{H}'_0 + \hat{H}_{IR} = 2\sum_{\vec{k}} \xi_{\vec{k}}\, \hat{c}^{\dagger}_{\vec{k}\uparrow} \hat{c}_{\vec{k}\uparrow} + \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} \hat{c}^{\dagger}_{\vec{k}'\uparrow}\, \hat{c}^{\dagger}_{-\vec{k}'\downarrow} \hat{c}_{\vec{k}\uparrow} \hat{c}_{-\vec{k}\downarrow}$ yields

$$\langle \hat{H}'_0 \rangle = \sum_{\vec{k}} \xi_{\vec{k}} \left[2v^2_{\vec{k}} + \left(u^2_{\vec{k}} - v^2_{\vec{k}}\right) \left(\langle \hat{\gamma}^{\dagger}_{\vec{k},\uparrow} \hat{\gamma}_{\vec{k},\uparrow} \rangle + \langle \hat{\gamma}^{\dagger}_{-\vec{k},\downarrow} \hat{\gamma}_{-\vec{k},\downarrow} \rangle \right) \right]$$

+(terms with unequal numbers of $\hat{\gamma}^{\dagger}_{\vec{k},\vec{\sigma}}$ and $\hat{\gamma}_{\vec{k},\vec{\sigma}}$).

And

$$\langle \hat{H}_{IR} \rangle = \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} \left[u^*_{\vec{k}} v_{\vec{k}} u_{\vec{k}'} v^*_{\vec{k}'} (1 - \langle \hat{\gamma}^{\dagger}_{\vec{k},\uparrow} \hat{\gamma}_{\vec{k},\uparrow} \rangle - \langle \hat{\gamma}^{\dagger}_{-\vec{k},\downarrow} \hat{\gamma}_{-\vec{k},\downarrow} \rangle)(1 - \langle \hat{\gamma}^{\dagger}_{\vec{k}',\uparrow} \hat{\gamma}_{\vec{k}',\uparrow} \rangle - \langle \hat{\gamma}^{\dagger}_{-\vec{k}',\downarrow} \hat{\gamma}_{-\vec{k}',\downarrow} \rangle) \right]$$

+(terms with unequal numbers of $\hat{\gamma}^{\dagger}_{\vec{k},\vec{\sigma}}$ and $\hat{\gamma}_{\vec{k},\vec{\sigma}}$).

Using eqs. (53a) and (53b) the expectation value of the reduced Hamiltonian is

$$\langle \hat{H}'_R \rangle = 2\sum_{\vec{k}} \xi_{\vec{k}} \left[v^2_{\vec{k}} + \left(u^2_{\vec{k}} - v^2_{\vec{k}}\right) f_{\vec{k}} \right]$$

$$+ \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} \left[u^*_{\vec{k}} v_{\vec{k}} u_{\vec{k}'} v^*_{\vec{k}'} (1 - 2f_{\vec{k}})(1 - 2f_{\vec{k}'}) \right] \text{.....(54)}$$

In this case the "Gap equation" becomes,

$$\Delta = V \sum_{\vec{k}} u_{\vec{k}} v_{\vec{k}}^{*} (1 - 2f_{\vec{k}}) \qquad \text{.........(55)}$$

This expression gives the temperature dependence of the energy gap. As $T \to 0$, the gap is $\Delta \to \Delta(0)$. With the help of eq. (22)

$$\Delta = V \sum_{\vec{k}} \frac{\Delta}{2E_{\vec{k}}} \left[1 - \frac{2}{\exp\left(E_{\vec{k}} / k_B T \right) + 1} \right]$$

Where $E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + \Delta^2(T)}$ by analogy to the case of zero temperature.

$$1 = V \sum_{\vec{k}} \frac{1}{2E_{\vec{k}}} \left[1 - \frac{2}{\exp\left(E_{\vec{k}} / k_B T \right) + 1} \right]$$

Replacing summation with the integration yields, after simple algebra,

$$1 = N(0)V \int_{-\hbar\omega_c}^{\hbar\omega_c} \frac{d\xi}{2(\xi^2 + \Delta^2(T))^{1/2}} \tanh \frac{\sqrt{\xi^2 + \Delta^2(T)}}{2k_B T} \qquad \text{.........(56)}$$

