THE VARIATION OF ISOTOPE EFFECT COEFFICIENT α IN IMPURE HIGH T_c SUPERCONDUCTORS

By

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Abstract

The value of the critical temperature T_c and isotope coefficient α could be greatly affected by a number of factors. Among them are the presence of magnetic impurities, non-magnetic impurities, disorder and defects. Following previous calculation of the critical temperature and isotope effect by Singh and Kishore (P. Singh and R. Kishore, J. Supercond. **8**, 9 (1995)), Singh *et al.* (S. P. Singh, R. K. Pandey, and P. Singh, J. Supercond. **9**, 277 (1996)), Openov (Phys. Rev. B **58**, 9468 (1998)) and Openov *et al.* (Phys. Rev. B **64**, 12513 (2001)) we have considered the effect of disorder (defect) on the superconducting transition temperature T_c and isotope coefficient α with in the BCS model. An expression for T_c and α as a function of potential and spin-flip scattering rates is derived by means of Green's functions technique. This is done with the introduction of the matrix Green function in the Nambu representation. The expression for $\ln\left(\frac{T_c}{T_{co}}\right)$ and $\left(\frac{\alpha}{\alpha_o}\right)$ is obtained for a superconductor with an arbitrary degree of anisotropy of the superconducting order parameter, ranging from isotropic s-wave to d-wave and including anisotropic s-wave and mixed (s+d)-wave as particular cases. The universal dependence of $\left(\frac{T_c}{T_{co}}\right)$ on φ (a factor proportional to $\frac{1}{\tau}$, where τ is the total relaxation time) and $\left(\frac{\alpha}{\alpha_o}\right)$ on δ or φ for a given value of χ (a coefficient for anisotropy of the order parameter) is shown in different plots for different cases.

Key words: AG-equation, Superconducting transition temperature T_c, Isotope effect coefficient, Impurity effect, Disorder (defect) effect.

Chapter 1

Introduction and Overview

In the history of understanding the phenomenon of superconductivity isotope effect plays an important role and also helps in the development of a theory describing the microscopic nature of the phenomenon. In 1950, Fröhlich [1] initiated the modern approach to the theory of superconductivity, by focusing attention on an interaction between electrons which had been completely ignored up till then. According to him; if an electron gets scattered by a lattice (superconducting one), emitting a quanta of elastic wave (phonon) in the process and another electron absorbs this very phonon there by itself being scattered, what we have in effect is an electron-electron interaction transmitted by phonons. One of the qualitative consequences of this theory is that superconductivity involves the motion, i.e, the dynamics, of the lattice ions. Due to this significant effects on the superconductivity of the dynamical properties of the lattice ions (in particular their mass) are expected. This was the anticipation of the isotope effect before it was observed.

Experimentally the isotope effect in superconductivity was simultaneously and independently discovered, in 1950 by Maxwell [2], and by Rynolds *et al.* [3]. It states that the critical temperature T_c is proportional to $M^{-\alpha}$ for isotopes of the same element:

$$T_c \quad \propto \quad M^{-\alpha} \quad \Leftrightarrow \quad T_c M^{\alpha} = const. \tag{1.0.1}$$

where M is the isotopic mass and $\alpha = \frac{1}{2}$ for phonon induced superconductivity. The effect was first observed in mercury and then in a number of other elements and compounds. This was also the first direct experimental indication of a particular mechanism of superconductivity.

There are several models used for treating superconductivity and its isotope effect.

The first and simplest model is the BCS one-square-well model, [4] in which the attractive electron-phonon interaction is cut off at the Debye energy $\hbar\omega_D$ and the repulsive coulomb interaction is neglected. The equation for the critical temperature (T_c), $T_c \propto \omega_D \exp[-\frac{1}{N(0)V}]$ implies that the isotope effect described by its isotope coefficient α, $\alpha = 0.5$ holds in this model. (N.B. In this thesis a system of units in which $\hbar = 1$ is used. Temperatures are expressed in energy units ($\kappa_B = 1$).) The inclusion of the repulsive coulomb interaction with the same energy cut off does not alter the isotope effect, since the only dependence on ionic mass is through the Debye frequency ω_D.

In the two-square well model [5], the Coulomb repulsion μ is assumed to have a separate energy cut-off $\omega_c \simeq \varepsilon_F$ which is independent of the ion masses. In this model

$$T_c \propto \omega_D \exp\left[-\frac{1}{(\lambda-\mu^*)}\right] \Rightarrow \alpha = \frac{1}{2}\left(1-\left[\frac{\mu^*}{\lambda-\mu^*}\right]^2\right) \tag{1.0.2}$$

where $\frac{1}{\mu^*} = \frac{1}{\mu} + \ln(\frac{\omega_c}{\omega_D})$.

The isotope effect α is therefore only limited to values of $-\infty < \alpha \leq 0.5$.

The McMillan [6] equation, which has been refined in [7], is an approximation for strong and weak coupling superconductors. It yields

$$T_c = \left(\frac{\omega}{1.2}\right) \exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right] \tag{1.0.3}$$

for the transition temperature and

$$\alpha_{McMillan} = \frac{1}{2}\left[1-\left(\frac{1.04(1+\lambda)(1+0.62\lambda)(\mu^*)^2}{[\lambda-\mu^*(1+0.62\lambda)]^2}\right)\right] \tag{1.0.4}$$

for the isotope effect parameter.

These equations all predict large deviations from the BCS value of $\alpha = 0.5$ at small λ for modest μ^*, with the magnitude of the deviations decreasing with increasing λ. Thus, for elements with large λ, these models predict an isotope shift close to 0.5 unless very large values of μ^* occur. For weak coupling superconductors, the models generally agree with the calculation [8] which also qualitatively predicts the values for strong-coupling materials and the transition metals. Table 1 shows characteristic values of the isotope coefficient (α) for different types of superconductors. Very different values of α have been observed in the range from -2 to +1. One notes that some systems have a negligible coefficients, some display even an "inverse isotope coefficient" ($\alpha < 0$), and some take values greater than 0.5, the value predicted by Fröhlich and the BCS model (for a monatomic system).

Superconductor	α	Superconductor	α
Hg	0.5 ± 0.03	Zr	0.0
Ti	0.5 ± 0.01	PdH(D)	-0.25
Cd	0.5 ± 0.01	U	-2
Mo	0.33 ± 0.05	$La_{1.85}Sr_{0.15}CuO_4$	0.07
Os	0.21 ± 0.01	$La_{1.89}Sr_{0.11}CuO_4$	0.75
Ru	0.0	($^{16}O -^{18}O$ subs.)	
		K_3C_{60}	0.37 or 1.4
		($^{12}C -^{13}C$ subs.)	

Table 1 Experimental values of the isotope coefficient of T_c [see [9]]

The understanding that α is a measure of the contribution of phonons to the pairing mechanism leads to confusions, which is particularly true for the high-temperature

superconductors. Indeed several factors not related to the pairing mechanism can alter the value of the isotope coefficient. So the value of α (even in its absence) does not allow any apriori conclusion about the pairing mechanism.
The calculation of α and its comparison with experimental results was used to determine the value of the Coulomb repulsion μ^* or the relative weight of different electron-phonon coupling strengths in superconductors. It can thus be used as a tool for the characterization of superconductors.

In 1986, J. George Bednorz and K. Alex Müller [10] made a starting discovery while studying the conductivity of the ceramic, lanthanum-barium copper-oxide ($La_{2-x}Ba_xCuO_4$). They discovered superconductivity in the ceramic at 35K for $x \simeq 0.15$. The result was very surprising for two reasons

- Ceramics are usually insulating rather than conducting, so that superconductivity was not expected at any temperature, and
- Such a high value of T_c had never been observed in any material in 75 years of active research on superconductivity.

Following this discovery a related material $YBa_2Cu_3O_7$ was discovered with the critical temperature of 92K! Many additional high-T_c superconductors have been discovered with T_c above 30K and different characterization of superconductors appear. Figure (1.1) shows the progress in T_c of superconductor materials with time.

Superconductivity is characterized by an order parameter $\Delta_{\alpha\beta}(\mathrm{r},r')$ that describes pairing of fermion with time-reversed momentum, **k** and -**k**.

If the order parameter is constant or nearly constant on the Fermi surface the superconductor is called s-wave (conventional) superconductor. They have even orbital function of momentum **k** with l = 0 analogy with the notation for the atomic states. In momentum space $\Delta(\mathbf{k}) = \Delta_o$. Conventional superconductors are characterized by isotropic s-state (wave) pairing which gives rise superconducting energy gap

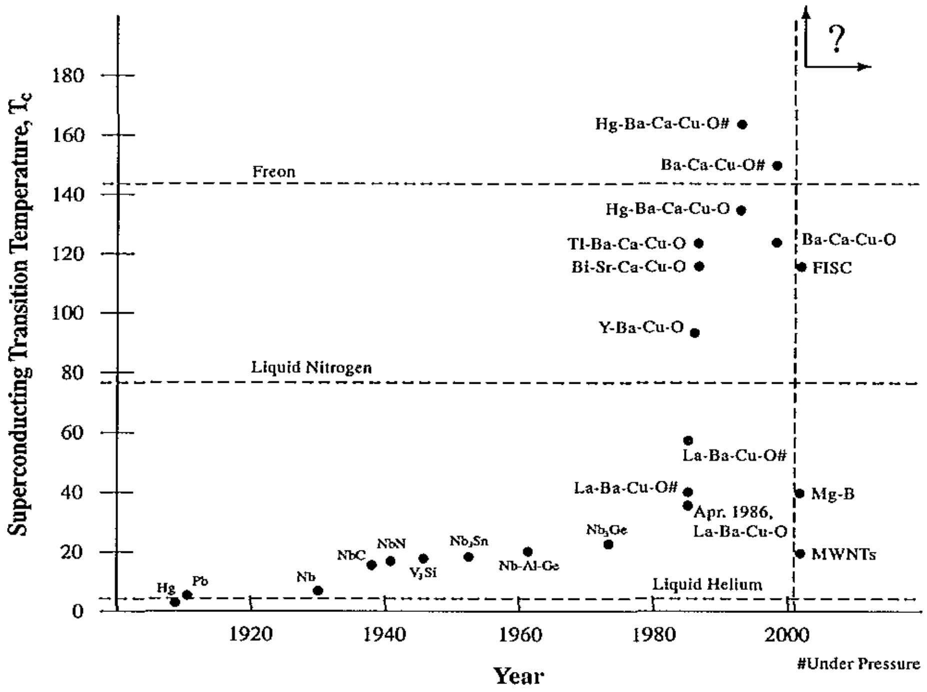

Figure 1.1: Graph showing the historical rise of the maximum known critical temperature including high-temperature superconductors.

which is every where finite (no nodes) over the Fermi surface and have an exponential temperature dependence (for the penetration depth) $\lambda(T) \propto \exp(-\frac{\Delta}{T})$.

A superconductor with vanishing order parameter averaged over the Fermi surface is called unconventional superconductor. Here $\sum_k < a_{k\alpha}, a_{-k\beta} >= 0$.

p-, d-, or higher waves where this relation holds are unconventional superconductor. Unconventional (specially cuprate) superconductors are characterized by apparent d-state (wave) pairing where there are nodes (i.e. states in overall gap) and the temperature dependence (for the penetration depth) is expected to be a power law $\lambda(T) \propto (\frac{T}{\Delta_{max}})^n$, with n=1 for line nodes.

Schematic comparison of the s-wave and $d_{x^2-y^2}$-wave pairing potentials and the corresponding quasiparticle tunnelling spectra are shown in Fig (1.2).

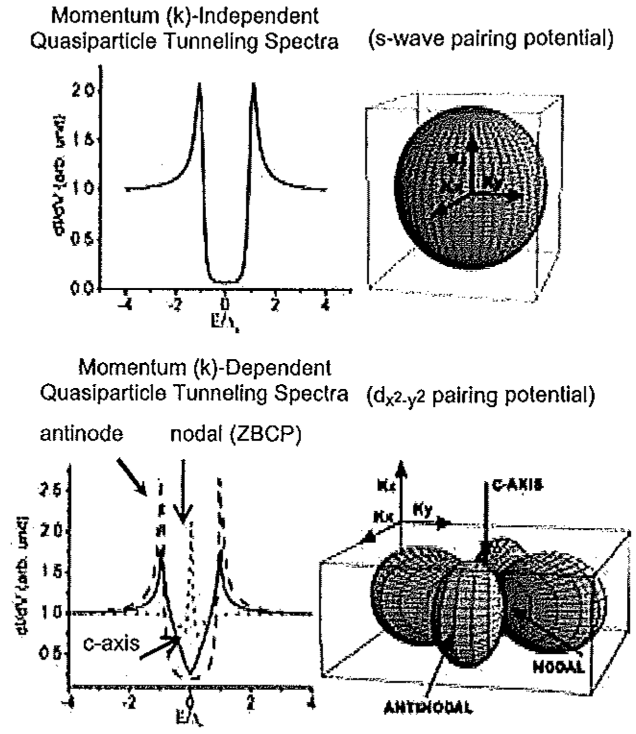

Figure 1.2: Comparison of s-wave and $d_{x^2-y^2}$-wave pairing potentials in the momentum (k) space and the corresponding quasiparticles tunnelling spectra for quasiparticles momentum along various principal axes.

Though conventional BCS mechanism is based on electron-phonon interaction this interaction is insufficient to explain high-T_c superconductivity. Superconducting transition can also be caused by a non-phonon mechanism [9]. Historically, the introduction of electronic mechanism started the race for higher T_c's. The pairing can be provided by the exchange of excitations such as exitons, plasmons, magnons etc. In general one can have a combined mechanism [11, 12] which may provide an explanation for the unusual occurrence of high T_c's and small isotope coefficient α.

Several non-phononic as well as combined mechanisms have been proposed that lead to a reduction of the isotope effect [13].

The main purpose of this paper is to explain how the isotope coefficient varies in impure and/or disordered superconductors. Specially it tries to treat high-T_c superconductors of different kind. The effect of impurity and/or disorder on the critical temperature as well as on the isotope coefficient of superconductors is treated deeply. In addition to that it tries to forward ideas on the role of the variation of α to high-T_c superconductivity and room temperature superconductivity.

The remaining part of this paper is presented as follows:

In chapter 2 we see a detailed literature review on isotope effect, critical temperature, mechanism of high-T_c superconductivity and effect of impurity,disorder and defect in superconductivity.

The remaining chapters are devoted to the description of the theoretical background, mathematical techniques, mathematical formulations, and the conclusion to the problem.

In chapter 3 we see the theoretical starting and forward the mathematical ways of treating superconductivity.

Chapter 4 is concerned with the mathematical formulation starting with the model and formalism used to see the effect of impurity and disorder in superconductors. Particularly we will look at the isotope effect and the critical temperature due to impurity and disorder of different types of superconductors. In the last section of this chapter the results are analyzed and discussed with the help of different graphs. Finally conclusion and short summary of the whole paper is given in chapter 5.

Chapter 2

Literature Review

Introduction

As indicated in the introduction part isotope effect of superconductivity plays an important role in developing a theory describing the microscopic nature of superconductivity. In this chapter we are going to observe the works of different authors around the area of superconductivity. As in any other rapidly developing field of research, many speculations and suggestions have been advanced in superconductivity. Though there are large number of papers written around superconductivity we have to restrict ourselves to areas related to the isotope effect, critical temperature of superconductors, high-T_c superconductivity and its nature (mechanism).

Having this in mind this chapter is presented in to three sections namely: isotope effect and critical temperature of conventional superconductors, high-T_c superconductivity and its mechanism, and effects of impurity, disorder and defect in superconductivity.

2.1 Isotope Effect and Critical Temperature in Conventional Superconductors

Here we treat works on isotope effect and critical temperature in conventional superconductors.

Fröhlich [1] forwards a theory describing the nature of the phenomena of superconductivity. He was the first to suggest the importance of the electron-phonon(el-ph) interaction in explaining superconductivity.

Experimentally Fröhlich's suggestion was confirmed by the discovery of the "isotope effect", i.e., the proportionality of T_c to $M^{-\frac{1}{2}}$ for isotopes of the same element, by Maxwell (1950) [2] and Reynolds, *et al.* (1950) [3] independently.

The basic idea that even a weak interaction can bind pairs of electrons into a bound state was presented by Cooper in 1956 [14]. What he showed was that the Fermi sea of electrons is unstable against the formation of at least one bound pair, regardless of how weak the interaction is, so long as it is attractive.

Bardeen *et al.*(1957) [4] present a theory of superconductivity which works well for low temperature superconductors. They show that electron-electron pairing interactions mediated by phonons neglecting Coulomb repulsion. The theory predicts that T_c can be expressed as

$$T_c = 1.13\omega \exp[-\frac{1}{N(0)V}] \tag{2.1.1}$$

and for a monatomic system the isotope coefficient is $\alpha = 0.5$. There are differences in the value of α between theory ($\alpha = 0.5$) and experiment (refer table 1). This may be due to the fact that BCS did not take Coulomb repulsion into account.

