THE STUDY OF CO-EXISTENCE OF SUPERCONDUCTIVITY AND FERROMAGNETISM IN UGE_2

By

Mesfin Asfaw Afrassa

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Supervisor: ______________________

Professor,P.Singh

Readers: ______________________

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Author: **Mesfin Asfaw Afrassa**

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Signature of Author

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Abstract

This work focuses on the study of co-existence of superconductivity and ferromagnetism in general and in UGe_2 superconductor in particular. Starting with a model Hamiltonian for the system and using Green functions formalism, we obtain expressions for T_c and superconductivity and magnetic order parameters Δ and η respectively.
For suitable value of the parameters the phase diagram is obtained which shows the possibility of the co-existence of superconductivity and ferromagnetism in UGe_2.

keywords: Superconductivity (SC), Ferromagnetism (FM), Co-existence, Green functions.

Introduction

Superconductivity (SC) is a phenomenon of zero resistance. The interplay between SC and magnetism long-range orderings has been an interesting topic in condensed matter physics. Magnetism is by now well understood than SC. Some of the basic features of SC were explained by Ginzburg and Landau, and by Bardeen, Cooper and Schriefer, but the basic mechanism of for example,spin triplet ferromagnetic superconductor is not well known. Thus, the interaction between SC and magnetism is studied to bring the mechanism for understanding and solving problems in superconductivity physics.

Superconductivity and magnetism would be antagonistic because of the competitive nature between the superconducting screening (Meissner effect) and the internal fields generated by magnetic ordering. How ever the discovery of a number of magnetic superconductors has allowed for a better understanding of how magnetic order and SC can coexist.

In this study we attempt to investigate theoreticaly the coexistence of superconductivity and ferromagnetism (FM) in a superconducting compound UGe_2. This compound have deferent characters which are impossible to explain by the existed theories. So we should look for better explanation.

This study is arranged in different chapters. The first chapter gives an overview of the SC, FM and there coexistence, review on the compound UGe_2 and the cooperative phenomenon on this compound, and highlight of phase transition and order parameter. Chapter 2 presents general discussion on the method we are using which is Green Functions. Chapter 3 yields the theoretical formulation and calculation of the problem.Chapter 4 contains a short presentation on the result of the calculation and discission. Finally, the fifth gives the summary of the whole thesis.

Chapter 1

Review Literature

1.1 Introduction

In this chapter, several important concepts will be introduced that will form the basis for understanding in this study. First, a general concept and history of superconductivity will be discussed, second, about ferromagnetism, third, a specific discussion on structure and electronic properties of UGe_2. Fourth, we will give a review of superconductivity and ferromagnetism on UGe_2. Following this discussion few concept of phase transition and order parameter will be presented. Finally, we will deal with few superconducting parameters.

1.2 Superconductivity and Ferromagnetism

Superconductivity

The history of superconductivity as a phenomenon is very rich, consisting of many events and discoveries. Therefore, it is not possible to describe all of them in this sub section but we can mention few by refereing [1,2] and other. Superconductivity was discovered in 1911 by Kamerling Onnes as the disappearance of resistivity in the metals mercury at a critical temperature, T_c. Subsequently perfect diamagnetism in superconductors was discovered by Meissner and Ochsenfield, 1933. In 1950 Ginzburg and Landau created a theory describing the transition between the superconducting and the normal phases.Isotopic effect is the other discovery in 1950. In

1957 Bardeen, cooper, and schrieffer(BCS) published a classic paper on the theory of superconductivity. In 1986 Bednorz and M$\ddot{u}$ller invented a new class of superconducting materials-high T_c cuprate superconductors(La-Ba-Cu-O,$T_c > 30k$). In 1987 a new kind of superconductivity were obtained in which bad conductors become superconductor. This was superconductivity in copper oxides. This hint the scientist to think that there must be a new mechanism, since phonon-mediated superconductivity is impossible at so high temperature.

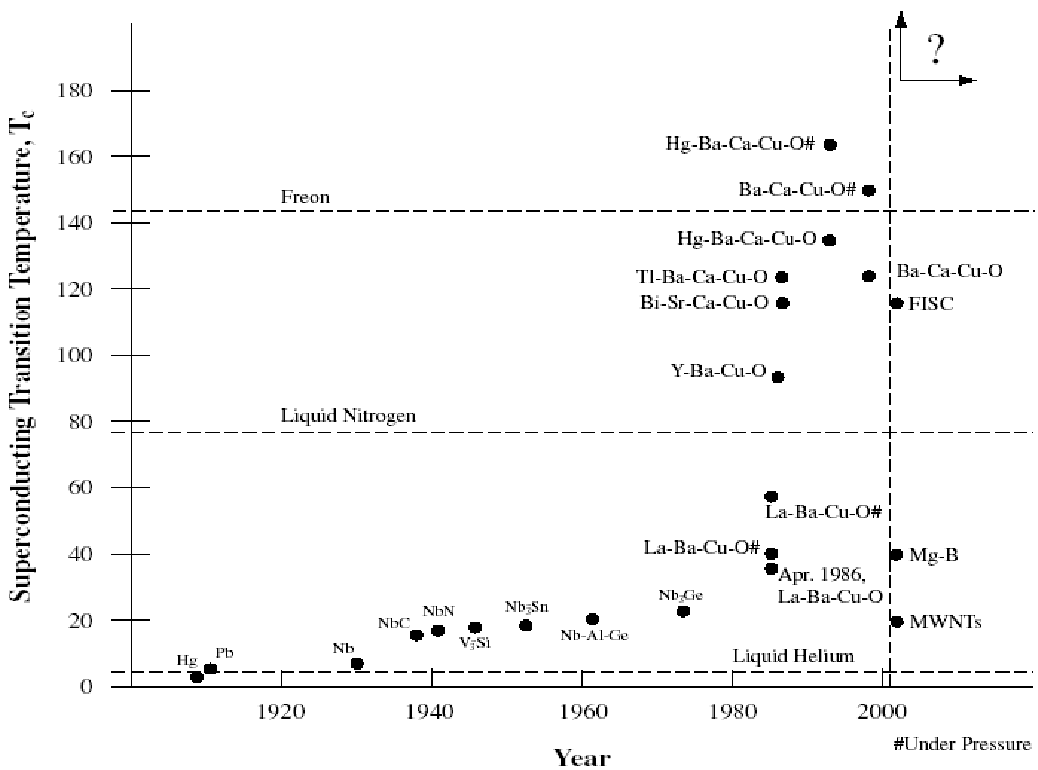

Figure 1.1: *History of the increase of superconducting temperature.*

The above figure shows the achivement in the history of superconductivity where different superconductors shows the phenomena of superconductivity at different temperatures. Kamerling obtained at low temperature but peoples have found at low and at high temperature. It is essential if superconductors are found at room temperature.

Superconductors are characterized by the transition temperature T_c, zero resistance, Cooper pairs, a diamagnetic behavior, the critical field and the energy gap. A complete understanding of these, is given by the first microscopic model developed by Bardeen, Cooper, Schriefer in 1957, and has as its center the occurrence of electron pairs due to the attractive electron-electron interaction mediated by virtual phonon.
In 1950 Fr$\ddot{o}$hlich suggested an electron-phonon interaction which is able to couple two electrons together in such a way that they behaved as if there was a direct interaction between them. We may think of the interaction between the electrons as being transmitted by phonon. Furthermore, Fr$\ddot{o}$hlich explained superconductivity by the lattice vibrations (phonon). Following Fr$\ddot{o}$hlich's discovery that the electron-electron interaction can be transmitted by phonon, the next step towards a microscopic theory of superconductivity was taken by Cooper, who discussed what happens when two electrons are added to a metal at absolute zero temperature so that they are forced by the Pauli principle to occupy states with $p > p_F$. He was able to show that if there is an attraction between them, however weak, they are able to form a bound state so that their total energy is less than $2\epsilon_F$. The largest number of allowed scattering processes, yielding the maximum lowering of the energy, is obtained by pairing electrons with opposite moments. Such a pair consisting of 2 electrons with equal and opposite momenta is known as a Cooper pair and is shown in fig.(1.2).

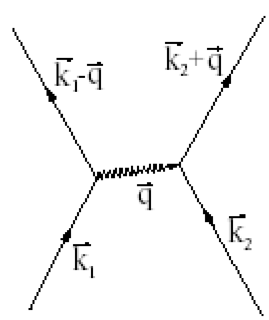

Figure 1.2: *Diagram illustrating electron-electron interaction via exchange of a virtual phonon of momentum $\hbar q$.*

The effective interaction of two electrons via a phonon can be visualized as the emission of a virtual phonon by one electron, and its absorption by the other, as shown in Fig.(1.2). An electron in a state k_1 (in momentum space) emits a phonon, and is scattered into a state $k\prime_1 = k_1 - q$. The electron in a state k_2 absorbs this phonon, and is scattered into $k\prime_2 = k_2 + q$.

Bardeen, Cooper and Schriefer(BCS theory) show how Cooper's simple result could be extended to apply to many interacting electrons. The idea of the BCS theory is that one conduction electron interacts with the ionic lattice and creates an excitation in the form of a phonon. This phonon propagates through the lattice and causes a local change of the charge density which will attract another electron, whereby an indirect interaction is established.

The great success of the BCS theory was to prove that the conduction electrons, collectively coupled in Cooper pairs by an attractive coupling (actually any attractive coupling, not necessarily phonon mediated), did indeed have a lower energy than the non-coupled electrons. It should be noted that the electrons in a Cooper pair have opposite spins and move in opposite directions, thus one may think of the condensate as a boson quasi particle state where the electrons are constantly changing partners. The fact that Cooper pairs are all in the same quantum state with the same energy is of great importance. Thus, the state of lowest energy (the ground state) occurs when all the electrons with momenta within a range $\Delta p = mhv_L/P_F$ about P_F are coupled together in Cooper pairs having opposite momentum and spin.

Ferromagnetism

Ferromagnetism is a phenomenon by which a material can exhibit a spontaneous magnetization and is one of the strongest form of magnetism. The distinct characteristic of ferromagnetic material are this spontaneous magnetization and existence of magnetic ordering temperature.

Ferromagnetism differs from the weaker diamagnetism and paramagnetism, in that the electrons of neighboring atoms interact with one another in a process called exchange coupling [3]. Ferromagnetism is strongly temperature dependent, and the magnetization of a ferromagnetic material is inversely related to temperature by:

$\chi = \frac{C}{T-\theta}$ where C is a constant and θ is close to the Curie temperature (θ_c) for the material.

Due to the dominance of thermal fluctuation,the spontaneous magnetization of a ferromagnetism disappears above a certain critical temperature, the curie point. The phase transition from the ferromagnetic to the paramagnetic phase is the classical example of a second-order phase transition.
The experimental value of θ_c for UGe_2 is 52k at ambient pressure [4,5,6].