By manipulating,

$$1 = N(0)V \left\{ \int_{-\hbar\omega_c}^{\hbar\omega_c} \frac{d\xi}{2\xi} \tanh \frac{\xi}{2k_B T} + k_B T \sum_{\omega} \int_{-\infty}^{+\infty} d\xi \left[\frac{1}{(E + i\hbar\omega)(E - i\hbar\omega)} - \frac{1}{(\xi + i\hbar\omega)(\xi - i\hbar\omega)} \right] \right\} \text{...(57)}$$

[It can be written that, $\tanh \frac{\xi}{2k_B T} = 2k_B T \sum_{\omega} \frac{1}{(\xi \pm i\hbar\omega)}$, where $\hbar\omega = 2\pi k_B T\left(n + \frac{1}{2}\right)$ [n is the set of all positive and negative integers] and it can be used to evaluate $\frac{1}{2\xi} \tanh \frac{\xi}{2k_B T}$ and $\frac{1}{2\xi} \tanh \frac{\xi}{2k_B T} = k_B T \sum_{\omega} \frac{1}{(\xi + i\hbar\omega)(\xi - i\hbar\omega)}$]

Where the second term is convergent and we may extend the limits of the integral to $\pm\infty$ with no significant loss in accuracy.

The 1st term in the square brackets has poles at $\xi = \pm i(\hbar^2\omega^2 + \Delta^2)^{\frac{1}{2}}$ with residues of $\pm \pi / (\hbar^2\omega^2 + \Delta^2)^{\frac{1}{2}} \cong \pm \pi / \hbar\omega \; (1 + \Delta^2 / 2\hbar^2\omega^2)$.

The corresponding poles of the second term are at $\xi = \pm i\hbar\omega$ with residues of $\pm \pi/\hbar\omega$. Using the property $\int_{-\hbar\omega_c}^{\hbar\omega_c} \frac{d\xi}{2\xi} \tanh\frac{\xi}{2k_BT} = \ln\left(\frac{1.13\hbar\omega_c}{k_BT}\right)$, which we shall calculate in the next topic.

Completing the contour in either half plane, we may write eq. (57)

$$\left[N(0)V\ln\left(\frac{1.13\hbar\omega_c}{k_BT}\right) - 1\right] + 2\pi N(0)Vk_BT\sum_{\omega}\left[\frac{1}{\hbar|\omega|\left(1+\frac{\Delta^2(T)}{2\hbar^2\omega^2}\right)} - \frac{1}{\hbar|\omega|}\right] = 0.$$

Expanding the denominator of the 1st term in the second square bracket to order $\frac{\Delta^2(T)}{\hbar^2\omega^2}$ yields

$$\left[1 - N(0)V\ln\left(\frac{1.13\hbar\omega_c}{k_BT}\right)\right] + \pi N(0)Vk_BT\Delta^2(T)\sum_{\omega}\frac{1}{\hbar^3|\omega|^3} = 0.$$

[Now, $\sum_{\omega}\frac{1}{\hbar^3|\omega|^3} = (\pi k_BT_c)^{-3}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^3} = (\pi k_BT_c)^{-3}\frac{7}{8}\zeta(3)$, T has been set equal to T_c.]

$$\Delta^2(T) = \frac{\left[N(0)V\ln\left(\frac{1.13\hbar\omega_c}{k_BT}\right) - 1\right]}{\pi N(0)Vk_BT(\pi k_BT_c)^{-2}\frac{7}{8}\zeta(3)}$$

When temperature is near T_c ($T \approx T_c$). We can write $T = T_c(1-\epsilon)$. Then taking upto 1st order of ϵ in $\ln(1-\epsilon)$ and $(1-\epsilon)^{-1}$, we get

$$\Delta^2(\epsilon) \approx \frac{(\pi k_BT_c)^2}{\frac{7}{8}\zeta(3)}\epsilon.$$

$$\Rightarrow \Delta^2(T) \approx \frac{(\pi k_BT_c)^2}{\frac{7}{8}\zeta(3)}\left(1-\frac{T}{T_c}\right) \text{.....(58)}$$

$$\text{So,} \quad \Delta(T) \approx \left(1-\frac{T}{T_c}\right)^{\frac{1}{2}} \text{.....(59)}$$

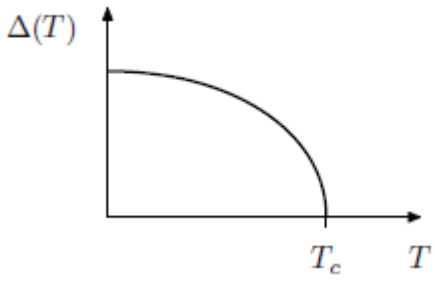

FIG 2: Temperature variation of energy gap predicted by BCS.