Inclusion of Coulomb interaction was first done by Morel and Anderson (1962) [15]. They propose the two-square-well model for which T_c is derived by including Coulomb interaction. Coulomb interactions are included by the introduction of the pseudo potential μ^* in the BCS equation for T_c as:

$$T_C = 1.13\Theta_D \exp(-\frac{1}{\lambda - \mu^*}) \tag{2.1.2}$$

where Θ_D is the Debye temperature and μ^* is the pseudo-potential given by

$$\mu^* = \frac{\mu}{1 + \mu \ln \frac{\varepsilon_F}{\omega_D}} \tag{2.1.3}$$

μ is the Coulomb potential and ε_F is the Fermi energy.

The corresponding IC is then

$$\alpha = \frac{1}{2}\Big[1 - \Big(\frac{\mu^*}{\lambda - \mu^*}\Big)^2\Big] \tag{2.1.4}$$

The effect of Coulomb interaction can be induced in a similar way in the strong coupling Eliashberg theory (1960) [16].

McMillan (1968) [6] calculate the superconducting transition temperature as a function of electron-phonon and electron-electron coupling constants within the frame work of the strong coupling theory. Using this result, he found empirical values of the coupling constants and the "band-structure" density of states for a number of metals and alloys. Having these results one can predict a maximum superconducting transition temperature.

Using the formula derived by McMillan

$$T_C = \frac{\omega}{1.2} \exp\big(-\frac{1.04(1+\lambda)}{\lambda - \tilde{\mu}}\big) \tag{2.1.5}$$

with $\tilde{\mu} = (1 + 0.62)\mu^*$ and μ^* given by Eq (2.1.3) the isotope coefficient is

$$\alpha = \frac{1}{2}\Big[1 - \frac{1.04(1+\lambda)\tilde{\mu}\mu^*}{[\lambda - \tilde{\mu}]^2}\Big] \tag{2.1.6}$$

An expression for T_c valid for the whole range of coupling strengths (from weak to very strong coupling) has been derived by Kresin (1987) [17]. According to him

$$T_c = \frac{6.25\omega}{\sqrt{e^{\frac{2}{\lambda_{eff}}} - 1}} \tag{2.1.7}$$

with

$$\lambda_{eff} = \frac{\lambda - \mu^*}{1 + 2\mu^* + \lambda\mu^* t(\lambda)}$$

and $t(\lambda) \simeq 1.5\exp(-0.28\lambda)$. The isotope effect coefficient resulting from this reads

$$\alpha = \frac{1}{2}\left[1 - \frac{(\mu^*)^2}{\lambda_{eff}(1 - e^{-\frac{2}{\lambda_{eff}}})}\left(\frac{1}{\lambda - \mu^*} + \frac{2 + \lambda t(\lambda)}{3 + \lambda t(\lambda)}\right)\right] \tag{2.1.8}$$

In all the above cases we see that the strongest deviation from the BCS monatomic value 0.5 occurs when μ^* (or $\tilde{\mu}$) is of the order of λ. Thus a small isotope coefficient is correlated to low T_c excluding anharmonic or band structure effects. In certain cases inverse (negative) isotope coefficient ($\alpha < 0$) is observed (refer table 1).

In conclusion we see that the Coulomb interaction and its logarithmic weakening leads to the deviation of the isotope coefficient from the value $\alpha = 0.5$ and to the non-universality of α.

2.2 High-Temperature Superconductivity

The field of superconductivity received an immense impetus from the discovery of the new high-temperature superconducting materials in 1986 by Bednorz and Müller [10]. The subsequent development has raised the transition temperature T_c to values as high as $T_c = 135K$. Examples are $La_{2-x}Sr_xCuO_4$ ($T_c \simeq 40K$), $YBa_2Cu_3O_7$ ($T_c \simeq 92K$), $Bi_2Sr_2Ca_2Cu_3O_{10}$ ($T_c \simeq 110K$), $Tl_2Ca_2Ba_2Cu_3O_{10}$ ($T_c \simeq 125K$), and $HgBaCaCuO$ ($T_c \simeq 135K$) [18, 19]. In fact materials have been found with T_c as high as 160K [20]. In these systems conduction is due to holes. An important property of these materials is the strength of their correlations. It was argued that strong correlations provide for the electron attraction which are required in order to obtain the high superconducting transition temperatures in the copper-oxide based materials [18]. In addition the electron-phonon interaction is also strong in these materials and therefore must contribute to T_c significantly.

Though there is a theory (i.e. BCS) that explains low temperature superconductivity large number of theories that will agree with some experiments and disagree with others are formulated to explain high temperature superconductivity. There is no complete microscopic description and certainly no consensus in the community in the mechanism of superconductivity. Different authors forward various theoretical ideas and experimental investigations on the mechanism and effects of high-T_c superconductors. Following are some of the main contributors.

2.2.1 Mechanism

Many mechanisms have been proposed by different workers by using different excitation mechanisms like phonons, polarons, bipolarons, biperoxitons, excitons, correlated charge (pair) transfer, plasmons, spin fluctuations, magnons, resonating valance bond states (see the references in [13]).

Singh *et al.* (1990) [13] proposed a combined phonon-biexiton mechanism to explain the high values of temperature transitions and small values of isotope effect coefficient of high-T_c superconductors. With this mechanism they explain the entire range of high-T_c values by their expression. The expression for (T_c), found by generalized BCS-type integral equation, looks like

$$T_c = 1.14\ \omega_p^{n_1}\omega_e^{n_2}\exp[-(\lambda_p^* + \lambda_e^*)^{-1}]$$

where $n_1 = \frac{\lambda_p}{\lambda_e+\lambda_p}$, $n_2 = \frac{\lambda_e}{\lambda_e+\lambda_p}$,
$\lambda_p^* = \frac{\lambda_p}{1+\lambda_p}$ and $\lambda_e^* = \frac{\lambda_e}{1+\lambda_e}$
In the model the α is given by $\alpha = \frac{n_1}{2}$.

By taking suitable values of the parameter of the system α values can be obtained for any Cu-O superconductors [21].

Rajiv Kumar Pandy, *et al.* (1998) [11] derive the expression for superconducting transition temperature T_c and isotope effect coefficient α from a generalized integral gap equation for a strongly coupled superconductors, when electrons, phonons and electrons biexitons are simultaneously present in high-T_c superconductors.

Shen *et al.* (2001) [22] use high resolution angle resolved photoemission (ARPES) data in conjunction with that from neutron and other probes to show that electron-phonon coupling is strong in cuprate superconductors and it plays an important role in pairing.

Zhao (2004) [23] has determined the polaron binding energy E_P for under doped parent cuprates from the unconventional oxygen-isotope effect on the antiferromagnetic ordering temperature (T_N). He showed that there is a very strong electron-phonon coupling feature at a phonon energy of about 20 meV along the antinodal direction and this coupling becomes weaker towards the diagonal direction. He also showed that high-temperature superconductivity in cuprates is caused by strong electron-phonon coupling, polaronic effect,and significant coupling with 2 eV Cu-O charge transfer fluctuation.

Alexandrov (2004) [24] briefly introduced the Fröhlich-Coulomb-multipolaron model of high-Temperature superconductivity, which include strong on site repulsive correlations and the long-range coulomb and electron-phonon interactions. The extension of the BCS theory to the strong-coupling region with long-range unscreened electron-phonon interaction naturally explains the isotope effects, unconventional thermomagnetic transport, and checkboard modulation of tunnelling density of states in cuprates.

Gweon *et al.* (2004) [25] provide a detailed comparison of the electron dynamics of Bi2212 samples containing different oxygen isotopes, using ARPES. On the basis of the results they propose a model dynamic spin-Peirls picture for the nature of electron-lattice coupling in high temperature superconductors.

Bill *et al.* (1997) [26] present a detailed study of the influence of non-adiabaticity and magnetic impurities on the values of the isotope coefficient (α) based on previous calculations of the the isotope coefficient (α).

Bill *et al.* (1998) [27] show that the various factors that can lead to an isotope dependence of the penetration depth δ. They presented a general equation relating the isotope coefficients of T_c and of δ for London superconductors.

Sorensen and Gygax (1995) [28] analyzed oxygen isotope effect measurements on $YBa_2Cu_3O_7$ substituted with Pr, Ca, and Zn to examine the validity of the large increases in the isotope coefficient at low critical temperature. They found that for Pr and Pr:Ca substitutions there is a correlation between the isotope shift and the width of transition.

Barbee III *et al.* (1998) [8] explored standard isotropic three-dimensional theory for the isotope effect with a purely electron-phonon attractive interaction. They found that additional features are necessary to account for the observed values of the isotope effect in high temperature superconducting oxides.

Zhao *et al.* (2002) [29] review various effects in the high temperature superconducting cuprates to asses the role of electron-phonon interaction. They suggest that for the observed unconventional isotope effects lattice vibrations play an important role in the microscopic pairing mechanism of high-Temperature superconductivity.

2.3 Effects of Impurity, Disorder and Defect in Superconductivity

Magnetic impurities are known to suppress conventional superconductivity and the detailed effects have been a topic of great research interest over the years.

The first experimental investigation on the relation between magnetism and superconductivity was initiated by Mathias *et al.* (1959) [30].

Abrikosov and Gor'kov (1960) [31] showed that there is a critical concentration of paramagnetic impurity which could destroy superconductivity.Below that critical concentration both superconductivity and magnetism can servive.

In (1961) [32] they show that T_c is lowered when paramagnetic impurities are introduced in to a superconductor and forward the known AG- equation given by

$$\ln\left(\frac{T_c}{T_{co}}\right) = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{1}{2\pi T_c \tau}\right) \tag{2.3.1}$$

where τ is the electron relaxation time for exchange interaction.

In (1962) [33] they also successfully explained the suppression of T_c by magnetic impurities by treating the doped magnetic impurities in superconductors as uncorrelated.

Skalski *et al.* (1964) [34] made additional calculations on the effects of paramagnetic impurities in superconductors using the Abrikosov-Gor'kov theory as their starting point.

In contrast, non-magnetic impurities in the dilute limit are found to have negligible effects on conventional superconductivity.

Anderson (1959) [35] showed that much change in T_c or Δ is not expected on going from a clean to a dirty specimen if impurities are non magnetic.

For high-T_c superconductivity different authors forward different ideas on isotope effect, transition temperature, mechanism and order parameter. Following are some of the main contributors.

Singh and Kishore (1995) [36] employ the generalized Abrikosov-Gor'kov theory to describe the isotope effect coefficient α by considering the dependence of the characteristic scattering time for Cooper pairs on the concentrations n of impurities by ignoring disorder.

Singh *et al.* (1996) [19] study the effect of pair breaking and isotope effect coefficient in $La_{2-x}Sr_xCuO_4$ and Pr-, Ca-, and Zn- doped $YBa_2Cu_3O_{7-\delta}$ and $EuBa_2Cu_3O_{7-\delta}$, using the generalized Abrikosov-Gor'kov theory including disorder.

Abrikosov (1996) [37] proposed a model of superconductivity in layered HTSC cuprates and studied the influence of impurity scattering on T_c, the order parameter at T=0 and the density of states, including the energy gap.

Openov (1998) [38] studies the combined effect of both non-magnetic and magnetic impurities on the superconducting transition temperature within the BCS model. He also derives an expression for the critical temperature as a function of potential and spin-flip scattering rates and generalizes the Abrikosov-Gor'kov formula for the critical temperature of impure superconductors. The effect of defects and impurities in HTSC is also discussed.

Openov *et al.* (2001) [39] obtain an expression for the isotope coefficient as a function of the critical temperature for a superconductor with an arbitrary contribution of spin-flip processes to the total scattering rate and an arbitrary degree of anisotropy of superconducting order parameter, ranging from isotropic s-wave and mixed (s+d) wave as particular cases. They found that both non-magnetic and magnetic impurities enhance the isotope coefficient, the enhancement due to magnetic impurities being generally greater than that due to non-magnetic impurities.

Chattophadhyay *et al.* [40] show that disordered short-coherence-length superconductors can exhibit pair breaking from spacial fluctuations in the pairing interaction, in a manner very similar to that found with magnetic impurities. They also studied the effects of a single state with up to three types of defect using the T-matrix approximation, and found bound states with in the superconducting gap arising from either pairing fluctuations or magnetic impurities.

Mierzynska and Wysokinski (2003) [41] study the influence of various kinds of impurities on the isotope shift exponent α of HTSC's. They considered the in-plane and out-of-plane impurities present in layered superconductors and showed that they differently affect T_c. In 2004 [42] they study the isotope effect in disordered weak and strong coupling superconductors of different symmetries of the order parameter. Here they found that weak localization corrections to Eliashberg equation describe a strong degradation of T_c with disorder of s-wave superconductors and isotope coefficient is relatively weak.

Shimahara (2003) [43] examine the isotope effect of superconductivity in systems with coexisting interactions of phonon and non-phonon mechanisms an addition to the direct Coulomb interaction. He proposed a model of superconductors with coexisting interactions of phonon and non-phonon origins. They also examined the impurity effects on the transition temperature T_c and the isotope effect in multiband superconductors with magnetic and non-magnetic impurities, where the effect of Coulomb repulsion is considered [44].

Kresin *et al.* (1997) [45] show that the presence of magnetic impurities affect the value of the IC and these effects can be observed for conventional as well as for the high-T_c superconductors.

Bayndir and Gedik (1999) [46] studied the effect of non magnetic impurities on high temperature superconductors by solving the Bogoliubov-de Gennes equations on a two dimensional lattice via exact diagonalization technique in a fully self-consistent way. They found that s-wave order parameter is almost un affected by impurities at low concentrations while $d_{x^2-y^2}$ wave order parameter exhibits a strong linear decrease with impurity concentration and they evaluated the critical impurity concentration n_i^c at which superconductivity ceases to be 0.1 which is in good agreement with experimental values.

Florens and Vojta (2004) [47] discuss d-wave states under the combined influence of impurities and competing instabilities; such as pairing in a secondary channel as well as lattice symmetry breaking. Using the self consistence T-matrix formalism, they show that disorder can strongly modify the competition between different pairing states.

Chapter 3

Mathematical Techniques

Introduction

In this chapter we are going to have basic fundamental mathematical techniques used to threat the problem that this paper solves. The chapter is subdivided in to sections. The first section is about preliminaries to mathematical techniques. The next mansions the main methods of solving the BCS Hamiltonian since the same methods are commonly applied to the studies of impurity effects in superconductors. The last section treats the solution of the BCS Hamiltonian by the Green's function formalism.

3.1 Preliminaries to Mathematical Techniques

As shown in the previous chapter the prediction and experimental verification of the isotope effect ([1, 2, 3]) led the way towards the BCS theory [4] of superconductivity. Frohlich used a Hamiltonian, now called the Frohlich Hamiltonian, in which interactions between electrons and phonons are included but Coulomb interactions are omitted except as they can be included in the energies of the individual electrons and phonons. He used a perturbation theory approach and found an instability of the ordinary Fermi-surface ground state of the electrons occupying states with equal and opposite momentum and spin if the electron-phonon interaction were sufficiently strong.

Now let us setup Frohlichs Hamiltonian for electron-phonon coupling and try to show that electron-phonon term can lead to an attractive force between electrons. Basically the idea is that an electron distorts or polarizes the positive ions in its vicinity, so that it carries with it an associated displacement field and this displacement field $\mathbf{P}(\mathbf{r})$ can be such that a net attraction between electrons is possible. i.e. when one electron leaves a region of the lattice, it leaves behind an excess of positive ion density, which in turn attracts another electron into this region. See figure (3.1).

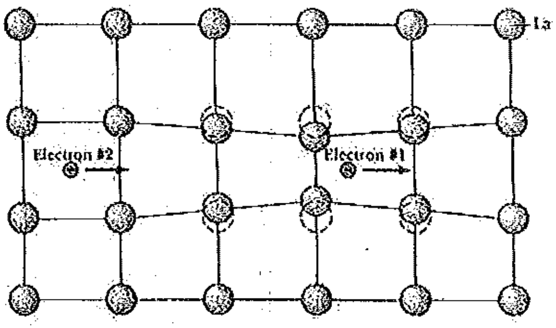

Figure 3.1: The phonon is created by the passing of a nearby electron attracting the positive lattice ions to itself. The higher density of positive charge is the quasi-particle called the phonon, and it propagates through the lattice with the electron

Basic Hamiltonian of Pairing Mechanism

The total Hamiltonian (Frohlich's Hamiltonian) of a superconductor (with electrons, phonons and their interaction) in second quantized form is

$$\hat{H} = \sum_k \epsilon_k a_k^\dagger a_k \; + \; \sum_q \omega_q b_q^\dagger b_q \; + \; \sum_{k,q} \chi_{kq} a_{k+q}^\dagger a_k (b_q + b_{-q}^\dagger) = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{ep} \quad (3.1.1)$$

where $\hat{H}_{el} = \sum_k \epsilon_k a_k^\dagger a_k$ is Hamiltonian of non interacting electrons,
$\hat{H}_{ph} = \sum_q \omega_q b_q^\dagger b_q$ is Hamiltonian of non interacting phonons, and

$\hat{H}_{ep} = \sum_{k,q} \chi_{k,q} a^{\dagger}_{k+q} a_k (b_q + b^{\dagger}_{-q})$ is the electron phonon interaction.