1.2.1 coexistence

The co-existence of superconductivity (SC) and ferromagnetism (FM) has been studied theoretically and experimentally. It is challenging problem in Condensed Matter Physics. In 1957 [7] Ginzburg pointed out the possibility of co-existence of SC and FM for magnetization less than the thermodynamic critical field, many experimental investigations have been made, for example, for impurity ferromagnetism in a superconductor [8]. Theoretical works also have shown the co-existence of weak itinerant FM with s-wave [9,10].
But, the discovery of the co-existence of FM and SC in UGe_2 [11,12] and subsequently in $ZrZn_2$ [13] and URhGe [14] has shown clearly the spin-triplet Superconducting state. T.Moges [34] also shows the co-existence of superconductivity and ferromagnetism theoretically by adding impurities in a compound.
Different approach have been used to show the co-existence,for example H.Kaneyaus and K.Yamada [15] shows using the two dimensional t-t' Hubard model. M.Cuoco [16] shows the co-existence assuming that the magnetic instability is due to kinetic exchange. In this study we use Green functions formalism to find the equation of motion and so to show the co-existence.

1.3 Superconductivity and Ferromagnetism in UGe_2

1.3.1 Structure and Electronic Property

Uranium is a chemical element in the periodic table that has the symbol U and atomic number 92. Heavy, silvery-white, metallic, naturally radioactive, pyrophoric, toxic and teratogenic, uranium belongs to the actinide series. Its isotopes ^{235}U and to a lesser degree ^{233}U are used as the fuel for nuclear reactors and the explosive material for nuclear weapons [17].

The Uranium atoms are arranged as zigzag chains of nearest neighbors that run along the crystallographic a axis, which is easy magnetization direction [12].

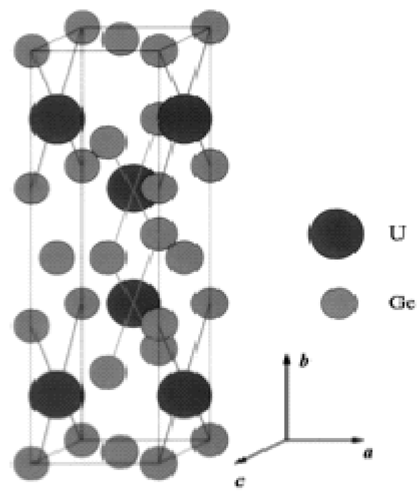

Figure 1.3: *crystal structure of* UGe_2 .

This figure is the conventional unit cell of UGe_2 with lattice parameter given by $a = 3.997\dot{A}$, $b = 15.039\dot{A}$, and $c = 4.087\dot{A}$. U atoms (large spheres) form zigzag lines along a, as shown in reference [18]
UGe_2 is a metalic ferromagnet with curie temperature $T_c = 52k$ and the spontaneous magnetization $1.14\mu_B/\mu$ at ambient pressure [5,6]. The magnetization is highly an isotropic along the easy a axis in orthorhombic crystal structure [11,12,4].
The electronic and the magnetic properties of the actinide metals and their compounds are largely determined by the partially filled 5f shell [19,20]. The 5f electrons in the actinides are less localized than the 4f electrons in the corresponding rare earth series.UGe_2 is light actinide compound [18].

Uranium compounds

$UGe_2, UIr, URhGe, UPd_2Al_3$, UBe_{13} and UNi_2Al_3 are the few of Uranium based compounds and grouped as Unconventional superconductors. $UPt_3, URu_2Si_2, UPd_2Al_3$

are also Uranium superconductors in which superconductivity co-exist with Anti ferromagnetism [18].
Both UGe_2 and $URhGe$ superconduct at ambient pressure, pairing is spin-triplet type, and both are orthorhombic structures and contain zigzag chains of nearest-neighbor uranium ions.

1.3.2 Experiment and Coexistence

The experimental discoveries of Uranium compounds have attracted interest in the relation between ferromagnetism and super conductivity. Generally, superconductivity does not favorably co-exist with ferromagnetism since the ferromagnetism moment gives rise to an internal magnetic field, which breaks the pairing state. However, superconductivity favorably coexists with ferromagnetism in UGe_2 [11,12] and URhGe [14]. superconductivity in these two materials is absent in paramagnetic phase. Such a co-existence is rarely found in a few materials belonging to a strongly correlated system.
Diffrent theoretical and experimental out come shows the co-existence of superconductivity and ferromagnetism in a compound UGe_2. For example with the use of ^{73}Ge nuclear-quadrupole-resonance(NQR) measurement were shown [21].
Co-existence of superconductivity and ferromagnetism was first verified by neutron scattering [12] by A. Huxley et al. It is thus concluded that superconductivity and ferromagnetism coexist below T_{SC}.And more recently by NQR experiments on Ge sites [4].
UGe_2 is pressure induced superconductor.Application of pressure suppresses T_C, and finally T_C becomes zero at the critical pressure P_C of 1.6-1.7GPa [22]. Superconductivity exist between pressure range from 1.0 to 1.6 GPa. In other words the present superconductivity disappears at $P > P_C$, namely in the paramagnetic state.
In URhGe, however, superconductivity at atmospheric pressure is completely suppressed with about 3-3.5GPa applied pressure, even though its T_c increases linearly to over 20k at 13GPa [23]. At ambient pressure, T_{sc}=0.25k for URhGe [14]
The superconducting transition temperature T_{SC} shows a maximum of 0.8 K around 1.2 GPa where the ferromagnetic state is still stable with $T_C = 32K$ [11,12,4] The heat capacity anomaly due to the superconducting transition was found at 1.13 GPa,

which indicates the bulk property of superconductivity [4].
Nayouki et al [24] performed the heat capacity measurement on UGe_2, under high pressure 1.13GP the superconducting temperature is 0.6k and confirm the bulk nature of the superconductivity in UGe_2.

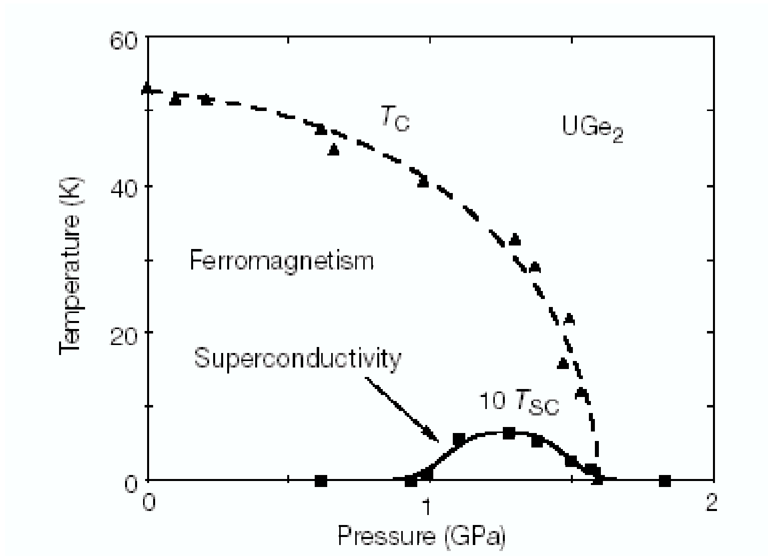

Figure 1.4: *phase diagram of* UGe_2 *given by Saxena et al .*

The temperature-pressure phase diagram of UGe_2 given by [11]. T_C denotes the Curie temperature and T_{SC} the superconducting transition temperature.

1.3.3 Mechanism

The onset of superconductivity occurs with the consideration of electron pairs. These electron pairs, called cooper pair [1], can be in a state of either total spin S=0 (spin singlet) or 1 (spin triplet). The standard S-wave pairing in usual (conventional) superconductors, the electron pairs are formed by an attractive electron-electron interaction due to a virtual phonon exchange.
In 1972 unconventional superfluidity due to a p-wave (spin triplet) cooper pairing of ^3He atom was experimentally predicted [25]. In this case the accepted mechanism of cooper pairing is based on attraction between the fermion (^3He atom) due to a virtual exchange of spin fluctuations. For unconventional superconductivity one can assume

the cooper pairing is mediated by spin fluctuation, which, like phonon are bosonic excitation.

Diffrent mechanism of unconventional cooper pairing of electrons/fermions (i.e., the formation of Cooper pairs with nonzero angular momentum) have been proposed. So that different expression were given to superconducting parameters, and let us see few for transition temperature, T_c.

BCS expresion:

$$k_B T_c = 1.14\hbar\omega e^{-1/NV}. \tag{1.1}$$

McMillan equation [26]:

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

Bogoliubov[2] model gives:

$$T_c \propto \omega_D exp[-\frac{1}{\lambda - \mu *}]. \tag{1.3}$$

Saxena et al [11] experiment shows the existence of spin triplet superconducting states in the metallic compound UGe_2 (see the fig.(1.4) given by [11]). This superconductivity is triggered by spontaneous magnetization of the ferromagnetic phase and co-exists with the superconducting phase. In this compound [11] the superconductivity seems to arise from the same electrons that create the band magnetism, and is most naturally understood as a triplet rather than a spin singlet pairing phonon.

As noted in Ref. [27] the superconductivity in these materials appears to be difficult to explain in terms of previous theories, and requires new concepts to interpret the experimental data. In the s-wave Cooper pairs are formed by conduction electrons while in UGe_2 and URhGe the 5f electrons of U atoms form both superconductivity and ferromagnetic order [11,12]. One may speculate about a spin-fluctuation mediated unconventional Cooper pairing as it is in the case of ^3He and heavy fermion superconductors. In this study we are not going to study the exact mechanism but to show the co-existence and to find the expression for transition temperature and the order parameter.

1.4 Phase Transition and Order Parameter

Phase transitions have played a role in modifying our world and we encountered it in day to day life. Since Superconductivity is a form of phase transition, we want to highlight phase transition in this section.

Phase Transition

In modern classification scheme, phase transition are divided in to two broad categories, named similarly to the Ehrenfest classes [28]:
The **first-order phase transitions** are those that involve a *latent heat*.
Second-order phase transitions have no latent heat nor Hysteresis. They are characterized by discontinuities in the heat capacity, which occur in super conducting, superfluid, magnetic, ferroelectric, order-disorder, and special kinds of structural transitions. An example which satisfy Ehrenfest classification scheme are first order solid-liquid-vapor transition and second order superconductiong transition.
In a system the normal phase can change due to the presence of interactions which cause the normal phase to become unstable. As a result of this instability, there is a phase transition to a new stable phase. The new phase is Fundamentally different to the original.Second-order transitions are the result of a competition between order and thermal fluctuations [29]. A discussion of the phase transition is beyond the scope of this work. we instead introduce the concept of order parameter.

Order Parameter

The more general description of phase transition than that provided be Ehrenfest is based on the fact that most phase transition are characterized by the appearance of some non-zero quantity in the order state. In a ferromagnetism this quantity is the spontaneous magnetization, such a quantity is called the *order parameter*.
In the theory of phase transitions, it is important to find order parameter which vanishes on one side of the transition, but takes a finite value on the other side. In a continuous phase transition, the order parameter may gradually evolve from zero at the critical point to a finite value on one side (usually the low-temperature side) of the transition. For different kinds of phases, different order parameters must be chosen.

From a phenomenological point of view, one must consider each physical system a new.
According to the standard theories of superconductivity, at low temperatures electrons with opposite spins form Cooper pairs. Thus, a possible order parameter would be the average probability amplitude to find a Cooper pair at a given lattice site in the crystal. Alternatively, one could characterize the phase transition through the gap parameter whose modulus is the difference in energy per electron of the Cooper pair condensate and the energy at the Fermi level.