2.7 Estimation of critical temperature:

At $T = T_c$, the gap is $\Delta = 0$. Hence, replacing T in eq. (56) with T_c and setting $\Delta = 0$ yields an equation with respect to T_c:

$$\frac{1}{N(0)V} = \int_0^{\hbar\omega_c} \frac{d\xi}{\xi} \tanh\frac{\xi}{2k_BT_c} \text{.....(60)}$$

$$\frac{1}{N(0)V} = \int_0^Z \frac{dz}{z} \tanh z \quad \text{where the cutoff, } Z = \frac{\hbar\omega_c}{2k_BT_c}$$

$$\frac{1}{N(0)V} = [\ln z \ \tanh z]_0^Z - \int_0^Z dz \ln z \ \text{sech}^2 z$$

The upper limit is very large and can be approximated as,

$$\frac{1}{N(0)V} = \ln\left(\frac{\hbar\omega_c}{2k_BT_c}\right) - \int_0^\infty dz \ln z \ \text{sech}^2 z$$

$$\left[\int_0^\infty dz \ln z \ \text{sech}^2 z = -\ln\frac{4e^\gamma}{\pi}\right]$$

$$k_BT_c = \frac{2e^\gamma}{\pi}\hbar\omega_c exp\left(-\frac{1}{N(0)V}\right) \qquad [e^\gamma \approx 1.781]$$

$$\Longrightarrow k_BT_c = 1.13\hbar\omega_c exp\left(-\frac{1}{N(0)V}\right) \text{.....(61)}$$

On the other hand, we already know (from eq. (30))

$$\Delta(0) = 2\hbar\omega_c exp\left(-\frac{1}{N(0)V}\right)$$

Then

$$2\Delta(0) = 3.54\ k_BT_c \text{.....(62)}$$

2.8 Isotope effect

Let say, $\hbar\omega_c$ energy is equal to Debye energy $\hbar\omega_D$, because the origin of attractive interaction is electron-phonon interaction and phonon comes due to vibration of lattices. Then from eq. (58)

$$T_c \propto \omega_D.$$

Recalling that the Debye frequency varies as:

$$\omega_D \propto M^{-\frac{1}{2}}.$$

Where M is the mass of the isotope.

So, $$T_c \propto M^{-\frac{1}{2}}.$$

The critical temperatures are different for different isotopes of the same superconducting element and following rule is satisfied.

$$T_c M^{\frac{1}{2}} = \text{constant.}$$

This is effect is called isotope effect.

2.9 Calculation of the free energy:

The entropy for Fermions is given by the usual expression from statistical mechanics:

$$S = -k_B \sum_{\vec{k},\vec{\sigma}} \left[f_{\vec{k}} ln f_{\vec{k}} + \left(1 - f_{\vec{k}}\right) \ln(1 - f_{\vec{k}}) \right]$$

$$= -2k_B \sum_{\vec{k}} \left[f_{\vec{k}} ln f_{\vec{k}} + \left(1 - f_{\vec{k}}\right) \ln(1 - f_{\vec{k}}) \right]$$

Putting the form of $f_{\vec{k}} = \frac{1}{\exp\left(E_{\vec{k}}/k_B T\right)+1}$

$$-TS = \sum_{\vec{k}} \left[E_{\vec{k}} \left(1 - 2f_{\vec{k}}\right) - 2k_B T ln \left(2 \cosh \frac{E_{\vec{k}}}{2k_B T}\right) \right] \text{.....(63)}$$

The Helmholtz free energy in the pairing approximation is given by

$$F = \langle \hat{H}'_R \rangle - TS.$$

The contribution of $\langle \hat{H}_{IR} \rangle$ to the energy can be obtained from eq. (54) and (55).

$$\langle \hat{H}_{IR} \rangle = -\sum_{\vec{k}} \frac{\Delta^2}{2E_{\vec{k}}} \left(1 - 2f_{\vec{k}}\right)$$

$$= -\frac{\Delta^2(T)}{V} \text{.....(64)}$$

And

$$\langle \hat{H}'_0 \rangle = 2 \sum_{\vec{k}} [\xi_{\vec{k}} v_{\vec{k}}^2 + f_{\vec{k}} E_{\vec{k}} - \frac{\Delta^2}{E_{\vec{k}}} f_{\vec{k}}] \text{.....(65)}$$