The following relation can be used

$$\sum_k a^{\dagger}_{k-q} a_k = \sum_k a_{k+q} a^{\dagger}_k$$

Consider $\hat{H}_o = \hat{H}_{el} + \hat{H}_{ph}$ as the un perturbed Hamiltonian and $\hat{H}_{ep}$ as the perturbation.

$\hat{H}_{ep}$ does not immediately show us that there is an electron-electron interaction between phonons. To make this interaction apparent, we can treat the problem by making a canonical transformation which is used to diagonalize the Hamiltonian. We use the generalized Lang-Firsov transformation which is such that

$$\tilde{Q} = e^{-s} Q e^{s} \tag{3.1.2}$$

Q being any operator. The unitary transformation is the special case where $s^* = -s$. Then we apply Baker-Hausdorff theorem that states

$$\tilde{Q} = e^{-s} Q e^{s} = Q + [Q, s] + \frac{1}{2!}[s, [s, Q]] + \frac{1}{3!}[s, [s, [s, Q]]] + ... = Q + \sum_{n=1}^{\infty} \frac{[s_n, Q]}{n!} \tag{3.1.3}$$

where s_n is defined by the recurrence relation $s_n = [s, [s_{n-1}]]$ with ($s_1 = s$). Using Eqs. (3.1.2, 3.1.3) we shall take a transformation on Eq. (3.1.1) in which there are no off diagonal terms of order χ.

We write Eq. (3.1.1) as

$$\hat{H} = \hat{H}_o \ + \ \hat{H}_{ep}$$

and then look for a transformation of the form

$$\tilde{H} = e^{-U} H e^{U} \tag{3.1.4}$$

that will eliminate $\hat{H}_{ep}$ to first order. Using Eq. (3.1.3) we have

$$\tilde{H} = e^{-U} Q e^{U} = \hat{H} \ + \ [\hat{H}, U] \ + \ \frac{1}{2!}[U, [U, H]] \ + \ ... \tag{3.1.5}$$

Substitute the value of $\hat{H}$ in Eq. (3.1.1) in to Eq. (3.1.5) to get

$$\tilde{H} = (\hat{H}_o + \hat{H}_{ep}) \; + \; [(\hat{H}_o + \hat{H}_{ep}), U] \; + \; \frac{1}{2!}[U, [U, (\hat{H}_o + \hat{H}_{ep})]] \; + \; ...$$

$$\tilde{H} = \hat{H}_o + \hat{H}_{ep} + [\hat{H}_o, U] + [\hat{H}_{ep}, U] + \frac{1}{2!}[U, ([U, \hat{H}_o] + [U, \hat{H}_{ep}])] + \; ... \tag{3.1.6}$$

Choose a condition such that

$$\hat{H}_{ep} + [\hat{H}_o, U] = 0 \tag{3.1.7}$$

so that U is in the first order. With this Eq. (3.1.6) becomes

$$\tilde{H} = \hat{H}_o \; + \; \frac{1}{2!}[\hat{H}_{ep}, U] \; + \; ... \tag{3.1.8}$$

the omitted terms being of the order of U^3 or higher. Since $\hat{H}_o$ and $\hat{H}_{ep}$ are expressed in Eq. (3.1.1) let us try to find the value of U. Assume that U can have the form

$$U \; = \; \sum_{kq} \chi_{kq} a^{\dagger}_{k+q} a_k (A b_q + B b^{\dagger}_{-q}) \tag{3.1.9}$$

with A and B coefficients to be determined. Substitute the value of $\hat{H}_o$,$\hat{H}_{ep}$ and U in to Eq. (3.1.7)

$$\hat{H}_{ep} + [\hat{H}_o, U] = 0$$

$$-\hat{H}_{ep} = [\hat{H}_o, U] = \Big[(\sum_k \epsilon_k a^{\dagger}_k a_k \; + \; \sum_q \omega_q b^{\dagger}_q b_q), \sum_{kq} \chi_{kq} a^{\dagger}_{k+q} a_k (A b_q + B b^{\dagger}_{-q})\Big]$$

$$-\hat{H}_{ep} = \Big[\sum_k \epsilon_k a^{\dagger}_k a_k, \sum_{k'q} \chi_{k'q} a^{\dagger}_{k'+q} a_{k'} (A b_q + B b^{\dagger}_{-q})\Big]$$

$$+ \; \Big[\sum_q \omega_q b^{\dagger}_q b_q, \sum_{kq'} \chi_{kq'} a^{\dagger}_{k+q'} a_k (A b_{q'} + B b^{\dagger}_{-q'})\Big]$$

To simplify this we use the following commutation relations

$$\left.\begin{array}{l}[a_k^\dagger, b_q] = [a_k^\dagger, b_q^\dagger] = [a_k, b_q] = [a_k, b_q^\dagger] \\ [b_q, b_{q'}^\dagger] = b_q b_{q'}^\dagger - b_{q'}^\dagger b_q = \delta_{q,q'} \\ [b_q, b_{q'}] = [b_q^\dagger, b_{q'}^\dagger] = [a_k, a_{k'}] = [a_q^\dagger, a_{q'}^\dagger] = 0 \\ [A, BC] = [A, B]C + B[A, C] \\ [AB, C] = A[B, C] + [A, C]B \\ [A, BC] = \{A, B\}C - B\{A, C\} \\ [AB, C] = A\{B, C\} - \{A, C\}B \end{array}\right\} \tag{3.1.10}$$

with these relations the above equation becomes

$$-\hat{H}_{ep} = \Big[\sum_k \epsilon_k a_k^\dagger a_k, \sum_{k'q} \chi_{k'q} a_{k'+q}^\dagger a_{k'}(Ab_q + Bb_{-q}^\dagger)\Big]$$

$$+ \Big[\sum_q \omega_q b_q^\dagger b_q, \sum_{kq'} \chi_{kq'} a_{k+q'}^\dagger a_k(Ab_{q'} + Bb_{-q'}^\dagger)\Big]$$

$$= \sum_{kk'q} \chi_{k'q}[\epsilon_k a_k^\dagger a_k, a_{k'+q}^\dagger a_{k'}](Ab_q + Bb_{-q}^\dagger) \ + \ \sum_{kqq'} \chi_{kq'} a_{k+q'}^\dagger a_k[\omega_q b_q^\dagger b_q, (Ab_{q'} + Bb_{-q'}^\dagger)]$$

$$= \sum_{kk'q} \big(\epsilon_k a_k^\dagger \delta_{k,k'+q} a_{k'} - \epsilon_k \delta_{k,k'} a_k a_{k'+q}^\dagger\big)(Ab_q + Bb_{-q}^\dagger) \ +$$

$$\sum_{kqq'} \chi_{kq'} a_{k'+q}^\dagger a_k\big(-\omega_q A \delta_{q,q'} b_q \ + \ \omega_{-q} B b_q^\dagger \delta_{q,-q'}\big)$$

$$= \sum_{k'q'} \chi_{k'q'} a_{k'+q'}^\dagger a_{k'}[(\epsilon_{k'+q'} - \epsilon_{k'})(Ab_{q'} + Bb_{-q'}^\dagger) \ + \ (-\omega_{q'} Ab_{q'} + \omega_{-q'} Bb_{-q'}^\dagger)$$

$$= \sum_{k'q'} \chi_{k'q'} a_{k'+q'}^\dagger a_{k'}\big(\epsilon_{k'+q'} - \epsilon_{k'} - \omega_{q'}\big)Ab_{q'} \ + \ \sum_{k'q'} \chi_{k'q'} a_{k'+q'}^\dagger a_{k'}\big(\epsilon_{k'+q'} - \epsilon_{k'} + \omega_{-q'}\big)Bb^{\dagger -q'}$$

changing the dummy indices k' to k, q to q' and using

$\hat{H}_{ep} = \sum_{k,q} \chi_{k,q} a_{k+q}^\dagger a_k(b_q + b_{-q}^\dagger)$ we get

$$-\sum_{k,q} \chi_{k,q} a_{k+q}^\dagger a_k(b_q + b_{-q}^\dagger) = \sum_{k,q} a_{k+q}^\dagger a_k(\epsilon_{k+q} - \epsilon_k - \omega_q)Ab_q + \sum_{k,q} a_{k+q}^\dagger a_k(\epsilon_{k+q} - \epsilon_k + \omega_{-q})Bb_{-q}^\dagger$$

$$\Rightarrow \ -1 = (\epsilon_{k+q} - \epsilon_k - \omega_q)A \quad and \quad -1 = (\epsilon_{k+q} - \epsilon_k + \omega_{-q})B$$

$$A = \frac{1}{\epsilon_{k+q} - \epsilon_k - \omega_q} \qquad B = \frac{1}{\epsilon_{k+q} - \epsilon_k + \omega_{-q}} \tag{3.1.11}$$

with these values Eq. (3.1.9) becomes

$$U \;=\; \sum_{kq} \chi_{kq} a^{\dagger}_{k+q} a_k (A b_q + B b^{\dagger}_{-q})$$

$$U = -\sum_{kq} \chi_{kq} a^{\dagger}_{k+q} a_k \Big(\frac{b_q}{\epsilon_{k+q} - \epsilon_k - \omega_q} \;+\; \frac{b^{\dagger}_{-q}}{\epsilon_{k+q} - \epsilon_k + \omega_{-q}} \Big) \tag{3.1.12}$$

Then we have to determine the reduced Hamiltonian ($\tilde{H}$) using Eq. (3.1.8)

$$\tilde{H} = \hat{H}_o \;+\; \frac{1}{2!}[\hat{H}_{ep}, U] \;+\; ...$$

$$\tilde{H} = \hat{H}_o \;+\; \frac{1}{2}\Big[\sum_{k,q} \chi_{k,q} a^{\dagger}_{k+q} a_k (b_q + b^{\dagger}_{-q}), -\sum_{kq} \chi_{kq} a^{\dagger}_{k+q'} a_k \Big(\frac{b_{q'}}{\epsilon_{k+q'} - \epsilon_k - \omega_{q'}}$$

$$+ \frac{b^{\dagger}_{-q'}}{\epsilon_{k+q'} - \epsilon_k + \omega_{-q'}} \Big) \Big] \tag{3.1.13}$$

In solving the commutator we have to examine particularly the set that arise from commuting the phonon operators.

$$[\hat{H}_{ep}, U] = -\Bigg(\Big[\sum_{k,q} \chi_{k,q} a^{\dagger}_{k+q} a_k (b_q + b^{\dagger}_{-q}), \sum_{kq} \chi_{kq'} a^{\dagger}_{k+q'} a_k \frac{b_{q'}}{\epsilon_{k+q'} - \epsilon_k - \omega_{q'}} \Big] \;+$$

$$\Big[\sum_{k,q} \chi_{k,q} a^{\dagger}_{k+q} a_k (b_q + b^{\dagger}_{-q}), \sum_{kq'} \chi_{kq'} a^{\dagger}_{k+q'} a_k \frac{b^{\dagger}_{-q'}}{\epsilon_{k+q'} - \epsilon_k + \omega_{-q'}} \Big] \Bigg)$$

$$= -\Bigg(\sum_{k,q} \chi_{k,q} a^{\dagger}_{k+q} a_k \frac{\chi_{q'} a^{\dagger}_{k+q'} a_k}{\epsilon_{k+q'} - \epsilon_k - \omega_{q'}} [b^{\dagger}_{-q}, b_{q'}] + \sum_{k,q} \chi_{k,q} a^{\dagger}_{k+q} a_k \frac{\chi_{q'} a^{\dagger}_{k+q'} a_k}{\epsilon_{k+q'} - \epsilon_k + \omega_{-q'}} [b_q, b^{\dagger}_{-q'}] \Bigg)$$

$$[\hat{H}_{ep}, U] = -\sum_{kqq'} \Bigg(-\chi_{kq} \chi_{kq'} \frac{a^{\dagger}_{k+q} a_k a^{\dagger}_{k+q'} a_{k'}}{\epsilon_{k+q'} - \epsilon_k - \omega_{q'}} \delta_{-q,q'} \;+\; \chi_{kq} \chi_{kq'} \frac{a^{\dagger}_{k+q} a_k a^{\dagger}_{k+q'} a_{q'}}{\epsilon_{k+q'} - \epsilon_k + \omega_{-q'}} \delta_{q,-q'} \Bigg)$$

$$= -\sum_{kqq'} |\chi_q|^2 a^\dagger_{k+q} a_k a^\dagger_{k'+q'} a_{k'} \left(-\frac{1}{\epsilon_{k+q'} - \epsilon_k - \omega_{q'}} + \frac{1}{\epsilon_{k+q'} - \epsilon_k + \omega_{-q'}} \right)$$

$$[\hat{H}_{ep}, U] = -\sum_{kqq'} |\chi_q|^2 a^\dagger_{k+q} a_k a^\dagger_{k+q'} a_{k'} \left(\frac{-\epsilon_{k+q'} + \epsilon_{k'} + \omega_{-q'} + \epsilon_{k+q'} - \epsilon_k - \omega_{q'}}{(\epsilon_{k+q'} - \epsilon_k - \omega_{q'})(\epsilon_{k+q'} - \epsilon_k + \omega_{-q'})} \right)$$

using $\omega_{q'} = \omega_{-q'} = \omega_q$ we arrive at

$$[\hat{H}_{ep}, U] \; = \; -\sum_{kqq'} |\chi_q|^2 a^\dagger_{k+q} a^\dagger_{k'-q} a_{k'} a_k \left(\frac{-2\omega_q}{(\epsilon_{k'+q} - \epsilon_{k'})^2 - \omega_q^2} \right) \qquad (3.1.14)$$

with this result Eq. (3.1.13) becomes

$$\tilde{H} = \hat{H}_o + \frac{1}{2}[\hat{H}_{ep}, U] = \hat{H}_o \; + \; \sum_{kqq'} |\chi_q|^2 a^\dagger_{k+q} a^\dagger_{k'-q} a_{k'} a_k \left(\frac{\omega_q}{(\epsilon_{k'+q} - \epsilon_{k'})^2 - \omega_q^2} \right) \qquad (3.1.15)$$

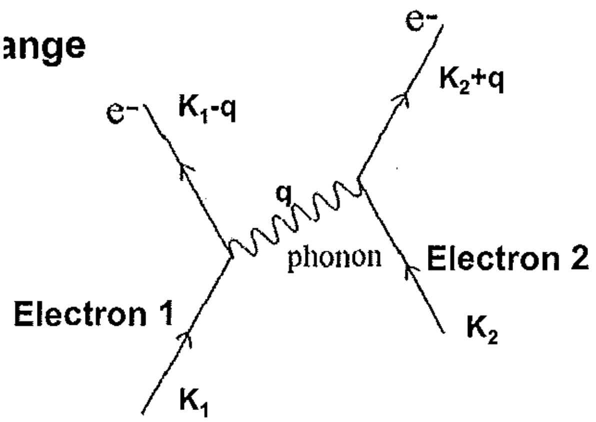

Figure 3.2: electron-electron interaction via phonons. In the process the electron 1 (with $\mathbf{k}_1$) emits a phonon of wave vector q. The phonon is absorbed later by the second electron 2 (with $\mathbf{k}_2$).

We know that superconductivity involves a phase transition in the electron gas brought about by attractive electron interactions. The interaction part is negative, i.e., attractive over the range of energies when $|\epsilon_{k+q} - \epsilon_k| < \omega_q$. It is in this narrow range that such an attraction leads to the condensation of electrons, which characterizes the superconducting phase. The existence of Cooper pairs, in which two electrons of opposite wave number and spin is the foundation for the BCS theory of superconductivity. The electron-electron indirect interaction through the lattice phonons is shown in Fig (3.2).

3.2 Methods of Solving BCS Hamiltonian

There are different methods of solving the BCS hamiltonian.The following methods are the main once:

- direct diagonalization via Bogoliubov-Valatin transformation
- BCS variational wave function in which there is variational determination of the ground state energy from the trial wave function and
- Green's function formalism.

The three approaches are complementary and equivalent in the case of homogeneous superconductors. However, some of them are better suited for addressing specific questions in the presence of impurities. In particular we will see the Green's function method which is some times advantageous for determining the thermodynamic properties of a material and averaging over many impurity configurations. The Green's function method originates with the work of Gor'kov.

3.3 BCS Hamiltonian by The Green's Function Formalism

Here we solve the BCS hamiltonian in a simpler way.

Consider the model Hamiltonian of a system (superconductor) having a form like Eq. (3.1.1). Using canonical transformation we approach to a result which looks like Eq. (3.1.15).

Let the reduced Hamiltonian have the form

$$\hat{H} = \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} - V \sum_{kk'} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} a_{-k'\downarrow} a_{k'\uparrow} \qquad (3.3.1)$$

where $\epsilon_k = \frac{\hbar^2 k^2}{2m}$.

To calculate the energy spectrum of the superconductor we construct the Green's function and search for the poles.