1.5 Superconducting Parameters

The superconducting energy gap plays a role when considering the electrons at the Fermi surface, which mediate the magnetic coupling. In the weak Superconductivity coupling limit the energy gap Δ is much smaller than the Debye phonon energy $k_B\theta_D$, and the BCS coupling parameter NV , is required to be smaller than unity where N is the number of one-electron states per energy range at the Fermi level, and V is the BCS coupling constant describing the attraction between electrons. The energy gap at zero temperature can be evaluated in the weak coupling limit [1](BCS model):

$$\Delta(T=0) = 2\hbar\omega e^{-1/NV}. \tag{1.4}$$

This isotropic gap at the Fermi surface may interfere with the magnetic superzone gaps, created by the Fermi surface nesting structure. The gap parameter at any temperature between the absolute zero and T_c is given by

$$\Delta(T) = 3.06 k_B T_c \sqrt{1 - T/T_c}. \tag{1.5}$$

The critical temperature of superconductivity T_c is evaluated as the temperature where $\Delta(T)$ is zero:

$$\Delta(T=0) = 1.76 k_B T_c. \tag{1.6}$$

T_c is suppressed when magnetic ions appear in the solid. For UGe_2 the transition of superconductivity were observed [4] at $T_C = 0.7k$, which implies that UGe_2 is a low temperature superconductor.

The model of BCS predicts that the ratio $2\Delta(0)/k_B T_c$ is a universal constant 3.53 independent of the interaction v and of the particular superconductor [1]. The figure below shows dependent on temperature.

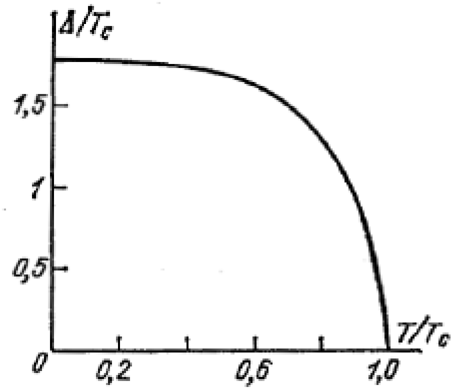

Figure 1.5: *Temperature dependence of the energy gap .*

The coherence length is a measure for the distance over which the two electrons in the Cooper pairs are correlated, given by:

$$\xi \sim \frac{\hbar\nu_f}{\Delta_{BCS}(0)}\sqrt{\frac{T_c}{T_c - T}} \tag{1.7}$$

where the coherence length at zero temperature is calculated in the BCS approximation, and the temperature dependence may be obtained using Ginzburg-Landau theory.

The Ginzburg-Landau parameter $\kappa = \frac{\xi}{\lambda}$ determines whether the superconductor is type I or II.

Chapter 2

Mathematical Methods

2.1 Introduction

There is a great deal of similarity between the quantum field theory and the theories based on Statistical Mechanics as far as the many-body aspect is concerned. The many-body problems is the study of the effect of interactions between the particles on the behavior of a many-particle system. The starting point for attacking the many-body problem is to express the Hamiltonian describing the system in terms of the creation and annihilation operators. In both quantum field theory and Statistical mechanics one is concerned with the averages of the quantum mechanical operator, but in the quantum field theory one usually consider the average over the ground state of the system $(T = 0)$ where as in statistical mechanics one is interested in the ensemble averages $(T \neq 0)$.

In this study we have used a Green functions technique to obtain the expression for super conducting transition temperature- T_c and order parameters (Δ, η). The Green's functions are useful because they are flexible enough to describe the effects of retarded interactions and all the quantities of physical interest can be derived from them [1].

2.2 Green Functions Formalism

Green functions or suitable modifications of these functions have been applied in quantum field theory to statistical problems. The Green functions are especially useful for summing over the restricted classes of perturbation theory diagrams, and are very powerful when combined with spectral representation. In quantum field theory the Green functions are the so called *Propagators* [30]. This name is based on the idea that, in order to fined the important physical properties of a system, it is essential to know, not the detailed behavior of each particle in the system, but rather just the average behavior of one or two typical particles. The quantities that describe this average behavior are called the one-particle and the two-particle propagators, respectively.

Green functions or propagators play the most important part in the field-theoretical treatment of the many-body problem. There are different types of Green functions: one-particle, two-particle...n-particle, advanced, retarded, causal, zero-temperature, finite-temperature, real-time, imaginary-time, and so on. The Green functions enjoy popularity between they yield, in a direct way, the most important physical properties of a system, have a simple physical interpretation, and can be calculated in a systematic way. In our discussion we used only the retarded Double-time Green function. It is defined as

$$G_r(t,t') \equiv \ll \hat{\mathbf{A}}(t); \hat{\mathbf{B}}(t') \gg$$
$$= -i\theta(t,t') < [\hat{\mathbf{A}}(t), \hat{\mathbf{B}}(t')] > . \tag{2.1}$$

Where$\ll ... \gg$ is the abbreviated notation for the Green functions, and$< ... >$ denotes averaging over a grand canonical ensemble. $\theta(t,t')$ is the step function.

$\mathbf{A}\hat{(t)}, \hat{\mathbf{B}}(t)$ are operators in the Heisenberg representation, which can be expressed as the product of the quantized field operators, that is,

$$\mathbf{A}(t) = exp(i\mathbf{H}t)\mathbf{A}(0)exp(-i\mathbf{H}t), h = 1$$

$$\theta(t) = \begin{cases} 0, & t < 0; \\ 1, & t > 0. \end{cases} \tag{2.2}$$

Also [**A**,**B**] is a commutator or anti commutator, that is, [**A**,**B**]=$AB - \eta BA$,$\eta = \pm 1$. The sign of η is positive if A and B are both BOSE operator and negative if they are FERMI operators.

In order to obtain the equation of motion we differentiate eq.(2.1) with respect to t as,

$$i\frac{d}{dt}G_r(t-t') = i\frac{d}{dt} \ll \hat{A}(t); \hat{B}(t') \gg$$
$$= \delta(t-t') < [\hat{A}(t); \hat{B}(t')] > + \ll [\hat{A}(t), \hat{H}]; \hat{B(t')} \gg . \tag{2.3}$$

Taking use of between Heaviside step function $\theta(t)$ and Dirac-δ function, $\theta(t) = \int_{-\infty}^{t} \delta(t)dt$, there fore $\frac{d}{dt}\theta(t) = \delta(t)$.

It is known that $A(t)$ and $B(t')$ satisfy equation of the form, $i\frac{dA}{dt} = [A, H]$. Now equation of motion becomes,

$$i\frac{d}{dt}G_r(t-t') = \delta(t-t') < [\hat{A}(t); \hat{B}(t')] > + \ll \hat{A}(t)\hat{H} - \hat{H}\hat{A}(t); \hat{B}(t') \gg . \tag{2.4}$$

To solve this equation it is convenient to work with Fourier transform of this equation. A careful analysis shows that the function depends on t and t' through$(t - t')$. Thus we can write $G_r(t, t') = G_r(t - t')$.

Now let $G_r(\omega)$ be the Fourier transform of $G_r(t - t')$ such that

$$G_r(t-t') = \int_{-\infty}^{\infty} G_r(\omega) exp(-i\omega(t-t'))d\omega. \tag{2.5}$$

$$G_r(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_r(t-t') exp(i\omega(t-t')d(t-t'). \tag{2.6}$$

And the δ function can be defined as

$$\delta(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} exp(-i\omega(t-t')d\omega. \tag{2.7}$$

Equation(2.5) becomes,

$$\omega G(\omega) =< [A(t), B(t')] > + \ll [A(t), H]; B(t') \gg_{\omega} .$$

Since the fourier transform of G(t) is $G(t) = \int G(\omega)exp(-i\omega t)d\omega$ from which it can be shown that
$\frac{\partial G}{\partial t} = -i\omega$ [fourier transform of $G(t)$] Then $\omega G(\omega)$ can be written as

$$\omega \ll A, B \gg_{\omega} =< [A, B] > + \ll [A, H], B \gg_{\omega} . \tag{2.8}$$

Since $\ll A, B \gg_{\omega}$ denotes the fourier transform of the Green functions involving the operator A and B. It satisfy the equation of motion eq.(2.3), where the double brackets $\ll ... \gg$ indicates the fourier transform of the corresponding Green function. The single brackets $< ... >$ indicate the thermal average over the canonical ensemble, that is ,

$$< F >= \frac{Trexp(-\beta H)F}{Trexp(\beta H)}.$$

Where $\beta = 1/(k_B T)$, k_B is the boltzman constant. H is the hamiltonian of the system considered.
From the analytical properties of the Green functions it follows that the correlation function $< \hat{B}(t')A(t) >$ can be obtained from the equation of Green functions by

$$< \hat{B}(t')A(t) >= i \lim_{\epsilon \longrightarrow 0} \int_{-\infty}^{\infty} \frac{(\ll \hat{A}; \hat{B} \gg_{\hbar\omega + i\epsilon} - \ll \hat{A}; \hat{B} \gg_{\hbar\omega - i\epsilon})}{exp(\beta\hbar\omega) - 1}. \tag{2.9}$$

In order to obtain the superconductivity properties, we have defined super conducting order parameters, Δ (energy gap), which is pairing of electron or spin and momentum by,

$$\Delta = \sum_k v < a_{k\uparrow} a_{-k\downarrow} > .$$

$$\Delta^* = \sum_k v < a^{\dagger}_{-k\downarrow} a^{\dagger}_{k\uparrow} > .$$

where $\Delta = \Delta^*$ (since Δ is real). The value of transition temperature T_c is calculated by using the condition, $T \longrightarrow T_c$, as $\Delta \longrightarrow 0$ from the BCS Hamiltonian which is given by

$$\hat{H}_{BCS} = \sum_{k} a^{\dagger}_{k\sigma} a_{k\sigma} - \sum_{kk\prime} v_{kk\prime} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} a_{k'\downarrow} a_{-k'\uparrow}.$$

Using the reduced BCS Hamiltonian, the equation of motion for $\ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg$ is given by

$$\omega \ll a_{k\downarrow}, a^{\dagger}_{k\uparrow} \gg = \delta_{kk'} + \ll [a_{k\uparrow}, H_{BCS}]; a^{\dagger}_{k\uparrow} \gg .$$

From this we can get

$$\ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg = -[\frac{\Delta}{\omega^2 - \in_k^2 - \Delta^2}].$$

$$\ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg = \frac{(\omega + \in_k)}{\omega^2 - \in_k^2 - \Delta^2}.$$

The super conducting order parameter Δ, can be given by the relation

$$\Delta = \frac{v}{\beta} \sum_{kn} \ll a^{\dagger}_{-k\downarrow}, a^{\dagger}_{k\uparrow} \gg . \tag{2.10}$$

Changing the summation in to an integral with cut off energy $\pm\hbar\omega_D$ from the fermi level it becomes

$$\Delta = N(0)v \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{tanh(\frac{\beta}{2}\sqrt{\in_k^2 + \Delta^2})}{2\sqrt{\in_k^2 + \Delta^2}} d \in_k .$$

As $T \longrightarrow T_c, \Delta \longrightarrow 0$

$\Longrightarrow \frac{1}{N(0)v} = \int_0^{\hbar\omega_D} \frac{tanh(\frac{\in_k}{2k_B T_c})}{\in_k} d \in_k$.