So,

$$\langle \hat{H}'_R \rangle = 2 \sum_{\vec{k}} [\xi_{\vec{k}} v_{\vec{k}}^2 + f_{\vec{k}} E_{\vec{k}} - \frac{\Delta^2}{E_{\vec{k}}} f_{\vec{k}}] - \frac{\Delta^2}{V} \text{.....(66)}$$

Using eq. (64) and (66) we obtain

$$\langle \hat{H}'_R \rangle = 2 \sum_{\vec{k}} [\xi_{\vec{k}} v_{\vec{k}}^2 + f_{\vec{k}} E_{\vec{k}} - \frac{\Delta^2}{2E_{\vec{k}}}] \text{.....(67)}$$

Using eq. (63) and (67) we get

$$F_s = \sum_{\vec{k}} \left[2\xi_{\vec{k}} v_{\vec{k}}^2 + E_{\vec{k}} - \frac{\Delta^2(T)}{E_{\vec{k}}} - 2k_B T ln\left(2\cosh\frac{E_{\vec{k}}}{2k_B T}\right)\right] \ldots\ldots\ldots\ldots\ldots\ldots (68)$$

This is the expression for free energy in the superconducting state.

In the normal state the expression for free energy can be obtained by setting $\Delta^2(T) = 0$ and $E_{\vec{k}} = \xi_{\vec{k}}$.

$$F_n = \sum_{\vec{k}} \left[\xi_{\vec{k}} - 2k_B T ln\left(2\cosh\frac{\xi_{\vec{k}}}{2k_B T}\right)\right] \ldots\ldots\ldots\ldots\ldots\ldots (69)$$

$$\therefore F_s - F_n = \sum_{\vec{k}} \left[2\xi_{\vec{k}} v_{\vec{k}}^2 + E_{\vec{k}} - \frac{\Delta^2(T)}{E_{\vec{k}}} - 2k_B T ln\left(2\cosh\frac{E_{\vec{k}}}{2k_B T}\right)\right] - \left[\xi_{\vec{k}} - 2k_B T ln\left(2\cosh\frac{\xi_{\vec{k}}}{2k_B T}\right)\right] \propto -\Delta^2$$

(Around T_c)

2.10 Temperature dependence of Critical magnetic field

We know that, $F_s - F_n = -\frac{H_c^2(T)}{8\pi}$.

$$\Longrightarrow H_c \propto \Delta. \qquad \text{(Near } T_c\text{)}$$

Actually, $H_c \propto \left(1 - \left(\frac{T}{T_c}\right)^2\right)$. Behavior of H_c is almost same as Δ with temperature.

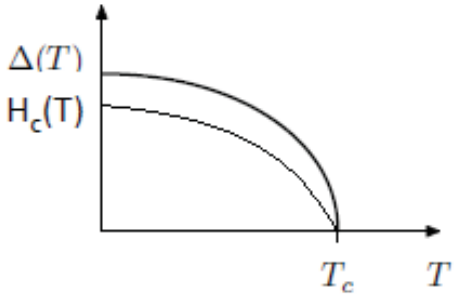

FIG 3: Variation of $\Delta(T)$ & $H_c(T)$ with temperature

2.11 Calculation of Specific heat

To calculate we have to use the expression for S:

$$S = -2k_B \sum_{\vec{k}} \left[f_{\vec{k}} ln f_{\vec{k}} + \left(1 - f_{\vec{k}}\right) \ln(1 - f_{\vec{k}})\right]$$

$$C_v = T\frac{dS}{dT}$$

$$= -2k_B T \sum_{\vec{k}} \left[ln f_{\vec{k}} - \ln(1 - f_{\vec{k}})\right] \frac{df_{\vec{k}}}{dT}$$

$$= 2k_BT\sum_{\vec{k}}\frac{E_{\vec{k}}}{k_BT}\frac{d}{dT}\left(\frac{1}{\exp\left(E_{\vec{k}}/k_BT\right)+1}\right)$$

$$= \frac{-2}{k_BT^2}\sum_{\vec{k}} f_{\vec{k}}\left(1-f_{\vec{k}}\right)\left(-E_{\vec{k}}{}^2 + T\Delta\frac{d\Delta}{dT}\right)$$

$$= \frac{2}{k_BT^2}N(0)\int_0^\infty d\xi\, f(E)[1-f(E)]\left(E^2 - T\Delta\frac{d\Delta}{dT}\right)$$

$$= \frac{2}{k_BT}N(0)\int_0^\infty d\xi\, f^2(E)\left(\frac{E^2}{T} - \frac{d\Delta^2}{2dT}\right)e^{\frac{E}{k_BT}} \text{.....(70)}$$