Defining is the temperature Green's function as

$$G_\sigma(k,\tau) = - < T_\tau a_{k\sigma}(\tau) a^\dagger_{k\sigma} >$$

as the usual single-particle Green's function and

$$F(k,\tau) = - < T_\tau a_{k\uparrow}(\tau) a_{-k\downarrow} > \quad ; \quad \tilde{F}(k,\tau) = - < T_\tau a^\dagger_{-k\downarrow}(\tau) a^\dagger_{k\uparrow} >$$

as the *anomalous* Green's function, which clearly vanish in the normal state, the Fourier transform with respect to frequency of the equations of motions for these Green's functions is calculated below. In the above definition$< >$stands for thermodynamic averaging with the Hamiltonian.

$$< a_{k\sigma}(\tau) a^\dagger_{-k\lambda} >= \frac{Tr[e^{-\beta\kappa} a_{k,\sigma}(t) a^\dagger_{-k\lambda}]}{Tr[e^{-\beta\kappa}]}$$

Using $G(k,\omega_n) \equiv \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega$ the equation of motion of the Green's function is given by

$$\omega \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega = \delta(t) < [a_{k\uparrow}, a^\dagger_{k'\uparrow}] > + < [a_{k\uparrow}, \hat{H}], a^\dagger_{k'\uparrow} >_\omega$$

$$\omega \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg_{\omega} = \delta_{kk'} + < [a_{k\uparrow}, \hat{H}], a^{\dagger}_{k'\uparrow} >_{\omega} \tag{3.3.2}$$

Now let us evaluate the commutator $[a_{k\uparrow}, \hat{H}]$

$$\begin{aligned}
[a_{k\uparrow}, \hat{H}] &= [a_{k\uparrow}, (\sum_{k\sigma} \epsilon_k a^{\dagger}_{k\sigma} a_{k\sigma} - V \sum_{kk'} a^{\dagger}_{k\uparrow} a^{\dagger}_{k'\downarrow} a_{k'\downarrow} a_{-k\uparrow})] \\
&= [a_{k\uparrow}, \sum_{p\sigma} \epsilon_p a^{\dagger}_{p\sigma} a_{p\sigma}] - [a_{k\uparrow}, V \sum_{pp'} a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow}] \\
&= \sum_{p\sigma} \epsilon_p [a_{k\uparrow}, a^{\dagger}_{p\sigma} a_{p\sigma}] - V \sum_{pp'} [a_{k\uparrow}, a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow}]
\end{aligned}$$

using Eq. (3.1.10) this becomes

$$= \sum_{p\sigma} \epsilon_p ([a_{k\uparrow}, a^{\dagger}_{p\sigma}] a_{p\sigma} + a^{\dagger}_{p\sigma} [a_{k\uparrow}, a_{p\sigma}]) - V \sum_{pp'} ([a_{k\uparrow}, a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\downarrow}] a_{p'\downarrow} a_{-p'\uparrow} + a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\downarrow} [a_{k\uparrow}, a_{p'\downarrow} a_{-p'\uparrow}])$$

$$[a_{k\uparrow}, \hat{H}] = \sum_{p\sigma} \epsilon_p \delta_{k,p} \delta_{\uparrow,\sigma} a_{p\sigma} - V \sum_{pp'} \left([a_{k\uparrow}, a^{\dagger}_{p\uparrow}] a^{\dagger}_{-p\downarrow} + a^{\dagger}_{p\uparrow} [a_{k\uparrow}, a^{\dagger}_{-p\downarrow}]\right) a_{p'\downarrow} a_{-p'\uparrow}$$

$$[a_{k\uparrow}, \hat{H}] = \epsilon_k a_{k\uparrow} - V \sum_{pp'} \delta_{kp} a^{\dagger}_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow} = \epsilon_k a_{k\uparrow} - V \sum_{kp'} a^{\dagger}_{-k\downarrow} a_{p'\downarrow} a_{-p'\uparrow} \tag{3.3.3}$$

So Eq. (3.3.2) becomes

$$\begin{aligned}
\omega \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg_{\omega} &= \delta_{kk'} + < [a_{k\uparrow}, \hat{H}], a^{\dagger}_{k'\uparrow} >_{\omega} \\
&= \delta_{k,k'} + < (\epsilon_k a_{k\uparrow} - V \sum_{kp'} a^{\dagger}_{-k\downarrow} a_{p'\downarrow} a_{-p'\uparrow}), a^{\dagger}_{k'\uparrow} >_{\omega} \\
(\omega + \epsilon_k) \ll a_{k\uparrow}, a^{\dagger}_{k'\uparrow} \gg_{\omega} &= \delta_{k,k'} \ - \ V \sum_{pp'} \ll a^{\dagger}_{-k\downarrow} a_{p'\downarrow} a_{-p'\uparrow}, a^{\dagger}_{k'\uparrow} \gg_{\omega} \qquad (3.3.4)
\end{aligned}$$

In order to reduce the second term of the RHS we have to use Wick's theorem which states that

In making all the possible pairing between creation and annihilation operators, each pairing should be time ordered. The time ordering of each pair gives the proper time ordering to the entire result.

For example

$$< |ABCD| > \simeq < |AB| >< |CD| > \pm < |AC| >< |BD| > \ + \ < |AD| >< |BC| >$$

So we can use the following decoupling

$$\ll a^\dagger_{-k\downarrow} a_{p'\downarrow} a_{-p'\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega \;\simeq\; < a_{p'\downarrow} a_{-p'\uparrow} > \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega \tag{3.3.5}$$

substitute this in to Eq. (3.3.4) to get

$$(\omega - \epsilon_k) \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega = \delta_{k,k'} \;-\; V \sum_{pp'} < a_{p'\downarrow} a_{-p'\uparrow} > \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega$$

Define the superconducting energy gap parameter as

$$V \sum_{pp'} < a_{p'\downarrow} a_{-p'\uparrow} > = \Delta \tag{3.3.6}$$

$$(\omega - \epsilon_k) \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega = \delta_{k,k'} \;-\; \Delta \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega \tag{3.3.7}$$

Next we need to evaluate $\ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = \tilde{F}(k, w_n)$ using the same procedure as above. Since our objective is to find the equation of motion for a cooper pair. i.e., an equation of the form $< a_{k\uparrow} a_{-k\downarrow} >$ or $< a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} >$. So the equation of motion for $\ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega$ is given by

$$\omega \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = \delta(t)[a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}] \;+\; < [a^\dagger_{-k\downarrow}, \hat{H}], a^\dagger_{k'\uparrow} >_\omega \tag{3.3.8}$$

$$\omega \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = - < [a^\dagger_{-k\downarrow}, (\sum_{p\sigma} \epsilon_p a^\dagger_{p\sigma} a_{p\sigma} - V \sum_{pp'} a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow})], a^\dagger_{k'\uparrow} >_\omega$$

where

$$\begin{aligned}
[a^\dagger_{-k\downarrow}, \hat{H}] &= [a^\dagger_{-k\downarrow}, (\sum_{p\sigma} \epsilon_p a^\dagger_{p\sigma} a_{p\sigma} - V \sum_{pp'} a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow})] \\
&= [a^\dagger_{-k\downarrow}, \sum_{p\sigma} \epsilon_p a^\dagger_{p\sigma} a_{k\sigma}] - [a^\dagger_{-k\downarrow}, V \sum_{pp'} a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow}] \\
&= \sum_{p\sigma} \epsilon_p [a^\dagger_{-k\downarrow}, a^\dagger_{p\sigma} a_{k\sigma}] - V \sum_{pp'} [a^\dagger_{-k\downarrow}, a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} a_{p'\downarrow} a_{-p'\uparrow}]
\end{aligned}$$

again we have to use the relation in Eq. (3.1.10) to get

$$[a^\dagger_{-k\downarrow}, \hat{H}] = \sum_{p\sigma} \epsilon_p (\{a^\dagger_{-k\downarrow}, a^\dagger_{p\sigma}\} a_{p\sigma} \;-\; a^\dagger_{p\sigma} \{a^\dagger_{-k\downarrow}, a_{p\sigma}\}) \;-$$

$$
\begin{aligned}
&V\sum_{pp'}([a^\dagger_{-k\downarrow}, a^\dagger_{p\uparrow}a^\dagger_{-p\downarrow}]a_{p'\downarrow}a_{-p'\uparrow} + a^\dagger_{p\uparrow}a^\dagger_{-p\downarrow}[a^\dagger_{-k\downarrow}, a_{p'\downarrow}a_{-p'\uparrow}]) \\
&= -\sum_{p\sigma}\epsilon_p\delta_{-k,p}\delta_{\downarrow,\sigma} \ - \ V\sum_{pp'}a^\dagger_{p\uparrow}a^\dagger_{-p\downarrow}\{a^\dagger_{-k\downarrow}, a_{p'\downarrow}\}a_{-p'\uparrow} \\
&[a^\dagger_{-k\downarrow}, \hat{H}] = -\epsilon_{-k}a^\dagger_{-k\downarrow} - V\sum_p a^\dagger_{p\uparrow}a^\dagger_{-p\downarrow}a_{k\uparrow}
\end{aligned}
\tag{3.3.9}
$$

Substitute this in to Eq. (3.3.8) we obtain

$$
\begin{aligned}
\omega \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega &= \delta(t)[a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow}] \ + \ < [a^\dagger_{-k\downarrow}, \hat{H}], a^\dagger_{k'\uparrow} >_\omega \\
&= \ll (-\epsilon_{-k}a^\dagger_{-k\downarrow} - V\sum_p a^\dagger_{p\uparrow}a^\dagger_{-p\downarrow}a_{k\uparrow}), a^\dagger_{k'\uparrow} \gg_\omega \\
(\omega + \epsilon_{-k}) \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega &= -V\sum_p \ll a^\dagger_{p\uparrow}a^\dagger_{-p\downarrow}a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega
\end{aligned}
$$

applying Wick's theorem to the RHS of this equation leads to

$$
(\omega - \epsilon_{-k}) \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = -V\sum_p < a^\dagger_{p\uparrow}a^\dagger_{-p\downarrow} > \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega
$$

But $V\sum_p < a^\dagger_{p\uparrow}a^\dagger_{-p\downarrow} >= \Delta^*$ and we can use

$$
\Delta = \Delta^*
$$

So we have

$$
(\omega + \epsilon_{-k}) \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = -\Delta \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega \tag{3.3.10}
$$

Finally from equations (3.3.7) and (3.3.10) we have

$$
\begin{aligned}
(\omega - \epsilon_k) \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega &= \delta_{k,k'} \ - \ \Delta \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega \\
(\omega + \epsilon_{-k}) \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega &= -\Delta \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega
\end{aligned}
$$

Since the term $\ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega$ participates in the formation of cooper pairs we need to solve these equations for $\ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega$. solving the second equation for $\ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega$ gives

$$
\ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega = -\frac{(\omega + \epsilon_{-k})}{\Delta} \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega .
$$

Substitute this into the first equation

$$(\omega - \epsilon_k) \ll a_{k\uparrow}, a^\dagger_{k'\uparrow} \gg_\omega = \delta_{k,k'} \; - \; \Delta \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega$$

$$-\frac{(\omega - \epsilon_k)(\omega + \epsilon_{-k})}{\Delta} \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = \delta_{k,k'} \; - \; \Delta \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega$$

since energy is an even function of k, $\epsilon_k = \epsilon_{-k} = \epsilon$ we have

$$\left(\Delta - \frac{(\omega^2 - \epsilon^2)}{\Delta}\right) \ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = \delta_{k,k'}.$$

For the case of $k = k'$ and $\delta_{k,k'} = 1$ we get

$$\ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = -\frac{\Delta}{\omega^2 - (\epsilon^2 + \Delta^2)}$$

$$\ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = -\frac{\Delta}{\omega^2 - \epsilon^2 - \Delta^2} = -\frac{\Delta}{\omega^2 - (\epsilon^2 + \Delta^2)}$$

$$\ll a^\dagger_{-k\downarrow}, a^\dagger_{k'\uparrow} \gg_\omega = -\frac{\Delta}{\omega^2 - \xi^2} \quad , \quad where \;\; \xi^2 = \epsilon^2 + \Delta^2 \tag{3.3.11}$$

We can generalize this result using matrix Green's function. A matrix Green's function was introduced by Nambu which are very useful to draw one's intuition about perturbation theory in normal metals to calculate various things in the superconducting state. He defined the two-component field spaning particle-hole space:

$$\mathrm{a}_k = \begin{pmatrix} a_{k\uparrow} \\ a^\dagger_{-k\downarrow} \end{pmatrix} \quad , \quad \mathrm{a}^\dagger_k = (a^\dagger_{k\uparrow} a_{-k\downarrow})$$

The Nambu or matrix Green's function is then defined as

$$\hat{G}_o \equiv - < T_\tau \mathrm{a}_k(\tau) \mathrm{a}^\dagger_k > = \begin{pmatrix} G_\uparrow(k,\tau) & -F(k,\tau) \\ -\tilde{F}(k,\tau) & G_\downarrow(-k,\tau) \end{pmatrix} \tag{3.3.12}$$

For a single homogeneous superconductor the Fourier transform with respect to frequency of the matrix elements are then given by (ω can be replaced by $i\omega$)

$$G_\uparrow(k,\omega) = -\frac{i\omega + \epsilon(k)}{\omega^2 + (\epsilon(k)^2 + |\Delta(k)|^2)} \quad , \quad \tilde{F}(k,\omega) = \frac{\Delta^*}{\omega^2 + (\epsilon(k)^2 + |\Delta(k)|^2)}$$

$$F(k,\omega)=\frac{\Delta}{\omega^2+(\epsilon(k)^2+|\Delta(k)|^2)}\quad,\quad G_{\downarrow}(-k,\omega)=-\frac{i\omega-\epsilon(k)}{\omega^2+(\epsilon(k)^2+|\Delta(k)|^2)}$$

So we have

$$\hat{G}_o=\begin{pmatrix} G_{\uparrow}(k,\omega) & -F(k,\omega) \\ -\tilde{F}(k,\omega) & G_{\downarrow}(-k,\omega) \end{pmatrix}=-\frac{1}{\omega^2-(\epsilon(k)^2+|\Delta(k)|^2)}\begin{pmatrix} i\omega+\epsilon(k) & \Delta(k) \\ \Delta^{*}(k) & i\omega-\epsilon(k) \end{pmatrix} \tag{3.3.13}$$

This can be written as

$$\hat{G}_o=-\frac{i\omega\tau_0+\epsilon(k)\tau_3+\Delta(k)\tau_1}{\omega^2-(\epsilon(k)^2+|\Delta(k)|^2)}$$

where τ_0 is a unit matrix and τ_i, i=1, 2, 3 are Pauli matrices.

The inverse of this matrix is determined using the fact that $\hat{G}_o\hat{G}_o^{-1}=\hat{1}$.

$$\begin{pmatrix} \frac{(i\omega+\epsilon(k))}{x} & \frac{\Delta(k)}{x} \\ \\ \frac{\Delta^{*}(k)}{x} & \frac{(i\omega-\epsilon(k))}{x} \end{pmatrix}\begin{pmatrix} G_{o11}^{-1} & G_{o12}^{-1} \\ \\ G_{o21}^{-1} & G_{o22}^{-1} \end{pmatrix}=\begin{pmatrix} 1 & 0 \\ \\ 0 & 1 \end{pmatrix}$$

where $x=-(\omega^2-(\epsilon(k)^2+|\Delta(k)|^2))$.

$$\begin{pmatrix} (\frac{(i\omega+\epsilon(k))}{x}G_{o11}^{-1}+\frac{\Delta(k)}{x}G_{o21}^{-1}) & (\frac{(i\omega-\epsilon(k))}{x}G_{o12}^{-1}+\frac{\Delta(k)}{x}G_{o22}^{-1}) \\ \\ (\frac{\Delta^{*}(k)}{x}G_{o11}^{-1}+\frac{(i\omega-\epsilon(k))}{x}G_{o21}^{-1}) & (\frac{\Delta^{*}(k)}{x}G_{o12}^{-1}+\frac{(i\omega-\epsilon(k))}{x}G_{o22}^{-1}) \end{pmatrix}=\begin{pmatrix} 1 & 0 \\ \\ 0 & 1 \end{pmatrix}$$

This gives the following systems of simultaneous equations:

$$\frac{(i\omega+\epsilon(k))}{x}G_{o11}^{-1}+\frac{\Delta(k)}{x}G_{o21}^{-1}=1$$

$$\frac{(i\omega-\epsilon(k))}{x}G_{o12}^{-1}+\frac{\Delta(k)}{x}G_{o22}^{-1}=0$$

$$\frac{\Delta^{*}(k)}{x}G_{o11}^{-1}+\frac{(i\omega-\epsilon(k))}{x}G_{o21}^{-1}=0$$

$$\frac{\Delta^{*}(k)}{x}G_{o12}^{-1}+\frac{(i\omega-\epsilon(k))}{x}G_{o22}^{-1}=1$$

Solving the equations leads to the following values

$$G_{o11}^{-1} = i\omega - \epsilon(k)\ ,\ G_{o21}^{-1} = -\Delta^{\star}(k)$$

and

$$G_{o12}^{-1} = -\Delta(k)\ ,\ G_{o12}^{-1} = i\omega + \epsilon(k)$$

So we have:

$$\hat{G}_o^{-1}(k,\sigma,\omega) = \begin{pmatrix} G_{o11}^{-1} & G_{o12}^{-1} \\ G_{o21}^{-1} & G_{o22}^{-1} \end{pmatrix}$$

$$\begin{pmatrix} G_{o11}^{-1} & G_{o12}^{-1} \\ G_{o21}^{-1} & G_{o22}^{-1} \end{pmatrix} = \begin{pmatrix} i\omega - \epsilon(k) & -\Delta(k) \\ -\Delta^{\star}(k) & i\omega + \epsilon(k) \end{pmatrix} \tag{3.3.14}$$

Therefore for a single homogeneous superconductor with a reduced mean field BCS Hamiltonian, the inverse of $\hat{G}_o$ is given by (from Maki, 1969) [48]

$$\hat{G}_o^{-1}(\mathrm{k}\omega) = i\omega_n\tau_o - \epsilon_{\mathrm{k}}\tau_3 - \Delta(\mathrm{k})\sigma_2\tau_1$$

Here $\omega_n = \pi T(2n+1)$ is the Matsubara frequency, σ_i are the Pauli matrices acting in spin space, and τ_i are the Pauli matrices in the particle-hole space, and $\tau_i\sigma_j$ denotes a direct product of the matrices operating in the four-dimensional Nambu space. The self-consistency equation (3.3.6) for a single superconductor takes the form

$$\Delta(\mathrm{k}) = -T\sum_{\omega_n}\int d\mathrm{k}'V(\mathrm{k},\mathrm{k}'Tr[\tau_1\sigma_2G_o]) \tag{3.3.15}$$

In BCS the interaction is restricted to a thin shell of electrons near the Fermi surface, and therefore,

$$\Delta(\hat{\Omega}) = -TN(0)\sum_{\omega_n}\int d\hat{\Omega}'V(\hat{\Omega}\hat{\Omega}')Tr\big[\tau_1\sigma_2\int d\epsilon_{\mathrm{k}}G_o\big]$$

where $\hat{\Omega}$ denotes a direction on the Fermi surface, and N(0) is the normal state density of states.