Integrating gives

$$k_B T_c = 1.14 \hbar\omega_D exp(\frac{-1}{N(0)v}). \tag{2.11}$$

Where N(0) is the density of state at the fermi level and the expression is BCS.

Chapter 3

Theoretical Formulation

3.1 The Model Hamiltonian

the purpose of this work is to study theoretically the co-existence of magnetic and superconductive properties in the compound UGe_2 in general and, to find expression for transition temperature and order parameter in particular. In this chapter we formulate a model Hamiltonian and do some calculation. Consider the Hamiltonian below:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3.$$

Where

$$\hat{H}_1 = \sum_{k,\sigma} \in_k a^{\dagger}_{k,\sigma} a_{k,\sigma} + \sum_{\ell} \in_\ell b^{\dagger}_{\ell,\sigma} b_{\ell,\sigma}, \tag{3.1}$$

which is the energy of free (conduction) electron and localized electron respectively.

$$\hat{H}_2 = -\sum_{k,k'} V(k,k') a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\uparrow} a_{-k'\uparrow} a_{k'\uparrow}, \tag{3.2}$$

which is the interaction (electron-electron) through boson (phonon) exchange and

$$\hat{H}_3 = \sum_{\ell,m} \alpha_{\ell,m} a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\uparrow} b_{\ell\uparrow} b_{m\uparrow} + hc, \tag{3.3}$$

which is the interaction term between conduction electrons and localized electrons due to some unspecified mechanism as may be due to spin fluctuation, with coupling

constant α.
$V(k,k')$ define the matrix element of the interaction potential. $a^{\dagger}_{k\sigma}(a_{k\sigma})$ is the creation (annihilation) operators of an electron specified by the wave vector k and the spin σ. $\in_k$ is the one electron energy measured relative to the chemical potential. $b^{\dagger}_{\ell}(b_{\ell})$ are creation (annihilation) operators of localized electrons. Both superconductivity and ferromagnetism is believed to be due to 5f electrons of uranium.

3.2 Equation of Motion

To get the equation of motion we use a Greens function which is defined as follows.

$$G_r(t,t') \equiv \ll \hat{\mathbf{A}}(t); \hat{\mathbf{B}}(t') \gg = -i\theta(t,t') < [\hat{\mathbf{A}}(t), \hat{\mathbf{B}}(t')] > .$$

After differentiating and taking the fourier transform of this equation (ch.2) we get eq.(2.8). Now we use in our calculation eq.(2.8) in the next sub sections.

3.2.1 For Mobile (conduction) Electrons

$$\omega \ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg_{\omega} = 1 + \ll [a_{k\uparrow}, \hat{H}], a^{\dagger}_{k\uparrow} \gg_{\omega} \tag{3.4}$$

for $[A,B] = \delta_{ij}$.
To solve eq.(3.4) let us evaluate the commutation relation with the use of

$$[A,BC] = [A,B]C + B[A,C],$$

$$[AB,C] = A[B,C] + [A,C]B,$$

$$[A,BC] = \{A,B\}C - B\{A,C\},$$

$$[AB,C] = A\{B,C\} - \{A,C\}B.$$

And $[a_k, a^{\dagger}_{k'}] = \delta_{kk'} = 1$, if $k = k'$, otherwise $= 0$,

$$[a_k, a_k] = [a^{\dagger}_k, a^{\dagger}_k] = 0.$$

Fermion use operators which satisfy anticommutation relation. $\{A, B\} = \{B, A\}$, $\{A, B\} = AB + BA$.

$$\begin{aligned}
[a_{k\uparrow}, \hat{H}_1] &= [a_{k\uparrow}, \sum_{p,\sigma} \in_p a^\dagger_{p,\sigma} a_{p,\sigma} + \sum_{\ell} \in_\ell b^\dagger_{\ell,\sigma} b_{\ell,\sigma}] \\
&= [a_{k\uparrow}, \sum_{p,\sigma} \in_p a^\dagger_{p,\sigma} a_{p,\sigma}] \\
&= \sum_{p,\sigma} \in_p \{a_{k\uparrow}, a^\dagger_{p,\sigma}\} a_{p,\sigma} - a^\dagger_{p,\sigma} \{a_{k\uparrow}, a_{p,\sigma}\} \\
&= \sum_{p,\sigma} \in_p \{a_{k\uparrow}, a^\dagger_{p,\sigma}\} a_{p,\sigma} \\
&= \sum_{p,\sigma} \in_p \delta_{kp} \delta_{\uparrow\sigma} a_{p,\sigma} \\
&= \sum_{p} \in_p \delta_{kp} a_{p,\uparrow} \\
&= \in_k a_{k\uparrow}.
\end{aligned} \tag{3.5}$$

$$\begin{aligned}
[a_{k\uparrow}, \hat{H}_2] &= [a_{k\uparrow}, -\sum_{p,p'} V(p,p') a^\dagger_{p\uparrow} a^\dagger_{-p\uparrow} a_{-p'\uparrow} a_{p'\uparrow}] \\
&= -\sum_{p,p'} V(p,p') [a_{k\uparrow}, a^\dagger_{p\uparrow} a^\dagger_{-p\uparrow}] a_{-p'\uparrow} a_{p'\uparrow} \\
&= -\sum_{p,p'} V(p,p') (\{a_{k\uparrow}, a^\dagger_{p\uparrow}\} a^\dagger_{-p\uparrow} - a^\dagger_{p\uparrow} \{a_{k\uparrow}, a^\dagger_{-p\uparrow}\}) a_{-p'\uparrow} a_{p'\uparrow} \\
&= -\sum_{p,p'} V(p,p') (\delta_{kp} a^\dagger_{-p\uparrow} - a^\dagger_{p\uparrow} \delta_{k,-p}) a_{-p'\uparrow} a_{p'\uparrow} \\
&= -\sum_{p'} V a^\dagger_{-k\uparrow} a_{-p'\uparrow} a_{p'\uparrow}.
\end{aligned} \tag{3.6}$$

$$[a_{k\uparrow}, \hat{H}_3] = [a_{k\uparrow}, \sum_{l,m,p} \alpha_{\ell,m} a^\dagger_{p\uparrow} a^\dagger_{-p\uparrow} b_{\ell\uparrow} b_{m\uparrow} + hc]. \tag{3.7}$$

where $hc = \sum_{l,m,p} \alpha^*_{\ell,m} a_{-k\uparrow} a_{k\uparrow} b^\dagger_{\ell\uparrow} b^\dagger_{m\uparrow}$,
assuming α is real we can take $\alpha = \alpha^*$ and the above equation becomes

$$\begin{aligned}
[a_{k\uparrow}, \hat{H}_3] &= [a_{k\uparrow}, \sum_{l,m,p} \alpha_{\ell,m} a^\dagger_{p,\uparrow} a^\dagger_{-p,\uparrow}] b_{\ell\uparrow} b_{m\uparrow} \\
&= \sum_{l,m,p} \alpha_{\ell,m} (\{a_{k\uparrow}, a^\dagger_{p,\uparrow}\} a^\dagger_{-p,\uparrow} - a^\dagger_{p,\uparrow}\{a_{k\uparrow}, a^\dagger_{-p,\uparrow}\}) b_{\ell\uparrow} b_{m\uparrow} \\
&= \sum_{l,m,p} \alpha_{\ell,m} (\delta_{kp} a^\dagger_{-p,\uparrow} - a^\dagger_{p,\uparrow} \delta_{k(-p)}) b_{\ell\uparrow} b_{m\uparrow} \\
&= \sum_{l,m,} \alpha_{\ell,m} a^\dagger_{-k,\uparrow} b_{\ell\uparrow} b_{m\uparrow}.
\end{aligned} \tag{3.8}$$

Now substituting equation (3.5) (3.6) and (3.8) in equation (3.4) yields that

$$\omega \ll a_{k\uparrow}, a^\dagger_{k\uparrow} \gg = 1 + \in_k \ll [a_{k\uparrow}, a^\dagger_{k\uparrow} \gg - \sum_{p'} V < a_{-p'\uparrow} a_{p'\uparrow} > \ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg$$

$$+ \sum_{l,m,} \alpha_{\ell,m} < b_{\ell\uparrow} b_{m\uparrow} > \ll a^\dagger_{-k,\uparrow}, a^\dagger_{k\uparrow} \gg .$$

which implies

$$(\omega - \in_k) \ll a_{k\uparrow}, a^\dagger_{k\uparrow} \gg = 1 - (\Delta - \eta) \ll a^\dagger_{-k,\uparrow}, a^\dagger_{k\uparrow} \gg . \tag{3.9}$$

where

$$\Delta = \sum_{p'} V < a_{-p'\uparrow} a_{p'\uparrow} > .$$

and $\eta = \sum_{l,m} \alpha_{\ell,m} < b_{\ell\uparrow} b_{m\uparrow} >$. One can also obtain the equation of motion for higher order Green's function $\ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg$ using

$$\omega \ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg_\omega = < [a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow}] > + \ll [a^\dagger_{-k\uparrow}, \hat{H}], a^\dagger_{k\uparrow} \gg_\omega . \tag{3.10}$$

Applying the same techniques;

$$\begin{aligned}
[a^{\dagger}_{-k\uparrow}, \hat{H}_1] &= [a^{\dagger}_{-k\uparrow}, \sum_{p,\sigma} \in_p\ a^{\dagger}_{p,\sigma} a_{p,\sigma} + \sum_{\ell} \in_\ell\ b^{\dagger}_{\ell,\sigma} b_{\ell,\sigma}] \\
&= [a^{\dagger}_{-k\uparrow}, \sum_{p,\sigma} \in_p\ a^{\dagger}_{p,\sigma} a_{p,\sigma}] \\
&= \sum_{p,\sigma} \in_p\ (\{a^{\dagger}_{-k\uparrow}, a^{\dagger}_{p,\sigma}\} a_{p,\sigma} - a^{\dagger}_{p,\sigma}\{a^{\dagger}_{-k\uparrow}, a_{p,\sigma}\}) \\
&= -\sum_{p,\sigma} \in_p\ a^{\dagger}_{p,\sigma} \delta_{-kp} \delta_{\uparrow\sigma} \\
&= -\sum_{p} \in_p\ a^{\dagger}_{p\uparrow} \delta_{-kp} \\
&= -\in_{-k}\ a^{\dagger}_{-k\uparrow}.
\end{aligned} \tag{3.11}$$