Because $\frac{d\Delta^2}{dT}$ vanishes in the normal state, we write difference between the heat capacity in the superconducting and normal states at T_c as,

$$(C_v^s - C_v^n)_{T=T_c} = -\frac{2}{k_BT}N(0)\int_0^\infty d\xi\, f^2(E)\frac{d\Delta^2}{2dT}e^{\frac{E}{k_BT}}$$

$$= N(0)\int_0^\infty d\xi\frac{df(E)}{dE}\frac{d\Delta^2}{dT}\bigg|_{T=T_c}$$

In the vicinity of $T = T_c$, the gap is well approximated by $\Delta^2 \sim \frac{(\pi k_B T_c)^2}{\frac{7}{8}\zeta(3)}\left|1-\frac{T}{T_c}\right|$. Then the discontinuity in the heat capacity is,

$$\Delta C_v = C_v^s - C_v^n \approx \frac{\pi^2 {k_B}^2 T_c N(0)}{\frac{7}{8}\zeta(3)} \text{.....(71)}$$

At very low temperature ($T \to 0$), $f(E) \ll 1$, $f(E) = e^{-\frac{E}{k_BT}}$ and $\Delta\frac{d\Delta}{dT} \cong 0$, and the heat capacity approaches the limiting form

$$C_v^s \cong \frac{2N(0)\Delta^2(0)}{k_BT^2}\int_0^\infty e^{-\left(\sqrt{\xi^2+\Delta^2(0)}/k_BT\right)}d\xi$$

$$\cong \frac{2N(0)\Delta^2(0)e^{-\frac{\Delta(0)}{k_BT}}}{k_BT^2}\int_0^\infty e^{-\left(\xi^2/2k_BT\Delta(0)\right)}d\xi$$

$$\cong 2N(0)\Delta(0)(2\pi)^{\frac{1}{2}}k_B\left(\frac{\Delta(0)}{k_BT}\right)^{\frac{3}{2}}e^{-\frac{\Delta(0)}{k_BT}}$$

which decays exponentially.

In the normal state $\Delta = 0$. So, $E = \xi$ and eq. (70) becomes

$$C_v^n = \frac{2}{k_BT}N(0)\int_0^\infty d\xi\, f^2(\xi)\frac{\xi^2}{T}e^{\frac{\xi}{k_BT}}$$

After carrying out the integration we get,

$$C_v^n = 4N(0){k_B}^2T$$

So, we get the following behavior of the variation of specific heat with temperature,

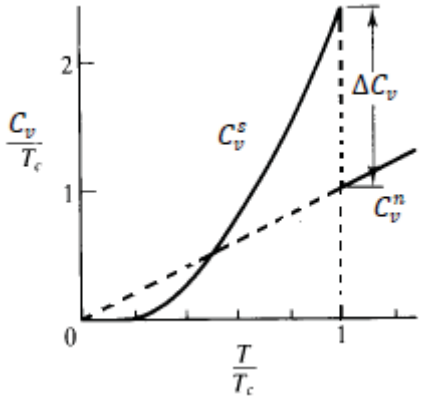

FIG 4: Temperature variation of heat Specific predicted by BCS.

3. Conclusion:

Thus, we can conclude that the BCS theory is a extraordinary powerful microscopic theory to understand the above various properties of superconductors. The original BCS theory predicts that the isotope exponent $\alpha = \frac{1}{2}$. Most common superconductors (Zn, Pb, Hg etc.) agree very well with this prediction. But there are exceptions of this prediction. Reduced effect is observed in Molybdenum and Osmium (Mo, Os) and zero isotope effect is observed in Ruthenium (Ru). In other systems such as the high temperature superconductor, $YBa_2Cu_3O_7$, the absence of isotope effect may indicate that the lattice phonons are not really involved in the pairing mechanism. In these materials applicability of BCS theory is limited, more sophisticated schemes need to be developed.

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