3.3.1 Gap Equation and T_c

The order parameter in the BCS theory is always determined self consistently by Eq (3.3.6) and must be temperature dependent since it vanishes at the transition. This dependence may be calculated by expressing the expectation value of the pair operator in terms of the Green's function which we have already calculated.

$$< a_{p'\downarrow}a_{-p'\uparrow} >= F(k,0^-) = T\sum_{\omega_n} e^{-i\omega_n 0^-}F(k,\omega_n)$$

$$= T\sum_{\omega_n} e^{-i\omega_n 0^-}\frac{\Delta}{\omega^2+(\epsilon^2+\Delta^2)}$$

$$= \oint \frac{dz}{2\pi i}f(z)e^{-z0^-}\frac{\Delta}{z^2-\xi^2} = \Delta(\frac{f(\xi)}{2\xi}-\frac{f(-\xi)}{2\xi}) = \frac{\Delta}{2\xi}\tanh\frac{\xi}{2T}$$

where f(x) is the Fermi function.

The gap equation then becomes

$$\Delta = V\sum_{pp'} < a_{p'\downarrow}a_{-p'\uparrow} >= V\frac{\Delta}{2\xi}\tanh\frac{\xi}{2T}$$

$$1 = V\sum_{pp'}\frac{1}{2\xi}\tanh\frac{\xi}{2T}$$

This equation may now be solved, first for the critical temperature itself, being the temperature at which $\Delta \to 0$, and then for the normalized order parameter $\frac{\Delta}{T_c}$ for any temperature T. At T_c the gap equation becomes

$$\frac{1}{N(0)V} = \int_0^{\omega_D} d\xi\frac{1}{\xi}\tanh\frac{\xi}{2T} \tag{3.3.16}$$

on integrating and rearranging we arrive at

$$T_c = 1.13\omega_D\exp(-\frac{1}{N(0)V}) \tag{3.3.17}$$

Near T_c we can do by expanding to leading order in the small quantity $\frac{\Delta}{T_c}$ to find a value

$$\frac{\Delta}{T_c} \simeq 3.40(1-\frac{T}{T_c})^{\frac{1}{2}}$$

At T=0 we have

$$\frac{1}{N(0)V} = \int_0^{\omega_D} d\epsilon_k \frac{1}{\xi} = \int_\Delta^{\omega_D} d\xi \frac{N(\xi)}{\xi}$$

$$= \int_\Delta^{\omega_D} \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} \simeq \ln(\frac{2\omega_D}{\Delta})$$

so that $\Delta(0) \simeq 2\omega_D \exp(-\frac{1}{N(0)V})$ or

$$\frac{\Delta(0)}{T_c} \simeq 1.76$$

The graph showing the variation of the order parameter Δ with temperature in the BCS approximation is shown in Fig. (3.3).

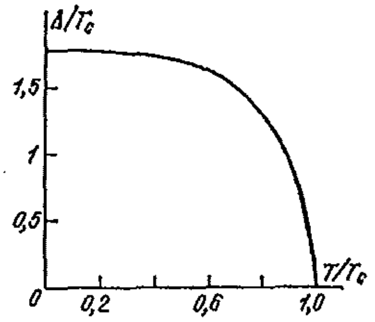

Figure 3.3: Temperature dependence of the energy gap

Chapter 4

Variation of α in Superconductivity

Introduction

This chapter is devoted to treat impurity and disorder effect in superconductivity. Specially it tries to find mathematical relations on the variation of the critical temperature as well as the isotope effect due to the presence of impurity and/or disorder in superconductors.

The model Hamiltonian and formalism used to solve the problem is set in the first section. This starts with a simpler case that there are magnetic impurities only. The second section is an extension. It is known that with in the Born approximation,the effects of pairing disorder and magnetic impurities are identical [40, 48, 49]. So contributions of magnetic impurities, non-magnetic impurities, disorders, defects etc. is studied in a similar manner. The relative shift of the Isotope coefficient ($\frac{\alpha}{\alpha_o}$) is also derived here. In the third section $\frac{\alpha}{\alpha_o}$ is derived by considering the total relaxation time τ as a function of isotopic mass M. Special cases are treated under this section. The chapter is finalized by the results and discussion section. Here the main results found in the third section are summarized using different graphs.

4.1 The Model Hamiltonian and Formalism

The Hamiltonian of a superconductor containing magnetic impurities is given by:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3 \tag{4.1.1}$$

where

- $\hat{H}_1 = \sum_{k,\sigma} \epsilon(k) a^{\dagger}_{k,\sigma} a_{k,\sigma}$ is the energy of the free electrons ,
- $\hat{H}_2 = \sum_{k,p,\sigma,\lambda} U(k,\sigma;p,\lambda) a^{\dagger}_{k,\sigma} a_{p,\lambda}$ is a term describing the effect of impurity scattering , and
- $\hat{H}_3 = \sum_{\mathbf{k},\mathbf{p}} V(\mathbf{k},\mathbf{p}) a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-k\downarrow} a_{\text{-}\mathbf{p}\downarrow} a_{p\uparrow}$ is the effective potential.

Magnetic impurities give rise to the potential scattering and exchange scattering. The total interaction between a conduction electron at $\mathbf{r}$ and all impurities in the sample is

$$U(r) = \sum_{\alpha} [u^{pot}(r - R_\alpha) + J(r - R_\alpha)\mathrm{s}.\mathrm{S}_\alpha] \tag{4.1.2}$$

In the momentum space this becomes

$$\begin{aligned} U(k,\sigma,p,\lambda) &= U_1(k,p,\sigma)\delta_{\sigma,\lambda} + U_2(k,p,\sigma)\delta_{\sigma,-\lambda} \\ &= [u^{pot} \sum_{\alpha} e^{-i(k-p).R_\alpha} + \frac{1}{2} J(k,p)\gamma_\sigma \sum_{\alpha} e^{-i(k-p).R_\alpha} S^z_\alpha]\delta_{\sigma,\lambda} \\ &+ \frac{1}{2} \sum_{\alpha} J(k,p) e^{-i(k-p).R_\alpha} (S^x_\alpha - i\gamma_\sigma S^y_\alpha)\delta_{\sigma,-\lambda} \end{aligned} \tag{4.1.3}$$

where

- $u^{pot}(r - R_\alpha)$ is the spin independent potential component
- $J(r - R_\alpha)\mathrm{s}.\mathrm{S}_\alpha$ is the exchange interaction with S_α spin of magnetic impurity at R_α and $\mathrm{s} = \frac{\sigma}{2}$ is operator of electron spin, and

- $\gamma_\sigma = +1$ and -1 for $\sigma =\uparrow$ and $\downarrow$ respectively.

Pairing interaction $V(k,p)$ is given by

$$V(k,p) = -V_o\phi(\hat{n})\phi(\hat{n}') \tag{4.1.4}$$

V_o - is pairing energy, $\hat{n} = \frac{\vec{k}}{|k|}$ is unit vector along $\vec{k}$.
The order parameter $\Delta(k)$ is given by

$$\Delta(k) = -\sum_p V(k,p) < a_{-p\downarrow}a_{p\uparrow} >= \Delta_0\phi(\hat{n}) \tag{4.1.5}$$

$\Delta_o = \Delta_o(T)$ and $\phi(\hat{n})$ specify anisotropy of $\Delta(k)$.

The self consistent equation for $\Delta(k)$ is derived by the Green's function technique. Define the normal and anomalous temperature Green's function as:

$$\left.\begin{aligned}
G(k,\sigma;p,\lambda;\tau) &= -< T_\tau a_{k\sigma}(\tau)a^\dagger_{p\lambda} > \\
F(k,\sigma;p,\lambda;\tau) &=< T_\tau a^\dagger_{-k-\sigma}(\tau)a^\dagger_{p\lambda} > \\
\tilde{G}(k,\sigma;p,\lambda;\tau) &= -< T_\tau a^\dagger_{-k-\sigma}(\tau)a_{-p-\lambda} > \\
\tilde{F}(k,\sigma;p,\lambda;\tau) &=< T_\tau a_{k\sigma}(\tau)a_{-p-\lambda} >
\end{aligned}\right\} \tag{4.1.6}$$

There Fourier transforms are $G(k,\sigma;p,\lambda;\omega), F(k,\sigma;p,\lambda;\omega), \tilde{G}(k,\sigma;p,\lambda;\omega)$ and $\tilde{F}(k,\sigma;p,\lambda;\omega)$ respectively. T_τ is time ordering operator given by

$$T_\tau(A(\tau_1),B(\tau_2)) = \begin{cases} A(\tau_1)B(\tau_2) & \text{if } \tau_1 > \tau_2 \\ B(\tau_2)A(\tau_1) & \text{if } \tau_2 > \tau_1 \end{cases} \tag{4.1.7}$$

The matrix Green's function $\hat{\mathrm{G}}(k,\sigma;p,\lambda;\omega)$ in the Nambu representation is given by:

$$\hat{\mathrm{G}}(k,\sigma;p,\lambda;\omega) = \begin{pmatrix} G(k,\sigma;p,\lambda;\omega) & -\tilde{F}(k,\sigma;p,\lambda;\omega) \\ -F(k,\sigma;p,\lambda;\omega) & \tilde{G}(k,\sigma;p,\lambda;\omega) \end{pmatrix}$$

$$\begin{pmatrix} G_\omega & -\tilde{F}_\omega \\ -F_\omega & \tilde{G}_\omega \end{pmatrix} = \begin{pmatrix} \ll a_{k\sigma}, a^\dagger_{p\lambda} \gg_\omega & -\ll a_{k\sigma}, a_{p\lambda} \gg_\omega \\ \\ -\ll a^\dagger_{-k-\sigma}, a^\dagger_{p-\lambda} \gg_\omega & \ll a^\dagger_{k\sigma}, a_{-p-\lambda} \gg_\omega \end{pmatrix} \tag{4.1.8}$$

Here $\hat{\mathrm{G}}$ is non diagonal in spin space as well as in K- space.

The matrix equation for $\hat{G}(k,\sigma;p,\lambda;\omega)$ can also be written as

$$\hat{\mathrm{G}}_o^{-1}(k,\sigma;p,\lambda;\omega)\hat{G}(p,\lambda;k',\sigma';\omega) - \hat{U}(k,\sigma;p,\lambda)\hat{G}(p,\lambda;k',\sigma';\omega) = \hat{1}\delta_{k,k'}\delta_{\sigma,\sigma'} \quad (4.1.9)$$

where:

$$\hat{\mathrm{U}}(k,\sigma;p,\lambda) = \begin{pmatrix} \mathrm{U}(k,\sigma;p,\lambda) & 0 \\ 0 & -\mathrm{U}(k,-\lambda;p,-\sigma) \end{pmatrix} \quad (4.1.10)$$

is the term describing the effect of impurity scattering,

$$\hat{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

is the 2×2 unit matrix, and

$$\hat{\mathrm{G}}_0(k,\sigma;p,\lambda;\omega) = \hat{\mathrm{G}}_0(k,\sigma,\omega)\delta_{k,p}\delta_{\sigma,\lambda}$$

is the Green function of the clean sample.

The Green function of the clean sample is already done in chapter three and is summarized by Eq. (3.3.13). By including the possibility of both up or down spins the equation can be modified as:

$$\hat{G}_o(k,\sigma,\omega) = -\frac{1}{\omega^2 + (\epsilon(k)^2 + \Delta(k)^2)} \begin{pmatrix} (i\omega + \epsilon(k)) & \gamma_\sigma\Delta(k) \\ \gamma_\sigma\Delta^*(k) & (i\omega - \epsilon(k)) \end{pmatrix} \quad (4.1.11)$$

The inverse of this matrix is also evaluated in chapter 3 by Eq. (3.3.14). To include the possibility of both spins we can modify the equation as:

$$\hat{G}_o^{-1}(k,\sigma,\omega) = \begin{pmatrix} G_{o11}^{-1} & G_{o12}^{-1} \\ G_{o21}^{-1} & G_{o22}^{-1} \end{pmatrix}$$

$$\begin{pmatrix} G_{o11}^{-1} & G_{o12}^{-1} \\ G_{o21}^{-1} & G_{o22}^{-1} \end{pmatrix} = \begin{pmatrix} i\omega - \epsilon(k) & -\gamma_\sigma\Delta(k) \\ -\gamma_\sigma\Delta^*(k) & i\omega + \epsilon(k) \end{pmatrix} \quad (4.1.12)$$

4.1.1 Averaging

To determine the average value of $\hat{G}(k,\sigma;p,\lambda;\omega)$ we have to consider the following simplifying assumptions:

- Consider short range scattering potentials so that matrix elements $u^{pot}(\mathbf{k},\mathbf{p})$ and $J(\mathbf{k},\mathbf{p})$ are $\mathbf{k}$ independent(momentum) and equal to u^{pot} and J respectively.
- Treat impurity scattering in the Born limit.
- Electron self energy and BCS pair potential are restricted to the Fermi surface.

Upon averaging the Green's function of the impure superconductor we obtain

$$< \hat{G}(k,\sigma;p,\lambda;\omega) >_{imp} = \hat{G}(k,\sigma,\omega)\delta_{k,p}\delta_{\sigma,\lambda}. \tag{4.1.13}$$

$\hat{G}(k,\sigma,\omega)$ can also be determined using the Dyson equation which is given by

$$\hat{G}^{-1}(k,\sigma,\omega) = \hat{G}_o^{-1}(k,\sigma,\omega) - \hat{\sum}(k,\sigma,\omega) \tag{4.1.14}$$

where $\hat{\sum}(k,\sigma,\omega)$ is the self-energy. In the self-consistent Born approximation it is given by

$$\hat{\sum}(k,\sigma,\omega) = < \hat{U}(k,\sigma;k',\sigma')\hat{G}(k',\sigma',\omega)\hat{U}(k',\sigma';k,\sigma) >_{imp} . \tag{4.1.15}$$

The product of the matrices on the right hand side is found using equations (4.1.8) and (4.1.10)

$$\hat{U}(k,\sigma;k'\sigma')\hat{G}(k',\sigma',\omega)\hat{U}(k',\sigma';k\sigma) =$$

$$\begin{pmatrix} U(k,\sigma;k'\sigma') & 0 \\ 0 & -U(k,-\sigma';k',-\sigma) \end{pmatrix} \begin{pmatrix} G(k',\sigma',\omega) & -\tilde{F}(k',\sigma',\omega) \\ -F(k',\sigma',\omega) & \tilde{G}(k',\sigma',\omega) \end{pmatrix}$$

$$\times \begin{pmatrix} U(k',\sigma';k,\sigma) & 0 \\ 0 & -U(k',-\sigma;k,-\sigma') \end{pmatrix}$$

$$= \begin{pmatrix} U(k,\sigma;k'\sigma')U(k',\sigma';k,\sigma)G(k',\sigma',\omega) & U(k,-\sigma';k',-\sigma)U(k',\sigma';k,\sigma)\tilde{F}(k',\sigma',\omega) \\ U(k,\sigma;k'\sigma')U(k',\sigma';k,\sigma)F(k',\sigma',\omega) & U(k,-\sigma';k',-\sigma)U(k',\sigma';k,\sigma)\tilde{G}(k',\sigma',\omega) \end{pmatrix} \tag{4.1.16}$$

Next we need to average this over the positions of the impurity configurations and directions of impurity spins (refer [32]).