$$\begin{aligned}
[a^{\dagger}_{-k\uparrow}, \hat{H}_2] &= [a^{\dagger}_{-k\uparrow}, -\sum_{p,p'} V(p,p') a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\uparrow} a_{-p'\uparrow} a_{p'\uparrow}] \\
&= -\sum_{p,p'} V(p,p')([a^{\dagger}_{-k\uparrow}, a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\uparrow}] a_{-p'\uparrow} a_{p'\uparrow} + a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\uparrow}[a^{\dagger}_{-k\uparrow}, a_{-p'\uparrow} a_{p'\uparrow}]) \\
&= -\sum_{p,p'} V(p,p') a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\uparrow}(\{a^{\dagger}_{-k\uparrow}, a_{-p'\uparrow}\} a_{p'\uparrow} - a_{-p'\uparrow}\{a^{\dagger}_{-k\uparrow}, a_{p'\uparrow}\}) \\
&= -\sum_{p,p'} V(p,p') a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\uparrow}(\delta_{-k(-p)'} a_{p'\uparrow} - a_{-p'\uparrow} \delta_{-kp'}) \\
&= -\sum_{p} V a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\uparrow} a_{k\uparrow}.
\end{aligned} \tag{3.12}$$

$$[a_{k\uparrow}, \hat{H}_3] = [a_{k\uparrow}, \sum_{l,m,p} \alpha_{\ell,m} a^{\dagger}_{p\uparrow} a^{\dagger}_{-p\uparrow} b_{\ell\uparrow} b_{m\uparrow} + hc]. \tag{3.13}$$

where $hc = \sum_{l,m,p} \alpha^*_{\ell,m} a_{-p\uparrow} a_{p\uparrow} + b^\dagger_{\ell\uparrow} b^\dagger_{m\uparrow}$.
Since α is real we can take $\alpha = \alpha^*$ so the above equation becomes

$$
\begin{aligned}
[a^\dagger_{-k\uparrow}, \hat{H}_3] &= [a^\dagger_{-k\uparrow}, \sum_{l,m,p} \alpha_{\ell,m} a^\dagger_{p\uparrow} a^\dagger_{-p\uparrow} b_{\ell\uparrow} b_{m\uparrow}] + [a^\dagger_{-k\uparrow}, \sum_{l,m,p} \alpha^*_{\ell,m} a_{-p\uparrow} a_{p\uparrow} b^\dagger_{\ell\uparrow} b^\dagger_{m\uparrow}] \\
&= \sum_{l,m,p} \alpha_{\ell,m} [a^\dagger_{-k\uparrow}, a_{-p,\uparrow} a_{p\uparrow}] b^\dagger_{\ell\uparrow} b^\dagger_{m\uparrow} \\
&= \sum_{l,m,p} \alpha_{\ell,m} (\{a^\dagger_{-k\uparrow}, a_{-p\uparrow}\} a_{p,\uparrow} - a_{-p\uparrow} \{a^\dagger_{-k\uparrow}, a_{p\uparrow}\}) b^\dagger_{\ell\uparrow} b^\dagger_{m\uparrow} \\
&= \sum_{l,m,p} \alpha_{\ell,m} (\delta_{-k(-p)} a_{p\uparrow} - a_{-p\uparrow} \delta_{-k,p}) b^\dagger_{\ell\uparrow} b^\dagger_{m\uparrow} \\
&= \sum_{l,m,} \alpha_{\ell,m} a_{k\uparrow} b^\dagger_{\ell\uparrow} b^\dagger_{m\uparrow}.
\end{aligned}
\tag{3.14}
$$

Substituting eq.(3.11), eq.(3.12) and eq.(3.14) in equation (3.10) yields that

$$
\begin{aligned}
\omega \ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg &= - \in_{-k} \ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg - \sum_p V < a^\dagger_{p\uparrow}, a^\dagger_{-p\uparrow} > \ll a_{k\uparrow}, a^\dagger_{k\uparrow} \gg \\
&+ \sum_{l,m,} \alpha_{\ell,m} < b^\dagger_{\ell\uparrow} b^\dagger_{m\uparrow} > \ll a_{k\uparrow}, a^\dagger_{k\uparrow} \gg .
\end{aligned}
\tag{3.15}
$$

Since $\in_k = \in_{-k}$ is the kinetik energy of the conduction electrons and $\Delta = \Delta^*$, $\eta = \eta^*$ (taking order parameter is real) then

$$
(\omega + \in_k) \ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg = -(\Delta - \eta) \ll a_{k\uparrow}, a^\dagger_{k\uparrow} \gg . \tag{3.16}
$$

Now using eq.(3.9) and eq.(3.16) we can obtain the following two equations:

$$
(\omega + \in_k) \ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg = -(\Delta - \eta)\left(\frac{1}{\omega - \in_k} - \frac{(\Delta - \eta)}{(\omega - \in_k)} \ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg\right)
$$

$$
\Longrightarrow (\omega^2 - \in_k^2 - (\Delta - \eta)^2) \ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg = -(\Delta - \eta).
$$

There fore,

$$
\ll a^\dagger_{-k\uparrow}, a^\dagger_{k\uparrow} \gg = \frac{-(\Delta - \eta)}{(\omega^2 - \in_k^2 - (\Delta - \eta)^2)} \tag{3.17}
$$

and

$$(\omega- \in_k) \ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg = 1 - (\Delta - \eta) \ll a^{\dagger}_{-k\uparrow}, a^{\dagger}_{k\uparrow} \gg$$
$$= 1 + \frac{(\Delta - \eta)^2}{(\omega+ \in_k)} \ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg$$
$$\Longrightarrow (\omega^2- \in_k^2 -(\Delta - \eta)^2) \ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg = (\omega+ \in_k)$$
$$\Longrightarrow \ll a_{k\uparrow}, a^{\dagger}_{k\uparrow} \gg = \frac{(\omega+ \in_k)}{(\omega^2- \in_k^2 -(\Delta - \eta)^2)}. \quad (3.18)$$

The equation of motion with green's function given by eq.(3.18)

$$\ll a^{\dagger}_{-k\uparrow}, a^{\dagger}_{k\uparrow} \gg = \frac{-(\Delta - \eta)}{(\omega^2- \in_k^2 -(\Delta - \eta)^2)}$$

where Δ is the supper conducting order parameter (analogue to the BCS order parameter) and η is the magnetic ordering. Using the relation for Δ,

$$\Delta = \frac{v}{\beta} \sum_{k,n} \ll a^{\dagger}_{-k\uparrow}, a^{\dagger}_{k\uparrow} \gg$$

and the sum may be changed in to an integral by introducing the density of states $N(\in)$, $\frac{1}{v}\sum_k \longrightarrow \frac{1}{(2\pi)^3}\int d^3k = \int_{-\varepsilon_F}^{\infty} d \in N(\in)$.
The summation with respect to k and n extends over all allowed pair states. There fore

$$\Delta = -\frac{1}{\beta}\sum_n \int_{-\varepsilon_F}^{\infty} d \in N(\in) v [\frac{\Delta - \eta}{\omega^2- \in_k^2 -(\Delta - \eta)^2}].$$

Attractive interaction is effective for the region $-\hbar\omega_b < \in < \hbar\omega_b$. And assuming the density of states does not vary over this integral. Then the expression becomes,

$$\Delta = -\frac{2}{\beta} N(\in) v \sum_n \int_0^{\hbar\omega_b} d \in [\frac{\Delta - \eta}{\omega^2- \in_k^2 -(\Delta - \eta)^2}]. \quad (3.19)$$

Now changing, $\omega \longrightarrow i\omega_n$ and using the Matsubara frequency

$$\omega_n = \frac{(2n+1)\pi}{\beta},$$

Eq.(3.19) becomes,

$$\Delta = 2N(0)v\beta \sum_n \int_0^{\hbar\omega_b} d\in [\frac{\Delta-\eta}{(2n+1)^2\pi^2+\beta^2E^2}],$$

where $E^2 = \in_k^2 + (\Delta-\eta)^2$.

Using the relation $\frac{1}{2x}tanh(x/2) = \sum_n \frac{1}{(2n+1)^2+x^2}$ we can write the above equation as follows.

$$\Delta = 2N(0)v\beta \int_0^{\hbar\omega_b} d\in (\Delta-\eta)\frac{1}{2\beta E}tanh(\beta E/2),$$

let $N(0)v = \lambda$

$$\Longrightarrow \frac{\Delta}{\lambda} = \int_0^{\hbar\omega_b} d\in \frac{(\Delta-\eta)}{\sqrt{(\in_k^2+(\Delta-\eta)^2)}}\tanh(\beta\sqrt{(\in_k^2+(\Delta-\eta)^2)}/2). \tag{3.20}$$

Let as study this equation (eq.(3.20)) in different cases: as $T \longrightarrow 0k$, and $T \longrightarrow T_c$.

(I) as $T \longrightarrow 0k, \beta = \infty$, so one can take

$$tanh(\beta E/2) \longrightarrow 1$$

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega_b} d\in \frac{(\Delta-\eta)}{\sqrt{(\in_k^2+(\Delta-\eta)^2)}}.$$

Using the integral $\int \frac{a}{\sqrt{a^2+x^2}}dx = asinh^{-1}(x/a)$,the above equation becomes

$$\frac{1}{\lambda} = (1-\frac{\eta}{\Delta})\sinh^{-1}(\frac{\hbar\omega_b}{\Delta-\eta})$$

$$= (1-\frac{\eta}{\Delta})\ln\{\frac{\hbar\omega_b}{\Delta-\eta} + \sqrt{(\frac{\hbar\omega_b}{\Delta-\eta})^2+1}\}$$

$$\approx (1-\frac{\eta}{\Delta})\ln\frac{2\hbar\omega_b}{\Delta-\eta}. \tag{3.21}$$

Which implies:

$$(\Delta-\eta) = 2\hbar\omega_b\exp(-\frac{1}{\lambda(1-\eta/\Delta)}). \tag{3.22}$$

Which is similar to BCS except the η and $(1-\eta/\Delta)$ term.

If we use $\Delta(0)$ of BCS at T=0, which is given by

$$2\Delta(0) = 3.5 k_B T_C,$$

for the compound we study (UGe_2) the experimental result of $T_C \approx 0.7k$, so that

$$\Delta(0) = 1.75 k_B T_C = 3.36 \times 10^{-23}.$$

At T=0 the expression for η using Eq.(3.22) becomes

$$\eta \simeq 1.75 k_B T_C - 2\hbar\omega_b exp(-\frac{1}{\lambda(1-\eta/1.75 k_B T_C)}). \quad (3.23)$$

(II) As T$\longrightarrow T_c, \Delta \longrightarrow 0$

Using equation(3.20)

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega_b} d\in \frac{(\Delta-\eta)}{\sqrt{(\in_k^2 + (\Delta-\eta)^2)}} \tanh(\beta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}/2)$$

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} d\in \frac{(1-\eta/\Delta)}{\sqrt{(\in_k^2 + (\Delta-\eta)^2)}} \tanh(\beta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}/2)$$

$$= \int_0^{\hbar\omega_b} d\in \frac{1}{\sqrt{(\in_k^2 + (\Delta-\eta)^2)}} \tanh(\beta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}/2)$$
$$- \int_0^{\hbar\omega_b} d\in \frac{\eta}{\Delta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}} \tanh(\beta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}/2). \quad (3.24)$$

At $T = T_c$,$\Delta = 0$

The first integral of eq.(3.24) becomes

$$\int_0^{\hbar\omega_b} d\in \frac{1}{\sqrt{(\in^2 + \eta^2)}} \tanh(\beta\sqrt{(\in^2 + \eta^2)}/2)$$

$$= \int_0^{\hbar\omega_b} d\in \frac{2}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{\omega_n^2 + \in^2 + \eta^2},$$

using Laplace's Transform, and Matsubara frequency, $\omega_n = (2n+1)\frac{\pi}{\beta}$, the above integral becomes

$$= \int_0^{\hbar\omega_b} d\in \frac{2}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{\omega_n^2 + \in^2} - \int_0^{\hbar\omega_b}\eta^2 d\in \frac{2}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{(\omega_n^2 + \in^2)^2} + ...$$

$$= \int_0^{\hbar\omega_b} d\in \frac{tanh(\frac{\beta}{2}\in)}{\in}$$

$$- \int_0^{\hbar\omega_b}\eta^2 d\in \frac{2}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{(((2n+1)\frac{\pi}{\beta})^2 + \in^2)^2} + ...$$

But,

$$\sum_{n=-\infty}^{\infty}\frac{1}{(((2n+1)\frac{\pi}{\beta})^2 + \in^2)^2} = 2\sum_{n=0}^{\infty}\frac{1}{(((2n+1)\frac{\pi}{\beta})^2 + \in^2)^2}$$

$$2\sum_{n=0}^{\infty}\frac{1}{(a^2+\epsilon^2)^2} = 2\sum_{n=0}^{\infty}\frac{1}{a^4(1+\frac{\epsilon^2}{a^2})^2} = 2\sum_{n=0}^{\infty}\frac{1}{a^4(1+x^2)^2}, x^2 = \frac{\epsilon^2}{a^2}$$

Then

$$\int_0^{\hbar\omega_b} d\in \frac{1}{\sqrt{(\in^2 + \eta^2)}}\tanh(\beta\sqrt{(\in^2 + \eta^2)}/2) = \int_0^{\hbar\omega_b} d\in \frac{\tanh(\frac{\beta}{2}\in)}{\in}$$

$$- \int_0^{\hbar\omega_b}\eta^2 d\in \frac{2}{\beta}2\sum_{n=0}^{\infty}\frac{1}{a^4(1+x^2)^2} + ... \quad (3.25)$$

$$= I_1 + I_2.$$

where

$$I_1 = \int_0^{\hbar\omega_b} d\in \frac{\tanh(\frac{\beta}{2}\in)}{\in}$$

$$= \int_0^{\frac{\beta}{2}\hbar\omega_b} dy\frac{\tanh y}{y}, y = \frac{\beta}{2}\in$$

$$= \ln y \tanh y|_0^{\frac{\beta}{2}\hbar\omega_b} - \int_0^{\frac{\beta}{2}\hbar\omega_b}\frac{\ln y}{\cosh^2 y}dy,$$

for low temperature $tanh(\frac{\hbar\omega}{2k_BT}) \to 1$

$$I_1 = \ln\frac{\beta}{2}\hbar\omega_b - ln(\pi/4)exp(-c) = \ln 1.14\frac{\hbar\omega_b}{k_BT_c}. \quad (3.26)$$

$$
\begin{aligned}
I_2 &= \int_0^{\hbar\omega_b} \eta^2 d\in \frac{2}{\beta} 2 \sum_{n=0}^{\infty} \frac{1}{a^4(1+x^2)^2} + ... \\
&= 4\eta^2 \sum_{n=0}^{\infty} (\frac{\beta}{\pi(2n+1)})^3 \int_0^{\infty} \frac{1}{(1+x^2)^2} dx + ... \\
&\approx \frac{4\beta^2}{\pi 3} \eta^2 \frac{7}{8} \zeta(3) \frac{\pi}{4} \\
&= (\frac{\eta}{\pi k_B T_c})^2 \frac{8.414}{8}.
\end{aligned} \tag{3.27}
$$

With the use of

$$
\int_0^{\infty} \frac{dx}{(x^2+1)^2} = \frac{\pi}{4},
$$

$$
\sum_0^{\infty} \frac{1}{(2n+1)^p} = (1-2^{-p})\zeta(p),
$$

$p = 3$, $\zeta(p) = 1.202$, ζ is a Zeta function.

Equation (3.25) using eq.(3.6) and eq.(3.27), becomes (**the first integral**)

$$
= ln 1.14 \frac{\hbar\omega_b}{k_B T_c} - \eta^2 (\frac{1}{\pi k_B T_c})^2 \frac{8.414}{8}.
$$

The second integral of eq.(3.24),

Applying L'Hopitals Rule (diffrentiating the numrator and denominator),

$$
\begin{aligned}
I &= \int_0^{\hbar\omega_b} \lim_{\Delta\to 0} [d\in \frac{\eta}{\Delta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}} tanh(\beta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}/2)] \\
&= \int_0^{\hbar\omega_b} \lim_{\Delta\to 0} [d\in \frac{\eta}{\Delta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}} tanh(\beta\sqrt{(\in_k^2 + (\Delta-\eta)^2)}/2)]' \\
&= \int_0^{\hbar\omega_b} \lim_{\Delta\to 0} [\frac{\eta sech^2 \frac{\beta}{2}\sqrt{(\in_k^2 + (\Delta-\eta)^2)} \frac{\beta}{2} \frac{2(\Delta-\eta)}{2\sqrt{\in_k^2 + (\Delta-\eta)^2}}}{\sqrt{\in_k^2 + (\Delta-\eta)^2} + \Delta \frac{2(\Delta-\eta)}{2\sqrt{\in_k^2 + (\Delta-\eta)^2}}}] d\in \\
&= -\int_0^{\hbar\omega_b} d\in \frac{\eta^2 \beta sech^2 \frac{\beta}{2}\sqrt{\in^2 + \eta^2}}{2(\in^2 + \eta^2)}.
\end{aligned} \tag{3.28}
$$

There fore combining the first and second integral result gives

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_BT_c}) - \eta^2(\frac{1}{\pi k_BT_c})^2\frac{8.414}{8} + \int_0^{\hbar\omega_b} d\in \frac{\eta^2\beta\sec h^2\frac{\beta}{2}\sqrt{\in^2+\eta^2}}{2(\in^2+\eta^2)}$$
$$= \ln(1.14\frac{\hbar\omega_b}{k_BT_c}) - \eta^2(\frac{1}{\pi k_BT_c})^2\frac{8.414}{8} + \int_0^{\hbar\omega_b} \frac{\eta^2}{2k_BT_c(\in^2+\eta^2)}d\in$$
$$- \int_0^{\hbar\omega_b} \frac{\eta^2\tanh^2\frac{\beta}{2}\sqrt{\in^2+\eta^2}}{2k_BT_c(\in^2+\eta^2)}d\in, \tag{3.29}$$

with the use of a relation $sech^2x = 1 - \tanh^2 x$.

The result of the third term from rhs of eq.(3.29) is

$$\int_0^{\hbar\omega_b} \frac{\eta^2}{2k_BT_c(\in^2+\eta^2)}d\in = \frac{\eta^2}{2k_BT_c}\arctan(\hbar\omega_b/\eta)$$
$$= \frac{\eta}{4k_BT_c}ln[\frac{\eta+\hbar\omega_b}{\eta-\hbar\omega_b}]. \tag{3.30}$$

And the fourth term rhs of eq.(3.29) can be integrated with the help of FORTRAN LANGUAGE using the following approximation:

$\hbar\omega_b \approx \hbar\omega_D = 10^{-3}ev$, (for BCS)

and, using superconducting critical temprature for $UGe_2, T_c = 0.7k$

so, $\frac{\hbar\omega_b}{2k_BT_c} \approx 0.00071,$

using $\eta = a = 0.05$ and $k_B = 1$.

With the afformantioned method and the above approximation we obtain

$$\int_{10^{-10}}^{0.00071} \frac{tanh^2(0.714\sqrt{x^2+a^2})}{2(x^2+a^2)}dx = 7.6\times10^{-18}. \tag{3.31}$$

Substituting eq.(3.30) and eq.(3.31) in eq.(3.29) and simplifying gives that

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_BT_c}) + \frac{\eta}{4k_BT_c}ln[\frac{\eta+\hbar\omega_b}{\eta-\hbar\omega_b}] - \eta^2(\frac{1}{\pi k_BT_c})^2\frac{8.414}{8} - \frac{7.6\times10^{-18}\eta^2}{(2k_BT_c)^2}. \tag{3.32}$$

For small η we can ignore the η^2 term, then eq.(3.32) becomes

$$\frac{1}{\lambda} = ln(1.14\frac{\hbar\omega_b}{k_BT_c}) + \frac{\eta}{4k_BT_c}ln[\frac{\eta+\hbar\omega_b}{\eta-\hbar\omega_b}]$$

$$k_B T_c = 1.14\hbar\omega_b e^{-(1/\lambda - a\eta)}. \tag{3.33}$$

where

$$a = \frac{1}{4k_B T_c} ln[\frac{\eta + \hbar\omega_b}{\eta - \hbar\omega_b}].$$

3.2.2 For localized Electrons

The equation of motion using Green functions technique for the Localized Electrons is as follows.

$$\omega \ll b_{l\uparrow}, b_{l\uparrow}^{\dagger} \gg_{\omega} = 1 + \ll [b_{l\uparrow}, \hat{H}], b_{l\uparrow}^{\dagger} \gg_{\omega} . \tag{3.34}$$

Now let we first evaluate the commutation $[b_{l\uparrow}, \hat{H}]$, using the Hamiltonian given at the beginning of this chapter.

$$\begin{aligned}
[b_{l\uparrow}, \hat{H}_1] &= \sum_{k,\sigma} \in_k [b_{l\uparrow}, a_{k,\sigma}^{\dagger} a_{k,\sigma}] + \sum_{p,\sigma} \in_p [b_{l\uparrow}, b_{p,\sigma}^{\dagger} b_{p,\sigma}] \\
&= 0 + \sum_{p,\sigma} \in_p [b_{l\uparrow}, b_{p,\sigma}^{\dagger} b_{p,\sigma}] \\
&= \sum_{p,\sigma} \in_p (\{b_{l\uparrow}, b_{p,\sigma}^{\dagger}\} b_{p,\sigma} - b_{p,\sigma}^{\dagger} \{b_{l\uparrow}, b_{p,\sigma}\}) \\
&= \sum_{p,\sigma} \in_p \delta_{l,p} \delta_{\uparrow,\sigma} b_{p,\sigma} \\
&= \sum_{p} \in_p \delta_{l,p} b_{p,\uparrow} \\
&= \in_l b_{l\uparrow}.
\end{aligned} \tag{3.35}$$