(1) The average over R_α vanishes when $|k-k'| \neq 0$ because the summation contains at least one scattering at R_α with $k' = k$. The result of the averaging for this particular case will be $n_m|u(k)|^2$ where n_m is the number of impurity atoms per unit volume (concentration).

(2) Averaging over the orientation of their spins (i.e. spin of impurity atom and spin of conduction electron).

Here we assume that spins are oriented arbitrarily relative to the lattice and that there is no correlation what ever between them. So we have a result given by $\bar{S} = 0$, $\overline{S_i S_k} = \frac{1}{4}S(S+1)\delta_{i,k}$ and from averaging in both cases we have a factor

$$n_m(|u|^2 + \frac{1}{4}S(S+1)) = n_m(|u^{pot}|^2 + |u^{ex}|^2)$$

Therefore, equation (4.1.16) becomes

$$\hat{\sum}(k,\sigma,\omega) = \begin{pmatrix} n_m(|u^{pot}|^2 + |u^{ex}|^2)\sum_{k'} G(k',\sigma,\omega) & n_m(|u^{pot}|^2 - |u^{ex}|^2)\sum_{k'} \tilde{F}(k',\sigma,\omega) \\ n_m(|u^{pot}|^2 - |u^{ex}|^2)\sum_{k'} F(k',\sigma,\omega) & n_m(|u^{pot}|^2 + |u^{ex}|^2)\sum_{k'} \tilde{G}(k',\sigma,\omega) \end{pmatrix}$$

here n_m is the concentration of magnetic impurities, $|u^{ex}|^2 = |J|^2\frac{S(S+1)}{4}$ it includes contributions from both spin-flip and spin conserving scattering of electrons due to their exchange interactions with magnetic impurities. The coefficient $n_m|u^{ex}|^2$ is entered in the normal and anomalous Green's functions with opposite signs, while $n_m|u^{pot}|^2$ which is due to the potential component of scattering by impurities appear with the same sign.

With the calculations performed above and using Eqs. (3.3.14), (4.1.15) and the above equation, we obtain

$$\begin{pmatrix} G_{11}^{-1} & G_{12}^{-1} \\ G_{21}^{-1} & G_{22}^{-1} \end{pmatrix} = \begin{pmatrix} i\omega+\epsilon & -\gamma_\sigma\Delta(k) \\ -\gamma_\sigma\Delta^*(k) & i\omega+\epsilon \end{pmatrix} - \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

$$\begin{pmatrix} G_{11}^{-1} & G_{12}^{-1} \\ G_{21}^{-1} & G_{22}^{-1} \end{pmatrix} = \begin{pmatrix} i\omega-\epsilon-\Sigma_{11} & -\gamma_\sigma\Delta(k)-\Sigma_{12} \\ -\gamma_\sigma\Delta^*(k)-\Sigma_{21} & i\omega+\epsilon-\Sigma_{22} \end{pmatrix}$$

From this we can determine $\hat{G}$ in terms of $k,\ \sigma,\ \omega$,and Δ as

$$\hat{G}(k,\sigma,\omega,\Delta) = \frac{1}{D}\begin{pmatrix} i\omega+\epsilon-\Sigma_{22} & \gamma_\sigma\Delta(k)+\Sigma_{12} \\ \gamma_\sigma\Delta^*(k)+\Sigma_{21} & i\omega+\epsilon-\Sigma_{11} \end{pmatrix} \tag{4.1.17}$$

where

$$D = (i\omega+\epsilon-\Sigma_{11})(i\omega+\epsilon-\Sigma_{22}) - (\gamma_\sigma\Delta(k)+\Sigma_{12})(\gamma_\sigma\Delta^*(k)+\Sigma_{21})$$

As it is seen above $\hat{G}$ has the same form as $\hat{G}_o$, except that ω and Δ_o are replaced by their renormalized equivalents ω' and Δ_ω respectively. i.e.

$$\hat{G}(k,\sigma,\omega,\Delta) = \hat{G}_o(k,\sigma,\omega',\Delta_\omega) \tag{4.1.18}$$

where $\omega' = \omega - i\Sigma_{11}$

$$\omega' = \omega - i(n_m|u^{pot}|^2 + n_m|u^{ex}|^2)\sum_k \frac{\Delta_\omega(k)}{\omega'^2+\epsilon^2+|\Delta_\omega(k)|^2} \tag{4.1.19}$$

and $\Delta_\omega = \Delta(k) + \Sigma_{12}$

$$\Delta_\omega = \Delta(k) + (n_m|u^{pot}|^2 - n_m|u^{ex}|^2)\sum_k \frac{\Delta_\omega(k)}{\omega'^2+\epsilon^2+|\Delta_\omega(k)|^2}. \tag{4.1.20}$$

The gap equation (order parameter) in Eq. (4.1.5) must also be averaged. So

$$\overline{\Delta(k)} = \overline{-\sum_p V(k,p) < a_{-p\downarrow}a_{p\uparrow} >}$$

$$\Delta(k) = -T\sum_{\omega'}\sum_p V(k,p)\frac{\Delta_\omega(p)}{\omega'^2+\epsilon^2+|\Delta_\omega(p)|^2} \tag{4.1.21}$$

The coefficients $n_m|u^{pot}|^2$ and $n_m|u^{ex}|^2$ can be expressed in terms of electron relaxation times τ^{pot} and τ^{ex} for potential and exchange scattering by magnetic impurities respectively. They are defined as

$$\frac{1}{\tau^{pot}} = 2\pi n_m|u^{pot}|^2 N(0) \quad ,and \quad \frac{1}{\tau^{ex}} = 2\pi n_m|u^{ex}|^2 N(0) \tag{4.1.22}$$

where N(0) is the density of electron states at the Fermi level. The total electron relaxation τ_m due to magnetic impurities in the sample can be found as

$$\frac{1}{\tau_m} = \frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}} \tag{4.1.23}$$

4.1.2 Critical Temperature

The critical temperature T_c can be found from Eq. (4.1.19), (4.1.20) and (4.1.21) as the temperature at which the order parameter goes to zero, i.e. $\Delta_o \to 0$ in Eq. (4.1.5). Setting $|\Delta_\omega(k)|^2 = 0$ in the denominators of Eq. (4.1.19) and (4.1.20) and taking Eq. (4.1.5) and (4.1.22) into account, we have at $T \to T_c$:

$$\omega' = \omega + \frac{1}{2}(\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}})sign(\omega) \quad , \quad \Delta_\omega(k) = \Delta(k) + \frac{1}{2|\omega'|}(\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}}) < \Delta_\omega(k) >_{FS} \tag{4.1.24}$$

where $< ... >_{FS}$ stands for a Fermi surface average defined by

$$< ... >_{FS} = \frac{\int_{FS}(...)\frac{d\Omega}{|\frac{\partial\epsilon}{\partial k}|}}{\int_{FS}\frac{d\Omega_k}{|\frac{\partial\epsilon}{\partial k}|}}.$$

Substitute Eq. (4.1.24) in to (4.1.20), set $|\Delta_\omega(k)|^2 = 0$ in the denominator of Eq. (4.1.20) and take Eq. (4.1.4) and (4.1.5) into account to get a result of the form

$$\frac{1}{N(0)V_o} = \pi T_c \sum_\omega \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])}[< \phi^2(\hat{n}) >_{FS} + < \phi(\hat{n}) >^2_{FS} (\frac{\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}}}{2[|\omega| + \frac{1}{\tau^{ex}}]})]$$

$$\frac{1}{\lambda} = \pi T_c \sum_\omega \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])}[< \phi^2(\hat{n}) >_{FS} + < \phi(\hat{n}) >^2_{FS} (\frac{\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}}}{2[|\omega| + \frac{1}{\tau^{ex}}]})] \tag{4.1.25}$$

where $\lambda = N(0)V_o$ is the electron-boson coupling constant. In the absence of impurities $\frac{1}{\tau^{pot}} = \frac{1}{\tau^{ex}} = 0$ and $T_c \to T_{co}$. So Eq. (4.1.25) becomes

$$\frac{1}{\lambda} = \pi T_{co} < \phi^2(\hat{n}) >_{FS} \sum_{\omega} \frac{1}{\omega}. \tag{4.1.26}$$

This can be written in the form of digamma function which is defined by

$$\psi(z) = \frac{d\ln(z!)}{dz} = -C - \sum_{n=1}^{\infty}(\frac{1}{z+n} - \frac{1}{n})$$

$$= -C + \sum_{n=1}^{\infty} \frac{z}{n(n+z)}$$

$$\psi(0) = -C = 0.577215... \ .$$

With this Eq. (4.1.26) becomes

$$\frac{1}{\lambda} = \psi(\frac{1}{2} + \frac{\omega}{\pi T_{co} < \phi^2(\hat{n}) >_{Fs}}) - \psi(\frac{1}{2}) \approx \ln(\frac{C\omega}{\pi T_{co} < \phi^2(\hat{n}) >_{FS}}). \tag{4.1.27}$$

Equation (4.1.25) can be modified by adding and subtracting the term

$$\pi T_c < \phi^2(\hat{n}) >_{FS} \sum_{\omega} \frac{1}{|\omega|}$$

$$\frac{1}{\lambda} = \pi T_c < \phi^2(\hat{n}) >_{FS} \sum_{\omega} \frac{1}{|\omega|} \ + \ \pi T_c \sum_{\omega} \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])} \times$$

$$\Big[< \phi^2(\hat{n}) >_{FS} + < \phi(\hat{n}) >_{FS}^2 (\frac{\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}}}{2[|\omega| + \frac{1}{\tau^{ex}}]})\Big] - \pi T_c < \phi^2(\hat{n}) >_{FS} \sum_{\omega} \frac{1}{|\omega|}$$

$$= \pi T_c < \phi^2(\hat{n}) >_{FS} \sum_{\omega} \frac{1}{|\omega|} \ + \pi T_c \sum_{\omega} \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])} \times$$

$$\Big[< \phi^2(\hat{n}) >_{FS} \ + < \phi(\hat{n}) >_{FS}^2 (\frac{\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}}}{2[|\omega| + \frac{1}{\tau^{ex}}]}) - < \phi^2(\hat{n}) >_{FS} \frac{|\omega| + \frac{1}{2}(\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}})}{|\omega|}\Big]$$

$$\frac{1}{\lambda} = \pi T_c < \phi^2(\hat{n}) >_{FS} \sum_{\omega} \frac{1}{|\omega|} \ + \ \pi T_c \sum_{\omega} \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])} \times$$

$$[\frac{<\phi^2(\hat{n})>_{FS}|\omega| - <\phi(\hat{n})>^2_{FS}(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}}])}{|\omega|} \quad + \quad <\phi(\hat{n})>^2_{FS}(\frac{\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}}}{2[|\omega| + \frac{1}{\tau^{ex}}]})]$$

$$\frac{1}{\lambda} = \pi T_c <\phi^2(\hat{n})>_{FS} \sum_{\omega} \frac{1}{|\omega|} \quad + \quad \pi T_c <\phi^2(\hat{n})>_{FS} \sum_{\omega} \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])}$$

$$[-\frac{1}{2|\omega|}(\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}) \quad + \quad \frac{<\phi(\hat{n})>^2_{FS}}{<\phi^2(\hat{n})>_{FS}} \frac{(\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}})}{2[|\omega| + \frac{1}{\tau^{ex}}]}] \tag{4.1.28}$$

The left hand side of Eq. (4.1.28) can be replaced by $\ln(\frac{C\omega}{\pi T_{co}<\phi^2(\hat{n})>_{FS}})$ on account of Eq. (4.1.26). With the same saying, the first term on the RHS of Eq. (4.1.28) equals $\ln(\frac{C\omega}{\pi T_c<\phi^2(\hat{n})>_{FS}})$. So Eq. (4.1.28) becomes

$$\ln(\frac{C\omega}{\pi T_{co} <\phi^2(\hat{n})>_{FS}}) = \ln(\frac{C\omega}{\pi T_c <\phi^2(\hat{n})>_{FS}}) + \pi T_c <\phi^2(\hat{n})>_{FS}$$

$$\sum_{\omega} \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])} \quad + \quad [-\frac{1}{2|\omega|}(\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}) \quad + \quad \frac{<\phi(\hat{n})>^2_{FS}}{<\phi^2(\hat{n})>_{FS}} \frac{(\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}})}{2[|\omega| + \frac{1}{\tau^{ex}}]}]$$

$$\ln(\frac{T_c}{T_{co}}) = \pi T_c <\phi^2(\hat{n})>_{FS} \sum_{\omega} \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])} \quad + \quad [-\frac{1}{2|\omega|}(\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}) \; +$$

$$\frac{<\phi(\hat{n})>^2_{FS}}{<\phi^2(\hat{n})>_{FS}} \frac{(\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}})}{2[|\omega| + \frac{1}{\tau^{ex}}]}]$$

$$\ln(\frac{T_{co}}{T_c}) = \pi T_c <\phi^2(\hat{n})>_{FS} \sum_{\omega} \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])} \quad + \quad [\frac{1}{2|\omega|}(\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}) \; -$$

$$\frac{<\phi(\hat{n})>^2_{FS}}{<\phi^2(\hat{n})>_{FS}} \frac{(\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}})}{2[|\omega| + \frac{1}{\tau^{ex}}]}] \tag{4.1.29}$$

Now introduce a coefficient χ for the anisotropy of the order parameter on the Fermi surface as

$$\chi = 1 - \frac{<\phi(\hat{n})>^2_{FS}}{<\phi^2(\hat{n})>_{FS}} = 1 - \frac{<\Delta(k)>^2_{FS}}{<\Delta^2(k)>_{FS}} \tag{4.1.30}$$

With this Eq. (4.1.29) becomes

$$\ln(\frac{T_{co}}{T_c}) = \pi T_c <\phi^2(\hat{n})>_{FS} \sum_{\omega} \frac{1}{(|\omega| + \frac{1}{2}[\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}])} \quad + \quad [\frac{1}{2|\omega|}(\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}) \; -$$

$$(1-\chi)\frac{<\phi(\hat{n})>^2_{FS}}{<\phi^2(\hat{n})>_{FS}} \frac{(\frac{1}{\tau^{pot}} - \frac{1}{\tau^{ex}})}{2[|\omega| + \frac{1}{\tau^{ex}}]}] \tag{4.1.31}$$

Since the RHS of this equation is convergent the cut of ω_c can be extended to infinity. This infinite sum can readily performed using the formula

$$\sum_{k=0}^{\infty}(\frac{1}{k+x} - \frac{1}{k+y}) = \psi(y) - \psi(x)$$

where ψ is the digamma function. Making use of this formula on Eq. (4.1.31) gives

$$\ln(\frac{T_{co}}{T_c}) = (1-\chi)\Big[\psi(\frac{1}{2} + \frac{1}{2\pi T_c \tau^{ex}}) - \psi(\frac{1}{2})\Big] + \chi\Big[\psi(\frac{1}{2} + \frac{1}{4\pi T_c}(\frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}})) - \psi(\frac{1}{2})\Big]$$

$$\ln(\frac{T_{co}}{T_c}) = (1-\chi)\Big[\psi(\frac{1}{2} + \frac{1}{2\pi T_c \tau^{ex}}) - \psi(\frac{1}{2})\Big] \;+\; \chi\Big[\psi(\frac{1}{2} + \frac{1}{4\pi T_c \tau_m}) - \psi(\frac{1}{2})\Big] \quad (4.1.32)$$

where $\frac{1}{\tau_m} = \frac{1}{\tau^{pot}} + \frac{1}{\tau^{ex}}$.

4.2 Contributions Due to All Effects

On the basis of Eq. (4.1.32) it is also possible to include all the contributions(of magnetic, non-magnetic impurities, disorders, defects etc.) that affect T_c by extending one term of the Hamiltonian in Eq. (4.1.1). In that equation $\hat{H}_2$ describes the effect of impurity (specially magnetic). The effect (contribution) of electron scattering by randomly distributed impurities which are non-magnetic, defects or disordered is included by inserting their respective interaction components in the total interaction in Eq. (4.1.2) and (4.1.3). Note that the non-magnetic, defects and disordered terms are spin-independent and contribute to the scattering matrix element $U(k,\sigma;p,\lambda) = U_1(k,p,\sigma)\delta_{\sigma,\lambda}$ in Eq. (4.1.3). Following the same procedure we arrive at the expression that can generalize Eq. (4.1.32). It looks like

$$\ln(\frac{T_{co}}{T_c}) = (1-\chi)\Big[\psi(\frac{1}{2} + \frac{1}{2\pi T_c \tau^{ex}}) - \psi(\frac{1}{2})\Big] \;+\; \chi\Big[\psi(\frac{1}{2} + \frac{1}{4\pi T_c \tau}) - \psi(\frac{1}{2})\Big] \quad (4.2.1)$$

where $\frac{1}{\tau} = \frac{1}{\tau_m} + \frac{1}{\tau_{nm}} + \frac{1}{\tau_D}$, $\frac{1}{\tau_i}$ is the electron relaxation time due to the factor i. This equation is a more general result than the AG equation (Eq. (2.3.1)). Note that the combined effect of magnetic, non-magnetic, disorder, and/or defect scattering on T_c can not be described by a single parameter depending on the value of τ_m, τ_{nm}, τ_D and χ (see [38]).