The commutation $[b_{l\uparrow}, \hat{H}_2] = 0$, so the remaining is:

$$\begin{aligned}
[b_{l\uparrow}, \hat{H}_3] &= \sum_{p,m} \alpha_{\ell,m}[b_{l\uparrow}, a^\dagger_{k\uparrow}a^\dagger_{-k\uparrow}b_{p\uparrow}b_{m\uparrow}] + \sum_{l,m,p} \alpha^*_{\ell,m}[b_{l\uparrow}, a_{-k\uparrow}a_{k\uparrow}b^\dagger_{p\uparrow}b^\dagger_{m\uparrow}] \\
&= 0 + \sum_{l,m,p} \alpha^*_{\ell,m}[b_{l\uparrow}, a_{-k\uparrow}a_{k\uparrow}b^\dagger_{p\uparrow}b^\dagger_{m\uparrow}] \\
&= \sum_{l,m,p} \alpha^*_{\ell,m}a_{-k\uparrow}a_{k\uparrow}[b_{l\uparrow}, b^\dagger_{p\uparrow}b^\dagger_{m\uparrow}] \\
&= \sum_{l,m,p} \alpha^*_{\ell,m}a_{-k\uparrow}a_{k\uparrow}(\{b_{l\uparrow}, b^\dagger_{p\uparrow}\}b^\dagger_{m\uparrow} - b^\dagger_{p\uparrow}\{b_{l\uparrow}, b^\dagger_{m\uparrow}\}) \\
&= \sum_{l,m,p} \alpha^*_{\ell,m}a_{-k\uparrow}a_{k\uparrow}(\delta_{lp}b^\dagger_{m\uparrow} - b^\dagger_{p\uparrow}\delta_{lm}) \\
&= \sum_{l,m} \alpha_{l,m}a_{-k\uparrow}a_{k\uparrow}b^\dagger_{m\uparrow}. \qquad (3.36)
\end{aligned}$$

Where $\alpha = \alpha^*$. Substituting eq.(3.35) and eq.(3.36) in eq.(3.34) yields

$$\omega \ll b_{l\uparrow}, b^\dagger_{l\uparrow} \gg = 1 + \in_l \ll b_{l\uparrow}, b^\dagger_{l\uparrow} \gg + \sum_{l,m} \alpha_{l,m} < a_{-k\uparrow}a_{k\uparrow} > \ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg$$

$$(\omega - \in_l) \ll b_{l\uparrow}, b^\dagger_{l\uparrow} \gg = 1 + \Delta_l \ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg .$$

This implies

$$\ll b_{l\uparrow}, b^\dagger_{l\uparrow} \gg = \frac{1}{(\omega - \in_l)} + \frac{\Delta_l}{(\omega - \in_l)} \ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg \qquad (3.37)$$

Where $\Delta_l = \sum_{l,m} \alpha_{l,m}a_{-k\uparrow}a_{k\uparrow}$.

One can also obtain the the equation of motion for higher order Green's function $\ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg$ using

$$\begin{aligned}
\omega \ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg &= < [b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow}] > + \ll [b^\dagger_{m\uparrow}, \hat{H}], b^\dagger_{l\uparrow} \gg \\
&= 0 + \ll [b^\dagger_{m\uparrow}, \hat{H}], b^\dagger_{l\uparrow} \gg . \qquad (3.38)
\end{aligned}$$

Applying the same techniques:

$$[b^{\dagger}_{m\uparrow}\hat{H}_1] = \sum_{k,\sigma} \in_k [b^{\dagger}_{m\uparrow}, a^{\dagger}_{k,\sigma}a_{k,\sigma}] + \sum_{l,\sigma} \in_l [b^{\dagger}_{m\uparrow}, b^{\dagger}_{l,\sigma}b_{l,\sigma}]$$
$$= 0 + \sum_{l,\sigma} \in_l [b^{\dagger}_{m\uparrow}, b^{\dagger}_{l,\sigma}b_{lp,\sigma}]$$
$$= \sum_{l,\sigma} \in_l (\{b^{\dagger}_{m\uparrow}, b^{\dagger}_{l,\sigma}\}b_{l,\sigma} - b^{\dagger}_{l,\sigma}\{b^{\dagger}_{m\uparrow}, b_{l,\sigma}\})$$
$$= -\sum_{l,\sigma} \in_l b^{\dagger}_{l,\sigma}\delta_{m,l}\delta_{\uparrow,\sigma}$$
$$= -\sum_{l} \in_l b^{\dagger}_{l\uparrow}\delta_{m,l}$$
$$= - \in_m b^{\dagger}_{m\uparrow}. \tag{3.39}$$

The commutation $[b^{\dagger}_{m\uparrow}, \hat{H}_2] = 0$, so the remaining is:

$$[b^{\dagger}_{m\uparrow}, \hat{H}_3] = \sum_{l,m,p} \alpha_{\ell,m}[b^{\dagger}_{m\uparrow}, a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\uparrow}b_{l\uparrow}b_{p\uparrow}] + \sum_{l,m,p} \alpha^{*}_{\ell,m}[b^{\dagger}_{m\uparrow}, a_{-k\uparrow}a_{k\uparrow}b^{\dagger}_{l\uparrow}b^{\dagger}_{p\uparrow}]$$
$$= \sum_{l,m,p} \alpha_{\ell,m}[b^{\dagger}_{m\uparrow}, a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\uparrow}b_{l\uparrow}b_{p\uparrow}] + 0$$
$$= \sum_{l,m,p} \alpha_{\ell,m}a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\uparrow}[b^{\dagger}_{m\uparrow}, b_{l\uparrow}b_{p\uparrow}]$$
$$= \sum_{l,m,p} \alpha_{\ell,m}a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\uparrow}(\{b^{\dagger}_{m\uparrow}, b_{l\uparrow}\}b_{p\uparrow} - b_{l\uparrow}\{b^{\dagger}_{m\uparrow}, b_{p\uparrow}\})$$
$$= \sum_{l,m,p} \alpha_{\ell,m}a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\uparrow}(\delta_{ml}b_{m\uparrow} - b_{l\uparrow}\delta_{mp})$$
$$= \sum_{l,m} \alpha_{\ell,m}a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\uparrow}b_{l\uparrow}. \tag{3.40}$$

Substituting eq.(3.39) and eq.(3.40) in eq.(3.38) and assuming $\in_m = \in_l$ yields that

$$\omega \ll b^{\dagger}_{m\uparrow}, b^{\dagger}_{l\uparrow} \gg = - \in_l \ll b^{\dagger}_{m\uparrow}, b^{\dagger}_{l\uparrow} \gg + \sum_{l,m} \alpha_{\ell,m} < a^{\dagger}_{k\uparrow}a^{\dagger}_{-k\uparrow} > \ll b_{l\uparrow}, b^{\dagger}_{l\uparrow} \gg$$

$$(\omega + \in_l) \ll b^{\dagger}_{m\uparrow}, b^{\dagger}_{l\uparrow} \gg = \Delta_l \ll b_{l\uparrow}, b^{\dagger}_{l\uparrow} \gg$$
$$\ll b^{\dagger}_{m\uparrow}, b^{\dagger}_{l\uparrow} \gg = \frac{\Delta_l}{(\omega + \in_l)} \ll b_{l\uparrow}, b^{\dagger}_{\uparrow} \gg. \tag{3.41}$$

Now combining eq.(3.37) and eq.(3.41) gives the following two equations.

$$\ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg = \frac{\Delta_l}{\omega + \in_l}\left(\frac{1}{(\omega - \in_l)} + \frac{\Delta_l}{(\omega - \in_l)} \ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg\right)$$

$$(1 - \frac{\Delta_l^2}{(\omega^2 - \in_l^2)}) \ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg = \frac{\Delta_l}{\omega + \in_l)(\omega - \in_l)}.$$

There fore,

$$\ll b^\dagger_{m\uparrow}, b^\dagger_{l\uparrow} \gg = \frac{\Delta_l}{\omega^2 - \in_l^2 - \Delta_l^2}. \tag{3.42}$$

And,

$$\ll b_{l\uparrow}, b^\dagger_{l\uparrow} \gg = \frac{1}{(\omega - \in_l)} + \frac{\Delta_l}{(\omega - \in_l)}\left(\frac{\Delta_l}{(\omega + \in_l)} \ll b_{l\uparrow}, b^\dagger_{l\uparrow} \gg\right)$$

$$(1 - \frac{\Delta_l^2}{(\omega^2 - \in_l^2)}) \ll b_{l\uparrow}, b^\dagger_{l\uparrow} \gg = \frac{1}{(\omega - \in_l)}$$

$$\ll b_{l\uparrow}, b^\dagger_{l\uparrow} \gg = \frac{(\omega + \in_l)}{\omega^2 - \in_l^2 - \Delta_l^2}. \tag{3.43}$$

Equation that show the correlation between conduction and mobile electrons:

From our previous definition for η we can write

$$\eta = \frac{\alpha}{\beta}\sum_{k,n} \ll b^\dagger_{\ell\uparrow}, b^\dagger_{m\uparrow} \gg = \frac{\alpha}{\beta}\sum_{k,n} \frac{\Delta_l}{\omega^2 - \in_l^2 - \Delta_l^2},$$

and the sum may be changed in to an integral by introducing the density of states $N(\in)$, $\frac{1}{v}\sum_{k,n} \longrightarrow \frac{1}{(2\pi)^3}\int d^3k = \int_{-\varepsilon_F}^{\infty} d\in N(\in)$
The summation with respect to k and n extends over all allowed pair states. There fore

$$\eta = \frac{\alpha}{\beta}\sum_{n}\int_{-\varepsilon_F}^{\infty} d\in N(\in)[\frac{\Delta_l}{\omega^2 - \in_l^2 - \Delta_l^2}].$$

For effective attractive interaction region and assuming the density of state constant,the expression becomes,

$$\eta = \frac{2}{\beta}N(\in)\alpha\sum_{n}\int_{0}^{\hbar\omega_b} d\in [\frac{\Delta_l}{\omega^2 - \in_l^2 - \Delta_l^2}]. \tag{3.44}$$

Now changing, $\omega_b \longrightarrow i\omega_n$ and using the Matsubara frequency

$$\omega_n = \frac{(2n+1)\pi}{\beta},$$

Eq.(3.44)becomes,

$$\eta = 2N(0)\alpha\beta \sum_n \int_0^{\hbar\omega_b} d\in [\frac{|\Delta_l|}{(2n+1)^2\pi^2 + \beta^2 E^2}]$$

where $E^2 = \in_l^2 + \Delta_l^2$.
Using the relation $\frac{1}{2x} tanh(x/2) = \sum_n \frac{1}{(2n+1)^2+x^2}$ we can write the above equation as follows.

$$\eta = 2N(0)\alpha\beta \int_0^{\hbar\omega_b} d\in \frac{|\Delta_l|}{2\beta E} tanh(\beta E/2)$$

Let $N(0)\alpha = \lambda_l$

$$\Longrightarrow \eta = \lambda_l \int_0^{\hbar\omega_b} d\in \frac{|\Delta_l|}{\sqrt{\in_l^2 + \Delta_l^2}} \tanh(\beta\sqrt{(\in_l^2 + \Delta_l^2)}/2). \quad (3.45)$$

Applying the method we have used (*on page 28-29 to calculate the first integral of equation (3.24)*), on the above equation(eq.3.45) at low T yields

$$\begin{aligned} \eta &\approx -\lambda_l\Delta_l(\ln 1.14\frac{\hbar\omega_b}{k_B T_m} - \Delta_l^2(\frac{1}{\pi k_B T_m})^2\frac{8.414}{8}) \\ &\approx -\lambda_l\Delta_l \ln 1.14\frac{\hbar\omega_b}{k_B T_m} + \lambda_l\Delta_l^3(\frac{1}{\pi k_B T_m})^2\frac{8.414}{8}. \end{aligned} \quad (3.46)$$

Since Δ_l is very small, we can ignore the second term of above equation. i.e.

$$\eta \approx -\lambda_l\Delta_l \ln 1.14\frac{\hbar\omega_b}{k_B T_m}.$$

This implies

$$k_B T_m = 1.14\hbar\omega_b exp(\frac{\eta}{\lambda_l\Delta_l}). \quad (3.47)$$

3.2.3 For pure superconducting system

For pure superconducting system (when magnetic order can not appear or magnetic effect is zero) we can ignore the η term and our previous calculation gives the following results which is similar to BCS.