From this general equation we can take the following limiting cases:

- Low impurity and disorder concentration.

  We can modify Eq. (4.2.1) as

$$-\ln\left(\frac{T_c}{T_{co}}\right) = (1-\chi)\Big[\psi(\frac{1}{2}+\frac{1}{2\pi\frac{T_c}{T_{co}}\tau^{ex}T_{co}})-\psi(\frac{1}{2})\Big] + \chi\Big[\psi(\frac{1}{2}+\frac{1}{4\pi\frac{T_c}{T_{co}}\tau})-\psi(\frac{1}{2})\Big] \tag{4.2.2}$$

At low impurity and disorder concentration $\frac{1}{2\pi T_{co}\tau^{ex}} \ll 1$, $\frac{1}{4\pi T_{co}\tau_{nm}} \ll 1$, $\frac{1}{4\pi T_{co}\tau_m} \ll 1$, $\frac{1}{4\pi T_{co}\tau_D} \ll 1$, and $T_{co}-T_c \ll T_{co}$. We can expand Eq. (4.2.2) using Taylor's expansion.

Expand the left hand side of the equation about T_c

$$\begin{aligned} -\ln\left(\frac{T_c}{T_{co}}\right) &= -(\ln T_c - \ln T_{co}) \\ &= -(\ln T_c - [\ln T_c - (T_{co}-T_c)(\ln T_c)']) \\ &= \frac{T_{co}-T_c}{T_c} \end{aligned}$$

Expand the right hand side of the equation about 1/2 using $\psi(x) \approx \psi(\frac{1}{2}) + (x-\frac{1}{2})\psi'(\frac{1}{2}) + ...$ and $\psi'(\frac{1}{2}) = \frac{\pi^2}{2}$.

$$\begin{aligned} &(1-\chi)\Big[\psi(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}})-\psi(\frac{1}{2})\Big] + \chi\Big[\psi(\frac{1}{2}+\frac{1}{4\pi T_c\tau})-\psi(\frac{1}{2})\Big] \\ &\approx (1-\chi)\Big[\psi(\frac{1}{2})+\frac{\pi}{4T_c\tau^{ex}}-\psi(\frac{1}{2})\Big] + \chi\Big[\psi(\frac{1}{2})+\frac{\pi}{8T_c\tau}-\psi(\frac{1}{2})\Big] \\ &\approx \frac{\pi}{4T_c}\left[\frac{(1-\chi)}{\tau^{ex}}+\frac{\chi}{2\tau}\right] \end{aligned}$$

Combining the above results we have

$$\frac{T_{co}-T_c}{T_c} \approx \frac{\pi}{4T_c}\left[\frac{(1-\chi)}{\tau^{ex}}+\frac{\chi}{2\tau}\right]$$

$$T_{co}-T_c \approx \frac{\pi}{4}\Big[\frac{\chi}{2}\big(\frac{1}{\tau^{pot}}+\frac{1}{\tau_{nm}}+\frac{1}{\tau_D}\big)+\frac{1-\frac{\chi}{2}}{\tau^{ex}}\Big] \tag{4.2.3}$$

- High impurity concentration.

  Here non-magnetic and disorder scattering are insufficient for the non-d-wave two dimensional superconductivity ($0 \leq \chi < 1$) to be destroyed completely; at $\frac{1}{\tau^{ex}} = 0$, the value of T_c asymptotically goes to zero as $\frac{1}{\tau_{nm}} + \frac{1}{\tau_D}$ increases.

From the generalized equation (Eq. (4.2.1)) we can also have the following particular cases

- If the scattering is in an isotropic s-wave superconductor.

  As mentioned above ($\chi = 0$) for s-wave superconductor and Eq. (4.2.1) reduces to

  $$\ln\left(\frac{T_{co}}{T_c}\right) = \psi\left(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}}\right) - \psi\left(\frac{1}{2}\right)$$

  which is the same as the already known AG equation (2.3.1).

  Limiting cases:

  (a) low impurity concentration

  Here $T_{co} - T_c \ll T_{co}$ and $\frac{1}{2\pi T_{co}\tau^{ex}} \ll 1$ and

  $$T_{co} - T_c \approx \frac{\pi}{4\tau^{ex}}$$

  (b) High impurity concentration

  Magnetic scattering in the absence of non-magnetic and disorder scattering ($\frac{1}{\tau_n} = \frac{1}{\tau_D} = 0$) is known to suppress the isotropic s-wave superconductivity with $\chi = 0$ at the critical value
  $\frac{1}{\tau^{ex}_{mc}} = \frac{\pi T_{co}}{2\gamma} \approx 0.882T_{co}$ with $\gamma = e^C \approx 1.781$

- For a d-(and/or p-)wave pairing state

  Here $\chi = 1$ and Eq. (4.2.1) becomes

$$\ln\left(\frac{T_{co}}{T_c}\right) = \psi\left(\frac{1}{2} + \frac{1}{4\pi T_c}\left(\frac{1}{\tau_{nm}} + \frac{1}{\tau_m} + \frac{1}{\tau_D}\right)\right) - \psi\left(\frac{1}{2}\right) \tag{4.2.4}$$

  We can have the following limiting cases:

  (a) Low impurity concentration

  If $\frac{1}{\tau_m} = 0$ we get

$$T_{co} - T_c \approx \frac{\pi}{8\tau}$$

  (b) High impurity concentration($T_c \to 0$)

  T_c vanishes at a critical value $\frac{1}{\tau_{nc}} = \frac{\pi T_{co}}{\gamma} \approx 1.764 T_{co}$

On the basis of Eq. (4.2.1), the general condition for impurity (disorder or defect) suppression of T_c for a superconductor having an arbitrary in-plane anisotropy coefficient χ and containing both nonmagnetic and magnetic scatterers is given by

$$\frac{1}{\tau_{eff,c}} = \frac{\pi}{\gamma} 2^{\chi-1} T_{co} \tag{4.2.5}$$

where $\frac{1}{\tau_{eff,c}}$ is the critical value of the effective relaxation time τ_{eff}, defined as (refer [38])

$$\frac{1}{\tau_{eff}} = \left(\frac{1}{\tau_m^{ex}}\right)^{1-\chi}\left(\frac{1}{\tau_n} + \frac{1}{\tau_{nm}} + \frac{1}{\tau_D}\right)^{\chi}. \tag{4.2.6}$$

From Eqs. (4.2.5) and (4.2.6) we can see that $\frac{1}{\tau_{eff,c}}$ increases monotonically with $\frac{1}{\tau_m}, \frac{1}{\tau_{nm}}$, and $\frac{1}{\tau_D}$ at any value of χ, with the exception of the case $\chi = 0$, where $\frac{1}{\tau_{eff,c}}$ doesn't depend on $\frac{1}{\tau_{nm}}$, and $\frac{1}{\tau_D}$, see Eq. (4.2.6). If χ is close to unity, then $\frac{1}{\tau_{eff}} \approx \frac{1}{\tau_m} + \frac{1}{\tau_{nm}} + \frac{1}{\tau_D}$, i.e., the contribution of disorder, non-magnetic and magnetic scattering to pair breaking is about the same. If $\chi \ll 1$, then $\frac{1}{\tau_{eff}} \approx \frac{1}{\tau^{ex}}$, i.e., τ_{eff} is determined primarily by magnetic scattering. The higher the the anisotropy coefficient χ, the greater is the relative contribution of disorder and non magnetic scatterers to T_c suppression as compared to magnetic scatterers.

4.2.1 Derivation of Isotope Coefficient α

The isotope effect of superconductivity is given by the relation

$$T_c \ \alpha \ M^{-\alpha} \ \Rightarrow \ T_c M^{\alpha} = const$$

$$\partial(T_c M^{\alpha}) = \partial(const) \ \Rightarrow \ M^{\alpha}\partial T_c + T_C\partial(M^{\alpha}) = 0$$

$$\alpha T_c M^{\alpha-1}\partial M = -M^{\alpha}\partial T_c \ \Rightarrow \ \alpha = -\frac{\partial \ln T_c}{\partial \ln M} \tag{4.2.7}$$

Using this we can find α for our case. To do this first assume that a slight change in the atomic mass does not affect the mechanism of the pairing interaction and the pair breaking effect by impurities.

Diffrentiate the LHS of Eq. (4.2.1) with respect to $\ln M$

$$\frac{\partial}{\partial \ln M}\left(\ln\left(\frac{T_{co}}{T_c}\right)\right) = \left(\frac{T_{co}}{T_c}\right)^{-1}\frac{\partial}{\partial \ln M}\left(\frac{T_{co}}{T_c}\right) = \frac{\partial \ln T_{co}}{\partial \ln M} - \frac{\partial \ln T_c}{\partial \ln M} = -\alpha_o + \alpha \tag{4.2.8}$$

where $\alpha_o = \alpha(M, 0)$ is the isotope coefficient in the absence of impurity and $\alpha = \alpha(M, \tau)$ is the isotope coefficient in the presence of impurity.

Next differentiate the RHS of Eq. (4.2.1) with respect to $\ln M$.

$$\frac{\partial}{\partial \ln M}\left[(1-\chi)\left[\psi\left(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}}\right) - \psi\left(\frac{1}{2}\right)\right] + \chi\left[\psi\left(\frac{1}{2}+\frac{1}{4\pi T_c\tau}\right) - \psi\left(\frac{1}{2}\right)\right]\right]$$

$$= (1-\chi)\psi'\left(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}}\right)\frac{\partial}{\partial \ln M}\left(\frac{1}{2\pi T_c\tau^{ex}}\right) + \chi\psi'\left(\frac{1}{2}+\frac{1}{4\pi T_c\tau}\right)\frac{\partial}{\partial \ln M}\left(\frac{1}{4\pi T_c\tau}\right)$$

$$= \alpha\left[(1-\chi)\frac{1}{2\pi T_c\tau^{ex}}\psi'\left(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}}\right) + \chi\frac{1}{4\pi T_c\tau}\psi'\left(\frac{1}{2}+\frac{1}{4\pi T_c\tau}\right)\right] \tag{4.2.9}$$

ψ' is the derivative of the psi function with respect to $\ln M$.

Combining equations (4.2.8) and (4.2.9) we have

$$-\alpha_o + \alpha = \alpha\left[(1-\chi)\frac{1}{2\pi T_c\tau^{ex}}\psi'\left(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}}\right) + \chi\frac{1}{4\pi T_c\tau}\psi'\left(\frac{1}{2}+\frac{1}{4\pi T_c\tau}\right)\right]$$

$$\frac{\alpha}{\alpha_o} = \left[1 \ - \ (1-\chi)\frac{1}{2\pi T_c\tau^{ex}}\psi'(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}}) \ - \ \chi\frac{1}{4\pi T_c\tau}\psi'(\frac{1}{2}+\frac{1}{4\pi T_c\tau})\right]^{-1} \qquad (4.2.10)$$

This equation can be used for an impure superconductor with arbitrary anisotropy of the superconducting order parameter and arbitrary relative contributions of potential and spin-flip scattering to the electron relaxation time. As in the case of T_c here we also have the following cases:

- For isotropic s-wave superconductor ($\chi = 0$) and

$$\frac{\alpha}{\alpha_o} = \left[1 - \frac{1}{2\pi T_c\tau^{ex}}\psi'(\frac{1}{2} + \frac{1}{2\pi T_c\tau^{ex}})\right]^{-1}$$

- For d- or p-wave superconductor ($\chi = 1$) and

$$\frac{\alpha}{\alpha_o} = \left[1 - \frac{1}{4\pi T_c\tau}\psi'(\frac{1}{2} + \frac{1}{4\pi T_c\tau})\right]^{-1}$$

4.3 Another Look at The Derivation of α

In the above section we derive the isotope coefficient by assuming that only T_c is a function of the mass M of the isotope. Now we are going to derive the isotope coefficient in an extended way.

Here we derive α by assuming that both T_c and τ are functions of the isotopic mass M($\ln M$).

Differentiating LHS of Eq. (4.2.1) with respect to gives Eq. (4.2.8).

Next we need to differentiate the RHS of Eq. (4.2.1) with respect to $\ln M$.

$$\frac{\partial}{\partial \ln M}(1-\chi)\left[\psi(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}}) - \psi(\frac{1}{2})\right] \ + \ \chi\left[\psi(\frac{1}{2}+\frac{1}{4\pi T_c\tau}) - \psi(\frac{1}{2})\right] =$$

$$= (1-\chi)\psi'(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}})\frac{\partial}{\partial \ln M}(\frac{1}{2\pi T_c\tau^{ex}}) \ + \ \chi\psi'(\frac{1}{2}+\frac{1}{4\pi T_c\tau})\frac{\partial}{\partial \ln M}(\frac{1}{4\pi T_c\tau})$$

$$= (1-\chi)\psi'(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}})(\frac{1}{2\pi T_c\tau^{ex}})\left[-\frac{\partial \ln T_c}{\partial \ln M} - \frac{\partial \ln \tau^{ex}}{\partial \ln M}\right] \ + \ \chi\psi'(\frac{1}{2}+\frac{1}{4\pi T_c\tau})\times$$

$$\frac{1}{4\pi}\Big(\frac{1}{\tau}\frac{\partial}{\partial \ln M}(\frac{1}{T_c}) \ + \ \frac{1}{T_c}\frac{\partial}{\partial \ln M}(\frac{1}{\tau})\Big)$$
$$= (1-\chi)\psi'(\frac{1}{2}+\frac{1}{2\pi T_c\tau^{ex}})(\frac{1}{2\pi T_c\tau^{ex}})\Big[\alpha - \frac{\partial \ln \tau^{ex}}{\partial \ln M}\Big] \ + \ \chi\psi'(\frac{1}{2}+\frac{1}{4\pi T_c\tau})\frac{1}{4\pi} \times$$
$$\left(\frac{\alpha}{T_c\tau}+\frac{1}{T_c}\Big(\frac{-\frac{\partial \ln \tau_m}{\partial \ln M}}{\tau_m} \ + \ \frac{-\frac{\partial \ln \tau_{nm}}{\partial \ln M}}{\tau_{nm}} \ + \ \frac{-\frac{\partial \ln \tau_D}{\partial \ln M}}{\tau_D}\Big)\right)$$

Using the following notations

$$\frac{1}{4\pi T_c\tau} = \varphi \ , \ \ \frac{1}{2\pi T_c\tau^{ex}} = \delta$$
$$-\frac{d\ln \tau^{ex}}{d\ln M} = \eta_{ex} \ , \ \ -\frac{d\ln \tau_{nm}}{d\ln M} = \eta_{nm}$$
$$-\frac{d\ln \tau_m}{d\ln M} = \eta_m \ , and \ \ -\frac{d\ln \tau_D}{d\ln M} = \eta_D$$

the equation reduces to

$$= (1-\chi)\delta\psi'(\frac{1}{2}+\delta)(\alpha+\eta_{ex}) \ + \ \chi\psi'(\frac{1}{2}+\varphi)\Big[\alpha\varphi \ + \ \varphi\tau\Big(\frac{\eta_m}{\tau_m} \ + \ \frac{\eta_{nm}}{\tau_{nm}} \ + \ \frac{\eta_D}{\tau_D}\Big)\Big] \quad (4.3.1)$$

Combining equation(4.2.1) and this last result (Eq. (4.3.1)) we have

$$-\alpha_o+\alpha = \alpha\Big[(1-\chi)\delta\psi'(\frac{1}{2}+\delta) \ + \ \chi\varphi\psi'(\frac{1}{2}+\varphi)\Big] \ + \ (1-\chi)\delta\eta_{ex}\psi'(\frac{1}{2}+\delta)+$$
$$\chi\varphi\tau\psi'(\frac{1}{2}+\varphi)\Big(\frac{\eta_m}{\tau_m} \ + \ \frac{\eta_{nm}}{\tau_{nm}} \ + \ \frac{\eta_D}{\tau_D}\Big)$$

After some arrangement we arrive at

$$\frac{\alpha}{\alpha_o} = \frac{1}{1-(1-\chi)\delta\psi'(\frac{1}{2}+\delta) \ - \ \chi\varphi\psi'(\frac{1}{2}+\varphi)}\Bigg[1 \ + \ \frac{1}{\alpha_o}\Bigg\{(1-\chi)\delta\eta_{ex}\psi'(\frac{1}{2}+\delta) +$$
$$\chi\varphi\tau\psi'(\frac{1}{2}+\varphi)\Big(\frac{\eta_m}{\tau_m} \ + \ \frac{\eta_{nm}}{\tau_{nm}} \ + \ \frac{\eta_D}{\tau_D}\Big)\Bigg\}\Bigg] \quad (4.3.2)$$

Like equation (4.2.1) this last equation (Eq. (4.3.2)) is a more general result than Eq. (4.2.10) for isotope effect comprising all types of superconductors (s- or d-wave or mixed). It can also be applied for different values of χ ranging from 0 to 1. From this we can single out so many different cases of interest.

For example if τ is not a function of M (or $\ln M$):

$\eta_{ex} = \eta_m = \eta_{nm} = \eta_D = 0$ and Eq. (4.3.2) reduces to

$$\frac{\alpha}{\alpha_o} = \frac{1}{1-(1-\chi)\delta\psi'(\frac{1}{2}+\delta)\ +\ \chi\varphi\psi'(\frac{1}{2}+\varphi)} = \Big[1-(1-\chi)\delta\psi'(\frac{1}{2}+\delta) + \chi\varphi\psi'(\frac{1}{2}+\varphi)\Big]^{-1}$$

This is trivially identical to Eq. (4.2.10).

Though there are numerous parameters independent of each other we can observe the general nature of the relation between $\frac{\alpha}{\alpha_o}$ and φ (See results and discussion part).

4.3.1 Special Cases

d-wave Superconductors

If the pairing mechanism is in such a way that $\chi = 1$ it is a d-wave superconductor. In this case we have to treat the effect of impurity, disorder, and defect in superconductivity. Specially the case of $\chi = 1$ (i.e., d- or p-wave superconductors) is our concern. Making use of this reduces the general relation in Eq. (4.3.2) to

$$\frac{\alpha}{\alpha_o} = \frac{1}{1-\psi'\varphi}\left(1+\frac{\psi'\varphi\tau\left(\frac{\eta_{nm}}{\tau_{nm}}+\frac{\eta_m}{\tau_m}+\frac{\eta_D}{\tau_D}\right)}{\alpha_o}\right) \qquad (4.3.3)$$

This is the equation showing relative shift of the isotope coefficient.

Effects Of Non-magnetic & Magnetic impurities in d-wave Superconductors

Here we neglect the effect of disorder, defect, etc. on doing this Eq. (4.2.1) reduces to

$$\ln\Big(\frac{T_{co}}{T_c}\Big) = (1-\chi)\Big[\psi(\frac{1}{2}+\delta) - \psi(\frac{1}{2})\Big] + \chi\Big[\psi(\frac{1}{2}+\varphi) - \psi(\frac{1}{2})\Big]$$

where now $\varphi = \frac{1}{4\pi T_c\tau} = \frac{1}{4\pi T_c}\left(\frac{1}{\tau_m} + \frac{1}{\tau_{nm}}\right)$.
The general relation describing the relative isotope change due to all contributions (4.3.2) is also reduced to

$$\frac{\alpha}{\alpha_o} = \left[1 - \frac{\psi'}{4\pi T_c\tau}\right]^{-1}\left[1 + \frac{\psi'\varphi\tau}{\alpha_o}\left(\frac{\eta_{nm}}{\tau_{nm}} + \frac{\eta_m}{\tau_m}\right)\right]$$

4.4 Results and Discussion

This section tries to generalize the main results obtained till now in this chapter and investigate the results with the help of different plots.

We put the theoretical formalism describing the variation of T_c and α in superconductivity. Starting with the model Hamiltonian that includes energy of free electrons, effective BCS potential and a term describing the effect of impurity, disorder, defect etc. we arrive at the general expression for variation of T_C given by

$$\ln(\frac{T_{co}}{T_c}) = (1-\chi)\Big[\psi(\frac{1}{2} + \frac{1}{2\pi T_c\tau^{ex}}) - \psi(\frac{1}{2})\Big] \;+\; \chi\Big[\psi(\frac{1}{2} + \frac{1}{4\pi T_c\tau}) - \psi(\frac{1}{2})\Big].$$

With the notations given in the above topics it can be written as

$$\ln(\frac{T_{co}}{T_c}) = (1-\chi)\Big[\psi(\frac{1}{2} + \delta) - \psi(\frac{1}{2})\Big] \;+\; \chi\Big[\psi(\frac{1}{2} + \varphi) - \psi(\frac{1}{2})\Big].$$

The universal dependence of $\frac{T_c}{T_{co}}$ on φ for a given value of χ and δ can be traced using certain sample values. Figure (4.1) shows the plot of $\frac{T_c}{T_{co}}$ versus φ when $\delta = 0.1$ and different values of χ. From this figure we can see that as χ increases from 0 to 1 the value of $\frac{T_c}{T_{co}}$ decreases.
At $\chi = 0$ (isotropic s-wave pairing) the value of $\frac{T_c}{T_{co}}$ does not depend on φ, while superconductivity is completely suppressed ($T_c = 0$) at a critical value of $\delta = \frac{1}{2\pi T_{co}\tau^{ex}} \approx \frac{1}{4\gamma}$.

Our next general result is the equation showing the variation showing the variation of the isotope effect on the assumption that both T_c and τ are functions of the isotopic

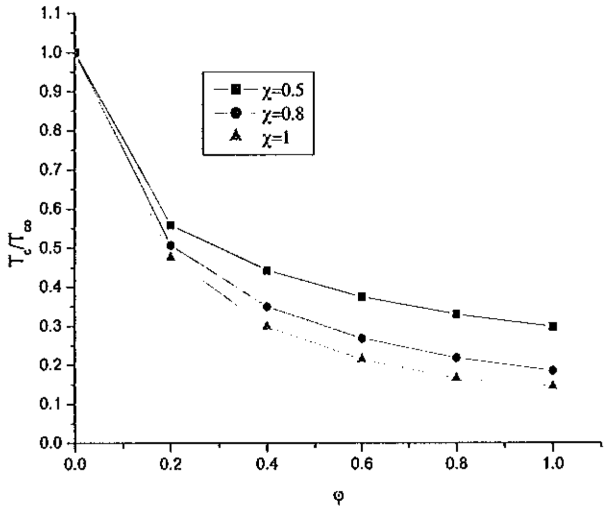

Figure 4.1: Variation of $\frac{T_c}{T_{co}}$ on φ

mass M ($\ln M$). In that case we get

$$\frac{\alpha}{\alpha_o} = \frac{1}{1-(1-\chi)\delta\psi'(\frac{1}{2}+\delta) - \chi\varphi\psi'(\frac{1}{2}+\varphi)}\left[1 + \frac{1}{\alpha_o}\left\{(1-\chi)\delta\eta_{ex}\psi'(\frac{1}{2}+\delta) + \chi\varphi\tau\psi'(\frac{1}{2}+\varphi)\left(\frac{\eta_m}{\tau_m} + \frac{\eta_{nm}}{\tau_{nm}} + \frac{\eta_D}{\tau_D}\right)\right\}\right]$$

Here there are numerous parameters independent of each other. We can observe the general nature of the relation between $\frac{\alpha}{\alpha_o}$ and φ by taking different conditions.

For $\eta_m = \eta_{nm} = \eta_D = \eta$ it reduces to

$$\frac{\alpha}{\alpha_o} = \frac{1}{1-(1-\chi)\delta\psi'(\frac{1}{2}+\delta) - \chi\varphi\psi'(\frac{1}{2}+\varphi)}\left[1 + \frac{1}{\alpha_o}\left\{(1-\chi)\delta\eta_{ex}\psi'(\frac{1}{2}+\delta) + \chi\varphi\eta\psi'(\frac{1}{2}+\varphi)\right\}\right] \qquad (4.4.1)$$

The plot in Fig. (4.2) shows the variation of $\frac{\alpha}{\alpha_o}$ on δ when $\chi = 0$ (isotropic s-wave pairing). Here $\frac{\alpha}{\alpha_o}$ doesn't depend on φ. From the figure it is seen that $\frac{\alpha}{\alpha_o}$increases as δ increases.

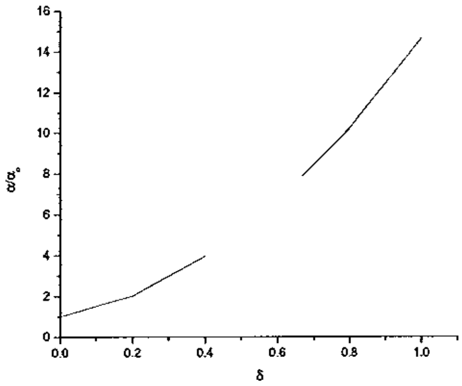

Figure 4.2: Variation of $\frac{\alpha}{\alpha_o}$ on δ for $\chi = 0$

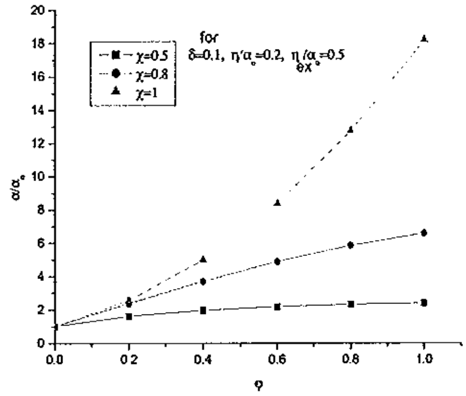

Figure 4.3: Variation of $\frac{\alpha}{\alpha_o}$ on φ for different values of χ

The sketch shown in Fig. (4.3) indicates the variation of $\frac{\alpha}{\alpha_o}$ on φ for $\chi = 0.5,\ 0.8,\ 1$ when $\frac{\eta}{\alpha_o} = 0.2$ and $\frac{\eta_{ex}}{\alpha_o} = 0.5$. From the graph it is shown that as φ increases $\frac{\alpha}{\alpha_o}$ also increases indicating the effect of impurity, disorder, and defect. It is also clear from the figure that α increases faster for magnetic impurities (less χ values) than for non-magnetic impurities and/or disorder.

In addition to $\eta_m = \eta_{nm} = \eta_D = \eta$ if $\chi = 1$ Eq. (4.4.1) gives

$$\frac{\alpha}{\alpha_o} = \frac{1}{1-\psi'\varphi}\left(1 + \frac{\psi'\varphi\tau\left(\frac{\eta}{\tau_{nm}} + \frac{\eta}{\tau_m} + \frac{\eta}{\tau_D}\right)}{\alpha_o}\right)$$

$$\frac{\alpha}{\alpha_o} = \frac{1}{1-\psi'\varphi}\left(1 + \frac{\psi'\varphi\eta\tau\left(\frac{1}{\tau_{nm}} + \frac{1}{\tau_m} + \frac{1}{\tau_D}\right)}{\alpha_o}\right)$$

$$\frac{\alpha}{\alpha_o} = \frac{1}{1-\psi'\varphi}\left(1 + \psi'\varphi\frac{\eta}{\alpha_o}\right)$$

By taking the two parameters (φ and $\frac{\eta}{\alpha_o}$) in to account we get the plot shown in Fig. (4.4). This is the full spectrum of the dependence of $\frac{\alpha}{\alpha_0}$ on φ for a d-wave pairing ($\chi = 1$). This plot shows that α is further enhanced by including $\frac{\eta}{\alpha_o}$. i.e., by taking the dependence of the scattering time τ on n (concentration).

The variation of $\frac{T_c}{T_{co}}$ of equation (4.2.4) on φ can also be seen by drawing the graph of $\frac{T_c}{T_{co}}$ versus φ. The plot is shown in Fig. (4.5).

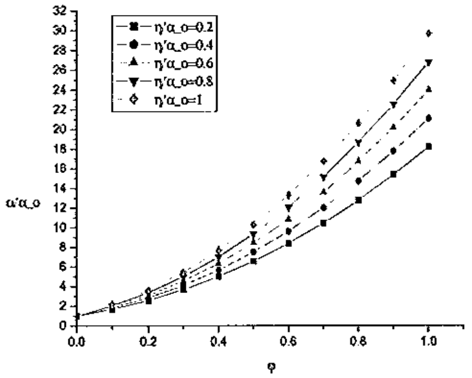

Figure 4.4: variation of α with φ for different values of $\frac{\eta}{\alpha_o}$

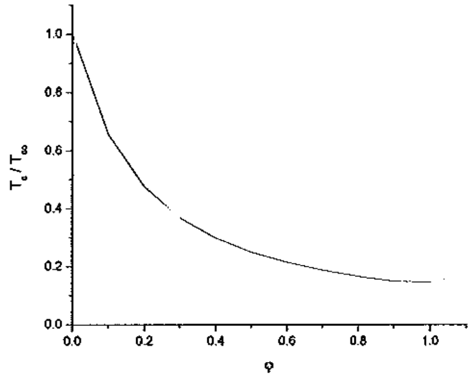

Figure 4.5: Variation of $\frac{T_c}{T_{co}}$ on φ

In addition to this we can take the following sample values $\alpha_o = 0.5$, $\delta = 0.1$, $\eta_m = \eta_{nm} = \eta_D = \eta$, and $\frac{\eta_{ex}}{\alpha_o} = 1$. In this regard Eq. (4.3.2) reduces to

$$\frac{\alpha}{\alpha_o} = \frac{1}{1 - \frac{1}{2}(0.1)\psi'(0.6) \;-\; 0.5\varphi\frac{\eta}{\alpha_o}\psi'(\frac{1}{2}+\varphi)}\Bigg[1 \;+\; 0.5\times 0.1\times\psi'(0.6) + 0.5\varphi\frac{\eta}{\alpha_o}\psi'(\frac{1}{2}+\varphi)\Bigg]$$

Figure (4.6) shows the graph of $\frac{\alpha}{\alpha_o}$ versus φ for different values of $\frac{\eta}{\alpha_o}$.

In all the above results we try to see the individual and combined effects of impurity and disorder on a superconductor. From these relations and plots it is possible

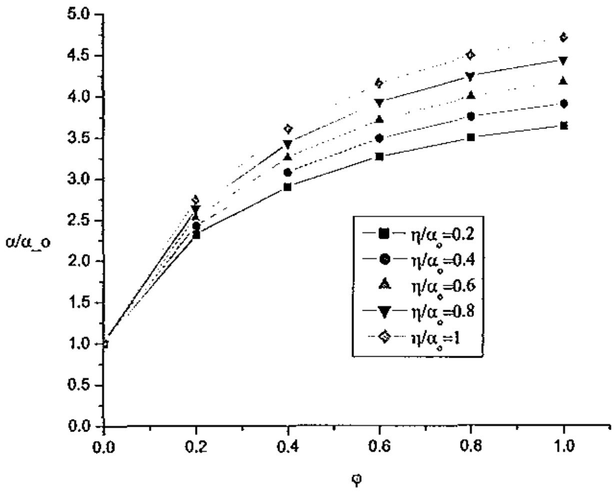

Figure 4.6: Variation of $\frac{\alpha}{\alpha_o}$ on φ

to predict different ways of enhancing the critical temperature T_c towards room temperature.

Chapter 5

Conclusion and Summary

Introduction

This part of our study is devoted to the conclusion and summary of the whole work of this thesis. So the chapter is presented under two sections one with the conclusion and the other with the summary.

5.1 Conclusion

In the last chapter (chapter4) we try to show the effect of impurity and/or disorder on the critical temperature and isotope effect coefficient. On the results and discussion part the outputs are described in words with the help of different plots. In general we may have the following concluding remarks:

As it is forwarded by the AG theory magnetic impurities destroy superconductivity by locally breaking the pairs, where as non-magnetic impurities are not pair breaking, according to Anderson's theorem. This is true for isotropic s-wave BCS superconductors, in which the order parameter is uniform and momentum independent.

In most high-transition-temperature superconductors the suppression of T_c with magnetic, non-magnetic impurities, and disorder effects are comparable in d-wave superconductivity.

We see that in the Born approximation, the effects of the random interactions (disorders) are exactly equivalent to those of magnetic impurities and in extremely disorder superconductors $\frac{T_c}{T_{co}}$ can be suppressed to zero even without any magnetic impurities.

We studied the effect of impurity and disorder and found that non-magnetic impurities and disorders (from spatial fluctuation in the pairing interaction) behaves as a strong pairing fluctuation defect or as a strong magnetic impurity.

By following different conditions that can enhance T_c it is possible to push the value of the critical temperature so that it is applicable for the advancement of this world.

5.2 Summary

Though this section is the last one it is not the least. Here we summarize the main ideas that the thesis tries to address.

In the introduction part historical development of superconductivity, the purpose of the paper, some explanation on s- and d-wave superconductors is treated.

Literatures about isotope effect, critical temperature, high-T_c superconductivity, and mechanism and effects of superconductivity are presented in the second chapter.

The third chapter lays basic mathematical grounds for treating the problem that this paper stands to solve.

It shows how electron-phonon interaction leads to the formation of Cooper pairs which are foundations for the BCS theory of superconductivity, methods of solving the BCS Hamiltonian and solving the Hamiltonian by the Green's function formalism.

The fourth chapter treats the problem that the paper is devoted to solve. Starting with the model and formalism it solves the Hamiltonian for the critical temperature and isotope effect in superconductors containing impurities, disorder,and'or defect.

Lastly the chapter presents the results with the help of different diagrams and discusses the results.

This last chapter deals with the concluding remarks.

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