Using the eq.(3.20), as $T \to 0, \eta \to 0$ and $\tanh(\beta E/2) \longrightarrow 1$ so the equation reduces to

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega_b} d\in_k \frac{\Delta}{\sqrt{(\in_k^2 + \Delta^2)}},$$

which implies

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} \frac{d\in_k}{\sqrt{(\in_k^2 + \Delta^2)}} = \sinh^{-1}(\frac{\hbar\omega_b}{\Delta}),$$

$$\Delta(0) \approx 2\hbar\omega_b e^{\frac{-1}{\lambda}}. \tag{3.48}$$

And as $T \to T_c$,using the same equation eq.(3.20) (for $\eta = 0$)

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} d\in_k \frac{\tanh(\beta \in_k /2)}{\in_k}$$

$$= \int_0^{\frac{\beta}{2}\hbar\omega_b} dy\frac{\tanh y}{y}, y = \frac{\beta}{2} \in$$

$$= \ln y \tanh y|_0^{\frac{\beta}{2}\hbar\omega_b} - \int_0^{\frac{\beta}{2}\hbar\omega_b} \frac{\ln y}{\cosh^2 y} dy$$

for low temperature $tanh(\frac{\hbar\omega}{2k_BT}) \to 1$

$$\frac{1}{\lambda} = \ln\frac{\beta}{2}\hbar\omega_b - ln(\pi/4)exp(-c) = \ln 1.14\frac{\hbar\omega_b}{k_BT_c},$$

which implies

$$k_BT_C = 1.14\hbar\omega_b e^{\frac{-1}{\lambda}}. \tag{3.49}$$

To obtain temperature dependent of energy gap of eq.(3.20), we used the same technique to solve the first integral of eq.(3.24), which is:

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_b} d\in \frac{1}{\sqrt{(\in^2 + \Delta^2)}} \tanh(\beta\sqrt{(\in^2 + \Delta^2)}/2)$$

$$= ln1.14\frac{\hbar\omega_b}{k_BT} - \Delta^2(\frac{1}{\pi k_BT})^2\frac{8.414}{8} + ...$$

But from BCS at $T = T_c, 1/\lambda = ln1.14\frac{\hbar\omega_D}{k_B T_c}$ and assuming $\omega_b = \omega_D$, simplifying the above equation yields that:

$$\ln(T/T_c) = -\Delta^2(\frac{1}{\pi k_B T})^2\frac{8.414}{8} + ...$$

Using $\ln(1-x) = -x - x^2/2 + ...$

Implies that, $\ln(T/T_c) = \ln(1-(1-T/T_c)) = -(1-T/T_c) - (1-T/T_c)^2/2 + ...$

$$\ln(T/T_c) \approx -(1-T/T_c)$$

$$\Rightarrow -(1-T/T_c) \approx -\Delta^2(\frac{1}{\pi k_B T})^2\frac{8.414}{8}.$$

Hence

$$\Delta(T) = 3.06 k_B T_c(1-\frac{T}{T_c})^{1/2}. \tag{3.50}$$

Chapter 4

Result and Discussion

Using the model Hamiltonian (ch.3) and retarded double time green's function formalism, we obtain an expression for superconductivity order parameter (Δ), magnetic order parameter (η), superconducting transition temperature (T_c), and magnetic ordering temperature (T_m).

The expression we get for pure superconductor (eq.3.48-3.50) (i.e.when magnetic effect is zero, $\eta = 0$), are in agreement with BCS expression.It is clear that the energy gap which is the measure of pairing energy, decreases with increasing temperature until it vanishes at the transition temperature, and Fig.(4.1) shows this fact.

Using the experimental value of T_c for superconductor UGe_2, $T_c \approx 0.7k$ and plausible approximation we plot Δ vs T_c (fig 4.1), T_c vs η (fig.4.3) and T_m vs η (fig.4.2). The combined graph (fig.4.4) shows possibility of the co-existence of Superconductivity and ferromagnetism, as the magnetic correlations are ferromagnetic in nature.

As the magnetic ordering (correlation) increases the transition temperature decreases [34] but the magnetic ordering temperature increases, which is shown in the fig.(4.2) and fig.(4.3). As revealed in [31] the magnetic moment of Uranium is due to f shells and so can be taken as localized. In our calculation, eq.(3.45) shows the correlation of the mobile and localized electrons.since η corresponds with localized electrons. So the two parameters are inter dependent. This implies the contribution of both electrons. In other word, the 5f electrons in UGe_2 seem to show dual activity for which two electrons being localized (magnetic) and the other being itinerant (and superconducting). This shows the combined phenomenon of superconductivity and ferromagnetism.

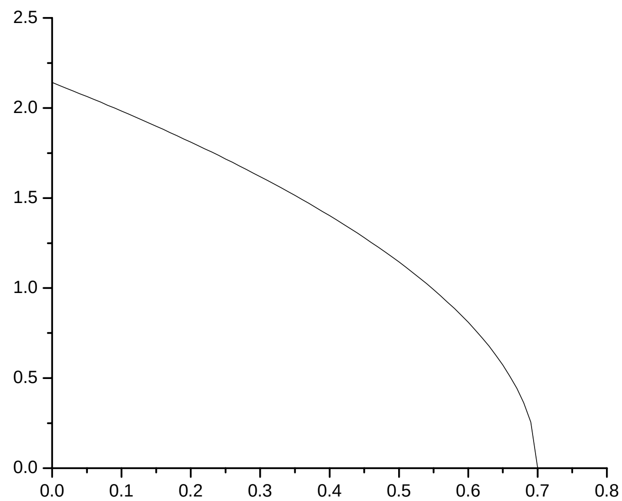

Figure 4.1: *gap energy (Δ) vs temperature for pure* UGe_2 *superconductor.*

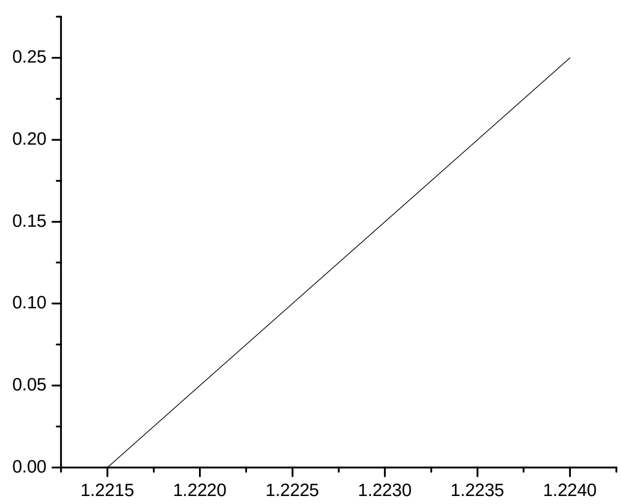

Figure 4.2: *magnetic ordering temperature (Tm) vs* η.

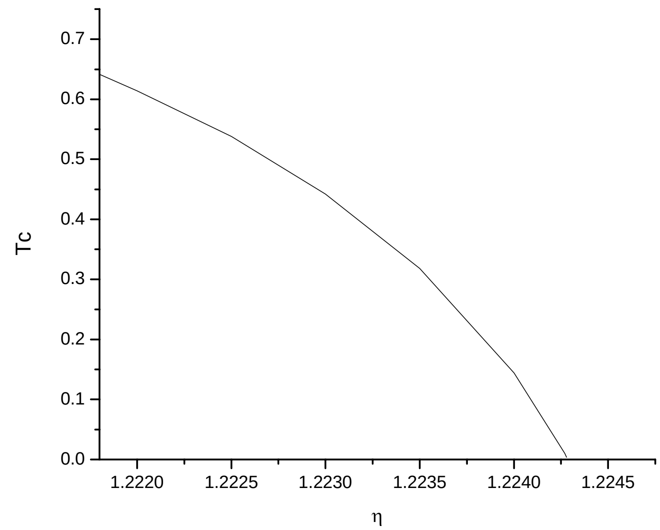

Figure 4.3: *temperature vs* η *(magnetic ordering).*

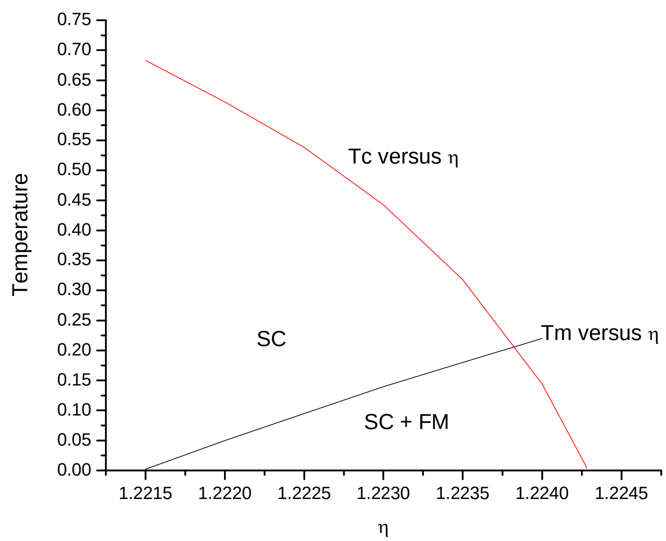

Figure 4.4: *co-existence of Ferromagnetism (FM) and Superconductivity (SC).*

Chapter 5

Conclusion

In the first place we introduce the basic concept of Superconductivity, Ferromagnetism, Phase transition, Order parameter and superconducting parameters in chapter one. We also reviewed the co-existence of superconductivity and ferromagnetism in general and in particular in the compound UGe_2. The second chapter discusses the formalism we use for calculation. The formulation of the Hamiltonian and calculation is done in chapter 3. In chapter 4 we presented the result and discussion.
In the model Hamiltonian we include spin triplet case and obtain an expression for the superconducting parameters T_c, Δ and η. We plot the obtained equation with suitable approximation and parameter values. The phase diagram shows the possibility of co-existence of Superconductivity and Ferromagnetism.
Eq.(3.45) shows the correlation of localized and conduction electrons. This supports our conclusion that Superconductivity and Ferromagnetism are possibly co-existing in a superconductor UGe_2. More refined and elegant experimental observations will assist more accurate investigation of this very exciting coexistence phenomenon.

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Declaration

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

Name: Mesfin Asfaw
Signature:

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This thesis has been submitted for examination with my approval as University advisor.

Name: Prof. P. Singh
Signature: