

COEXISTENCE OF FERROMAGNETISM AND
SUPERCONDUCTIVITY IN $ZrZn_2$

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By

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The undersigned hereby certify that they have read and recommended to the Faculty of Science School of Graduate Studies for acceptance a thesis entitled “**COEXISTENCE OF FERROMAGNETISM AND SUPERCONDUCTIVITY IN $ZrZn_2$** ” by **Birhanu Demeke** in partial fulfillment of the requirements for the degree of **Master of Science in Physics**.

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*This work is dedicated to **My Parents***

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Abstract

Ferromagnetism and superconductivity had been thought to be mutually repulsive. Even when superconductivity has been thought as arising from magnetic mediation of paired electrons, it was believed that superconductivity occurs in the paramagnetic phase. A great effort has been made to prove this, On the contrary in 2000 the two phenomena were found to coexist in UGe_2 and in others as URhGe and $ZrZn_2$ in which the same electrons are responsible for both phenomenon. We study the coexistence of the two phenomena particularly in $ZrZn_2$ and demonstrate that for certain values of the parameters of triplet superconductivity and ferromagnetism is a possibility.

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Introduction

Superconductivity is a phenomenon occurring in certain materials at extremely low temperatures, characterized by exactly zero electrical resistance. The phenomenon was discovered in mercury in 1911 by the Dutch physicist Heike Kamerlingh Onnes while studying the resistivity of metals at low temperatures [1].

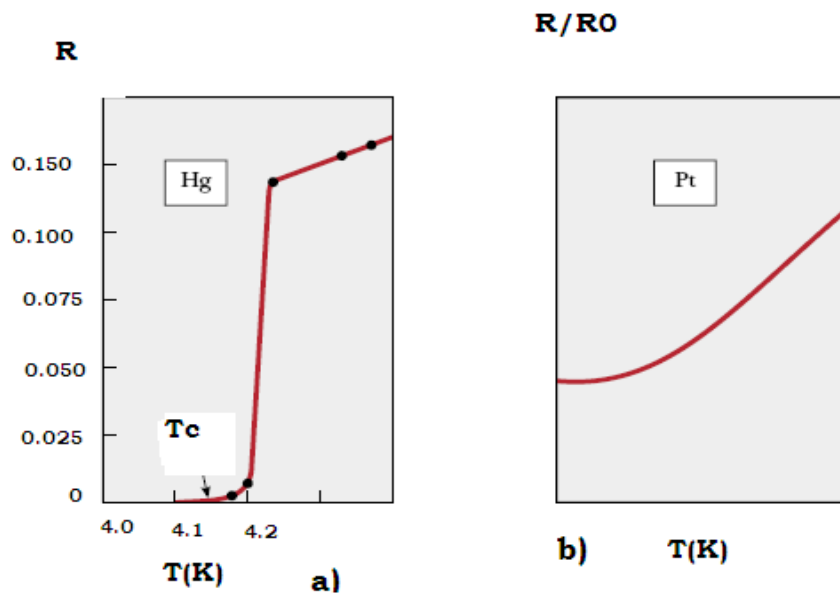


Figure 1: (a) Resistance R versus $T(K)$ for mercury (b) The resistance $\frac{R}{R_0}$ versus $T(K)$ of platinum of resistance R_0 at very low temperature

Since the resistivity of the firstly studied platinum metal, when extrapolated to 0 K, depend on purity. Mercury in which a very pure samples could easily be prepared chosen and the resistance of the mercury sample dropped to a very small value sharply at 4.15 K as shown in the figure above. In 1913 Kamerlingh Onnes was awarded the Nobel prize in physics for the study of matter at low temperatures and the liquefaction of helium. Soon after the discovery by Kamerlingh Onnes, many other elemental metals as Pb, Ti, V, Zn, Nb, Tc, Ru, Cd and compounds NbGe, Nb_3 Sn, Nb_3 Al, Nb_3 Au, NbN, MoN, V_3 Ga, V_3 Si, UCo, Ti_2 Co, La_3 In [22] were found to exhibit zero resistance when their temperatures were lowered below a certain characteristic temperature of the material, called the critical temperature T_c .

In 1933 W. Hans Meissner and Robert Ochsenfeld studied the magnetic behavior of superconductors and found that when certain materials are cooled below their critical temperatures in the presence of a magnetic field, the magnetic flux expelled from the interior of the superconductor [2]. Moreover, these materials lost their superconducting behavior above a certain temperature-dependent critical magnetic field, $B_c(T)$. In 1935 Fritz and Heinz London developed a phenomenological theory of superconductivity [3]. In 1950, the phenomenological Ginzburg-Landau theory of superconductivity was devised by Landau and Ginzburg. This theory, which combined Landau's theory of second-order phase transitions with a Schrödinger-like wave equation, had great success in explaining the macroscopic properties of superconductors. The actual nature and origin of the superconducting state were first explained by John Bardeen, Leon N. Cooper, and J. Robert Schrieffer in 1957 [4]. A central feature of this theory, commonly referred to as the BCS theory, is the formation of bound two-electron states called Cooper pairs. In 1962 Brian D. Josephson predicted a tunneling

current between two superconductors separated by a thin insulating barrier, where the current is carried by these paired electrons [5]. Shortly thereafter, Josephson's predictions were verified, and today there exists a whole field of device physics based on the Josephson effect as SQUID (superconducting quantum interference devices), the most sensitive magnetometer known.

Since early in 1986 J. Georg Bednorz and Karl Alex Muller reported evidence for superconductivity in an oxide of lanthanum, barium, and copper at a temperature of about 30 K [6] which was a major breakthrough in superconductivity because the highest known value of T_c at that time was about 23 K in a compound of niobium and germanium (Nb_3Ge) discovered in 1973. This remarkable discovery, which marked the beginning of a new era of high-temperature superconductivity, received worldwide attention in both the scientific community and the business world. And in 1987 Chu and others found a new material, $YBa_2Cu_3O_7$ with critical temperature of 90K. Tremendous advances were made in theoretical and experimental physics in quick succession. As a result the critical temperature reached 112K in Bi-compound, 126K in Ti-compound, and 135K in Hg-compound.

Recently, researchers have reported critical temperatures as high as 150 K in more complex metallic oxides as $InSnBa_4Tm_4Cu_6O_{18}$, but the mechanisms responsible for superconductivity in these materials remain unclear. The physical properties of these compounds were also investigated very intensively and it was confirmed that in all cuprate superconductors the superconductivity occurs in the thin layers including CuO_2 until the discovery of high-temperature superconductors, the use of superconductors required coolant baths of liquefied helium (rare and expensive) or liquid hydrogen (very explosive). On the other hand, superconductors with T_c 77 K

require only liquid nitrogen, which boils at 77 K and is comparatively inexpensive, abundant, and relatively inert. If superconductors with T_c above room temperature are ever found, technology will be drastically altered.

The other progress in the study of low temperature physics is the discovery of coexistence of ferromagnetism and superconductivity. As early as the 1950s, when the Bardeen-Cooper-Schrieffer (BCS) [4] theory of superconductivity (SC) was still being formulated and ferromagnetic correlations in solids were being treated in a (Weiss) mean-field manner, theories about the coexistence of these two phenomena in materials had begun surfacing [7]. This is somewhat surprising given that it had always been known that magnetic fields always suppress superconductivity. Nevertheless, proposed theories and speculations continued in the following decades but it was not until around 2000 when superconductivity and ferromagnetism were found to coexist in the material UGe_2 [8]. Superconductivity had not yet been observed in UGe_2 because it does not become superconducting until the temperature is lowered below about 0.8K at an optimal pressure of 13kbar, experimental conditions only available in the best laboratories. Following this discovery, SC was also found to coexist with ferromagnetism (FM) in the well-known compound URhGe [9] and also in $ZrZn_2$ [10].

We will focus on the history of the physics of the magnetic ordering in itinerant ferromagnetic metals and the interplay with superconductivity. Itinerant ferromagnetic systems are somewhat more complex than ferromagnetic insulators in that there are extra degrees of freedom due to charge mobility. One of the first people to look at the ferromagnetic-superconducting possibility was Ginzburg [7] in the Soviet Union, simultaneously with the development of the BCS theory of superconductivity in the

late 1950. The concept of superconductivity that Ginzburg was working with was with the electrodynamics of superconductors, particularly the behavior of a magnetic field response. He pointed out the possibility of its coexistence under the condition that the magnetization is less than the thermodynamical critical field. He also utilized his theory of phase transitions developed at that time in collaboration with Landau [11]. The search for ferromagnetic superconductors continued and superconducting materials with magnetic impurities were studied [12]. The research in this direction has led to the work of Larkin and Ovchinnikov [13] and Fulde and Ferrell [14], who studied a simple model of effective field theory of superconductivity fermions coupled to magnetic impurities.

Once it was realized that it was possible that Cooper pairing could come from non-phononic sources, unlike in the conventional BCS superconductors. In the late 1970, Enz and Matthias were studying the weak ferromagnet $ZrZn_2$ [15] and there were theories put forth of spin fluctuation mediated superconductivity in itinerant ferromagnet by Appel and Fay [18]. They argued that s-wave pairing is highly unlikely since most spins are aligned rather than anti-aligned, leaving the possibility open for triplet pairing and predicted that p-wave triplet superconductivity should be observed and, they found that the exchange of longitudinal spin fluctuations near a magnetic critical point leads to attractive p-wave coupling. They took possible examples $ZrZn_2$ which is suitable for a triplet pairing. Since this type of pairing is strongly suppressed by impurity scattering and since it was not clear that $ZrZn_2$ can be made clean enough to accurately observe the above effect, they investigated the possibility of triplet pairing state in Ni which can be made quite clean. The equal spin pairing (ESP) that they considered is like the A1 phase of 3He in a magnetic field. At the

time their very good supposition of T_c of $ZrZn_2$ was $< 0.5K$ which is proved to be $0.29K$ after 27 years [10]. And A.A. Abrikosov considered superconductivity arising within a background of ferromagnetic ordering [19]. He showed that coexistence of SC/FM can indeed occur for certain values of the coupling parameters but his work has not yet been experimentally proved. It had been known for a while that in some rare earth ternary compounds like $ErRh_4B_4$ and $HoMo_6S_8$ [20], superconductivity was suppressed as soon as ferromagnetic order set in, when the rare earth 4f moments completely align at low temperature, superconductivity is wiped out by strong internal field. The recently discovered $RuSr_2GdCu_2O_8$ also shows either ferromagnetism or superconductivity [10]. So these two phases seemed exclusive and incompatible. So far there is no known Superconductor which can fully sustain such a large molecular field [20]. The big surprise was that SC was finally found on the ferromagnetic side in UGe_2 [8]. Then, soon after, the same general phenomenon was found in two more materials, URhGe [9] and $ZrZn_2$ [10] .

In the present work We study the coexistence of ferromagnetism and superconductivity in $ZrZn_2$. In the review part of the paper we presented the basic findings in superconductivity and the study on ferromagnetic superconductors especially on $ZrZn_2$. In chapter two we describe green's function formalism necessary to study the problem, and in chapter three we investigated the problem using green's function method, in chapter four we presented a result and discussion, finally we made a conclusion in chapter five.

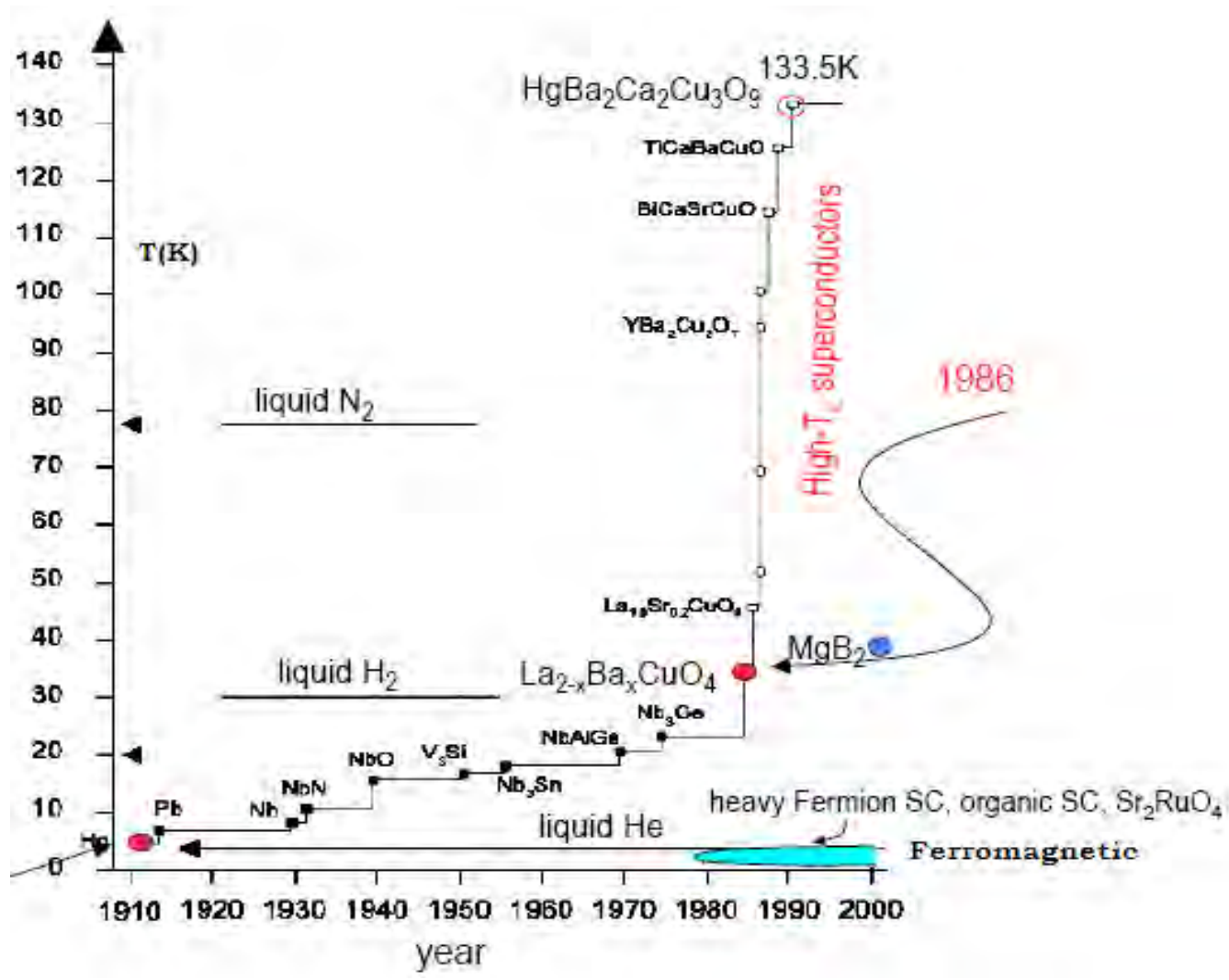


Figure 2: History of discovery in superconductivity

Chapter 1

Literature of Review

In this chapter we present a brief review of the problem of interplay of superconductivity and magnetism especially with regard to $ZrZn_2$.

1.1 BCS Theory

According to classical physics, part of the resistivity of a metal is due to collisions between free electrons and thermally displaced ions of the metal lattice, and part is due to scattering of electrons from impurities or defects in the metal. This classical model could never explain the superconducting state, because the electrons in a material always suffer some collisions, and therefore resistivity can never be zero. Until the discovery of BCS theory no one could explain why electrons enter the superconducting state and why electrons in this state are not scattered by impurities and lattice vibrations. The microscopic theory of superconductivity (BCS) [4] presented in 1957 by Bardeen, Cooper, and Schrieffer has had good success in explaining the features of superconductors. According to which two electrons in the superconductor are able to form a bound pair called a Cooper pair which experiences an attractive interaction. This notion at first seems counterintuitive since electrons normally repel one another

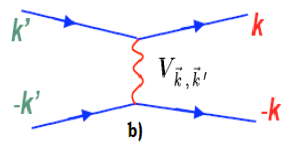
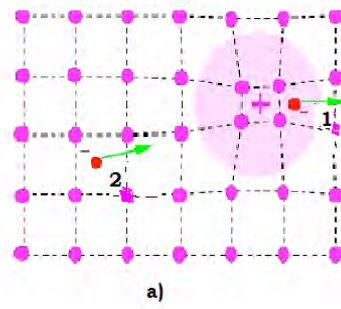


Figure 1.1: (a) A schematic diagram of an electron polarizing a positive ions in its vicinity to create an attractive potential for a second electron following the first electron (b) A schematic diagram of Electron phonon interaction

because of their like charges. However, a net attraction is achieved when the electrons interact with each other via the motion of the crystal lattice as the lattice structure is momentarily deformed by a passing electron as shown in the figure (1.1). The passage of electron 1 causes nearby ions to move inward toward the electron, resulting in a slight increase in the concentration of positive charge in this region. When electron 2 (the second electron to form the Cooper pair), approaching before the ions have had a chance to return to their equilibrium positions, it will be attracted to the distorted (positively charged) region. The net effect is a weak attractive force between the two electrons (cooper pairs). It can be said that the attractive force between two Cooper electrons is an electron-lattice-electron interaction (phonon mediated), where the crystal lattice serves as the mediator of the attractive force. A Cooper pair in a [22] superconductor consists of two electrons having opposite momenta and spin. Cooper pairs are formed in a shell of width of order $k_B T_c$ around the fermi surface. Their radius is small as compared to the average distance between electrons hence between electrons forming cooper pairs their are billions of cooper. The very essential feature of BCS theory is that the cooper pairs once formed they will have the same wave function, as regards both the center of mass and the relative coordinate.

1.2 Meissner effect

It was assumed that superconductivity was a manifestation of perfect conductors, that if a perfect conductor is cooled below a critical temperature in the presence of an applied magnetic field, the field should be trapped interior of the conductor, but it will be expelled if the field is applied after it cooled below the critical temperature. In 1933 Meissner and Ochsenfeld [2], discovered that Meissner superconductors are

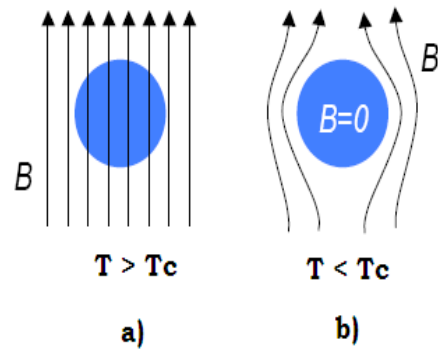


Figure 1.2: Meissner effect (a) Magnetic field penetrating a superconductor above critical temperature (b) Magnetic field expelled from it below critical temperature

materials that expell magnetic field (become perfect diamagnet) from their interior below their critical temperature wether the field is applied before or after. This property not only implies that magnetic fields are excluded from superconductors, but also that any field originally present in the metal is expelled from it when lowering the temperature below its critical value.

1.3 Superconductors and magnetism

Magnetic field plays an important role in the field of superconductivity . According to the way superconductors behave in an applied magnetic field can be classified as type I or type II superconductors. The application of strong magnetic field to superconductor destroys its superconductivity. For a type I [23] superconductor there is one small critical applied magnetic field above which the superconductor becomes normal metal. They expell the magnetic field if it is less than the critical field. Hence type I superconductors exhibit complete Meissner effect (perfect diamagnetism). This is the characteristic of many pure elemental superconductors like Al, Ga, In, Zr, Zn. The critical temperature T_c in the materials decreases with increasing of applied magnetic field, and the magnitude of the critical magnetic field varies with temperature according to the expression [24]

$$B_c(T) = B_c(0)[1 - (\frac{T}{T_c})^2]$$

Where $B_c(0)$ is the maximum value of the applied magnetic field above which superconductivity is destroyed. The other type of superconductor is type II. It is characterized by two critical magnetic fields, designated by B_{c1} and B_{c2} . If the applied magnetic field is less than the lower critical field B_{c1} , they superconduct perfectly as type I and there will be perfect diamagnetism. When the applied magnetic field is in between the two critical fields the materials superconduct but there will be flux penetration, and known as mixed (vortex) state. Hence meissner effect (perfect diamagnetism) is not complete. If the applied magnetic field exceeds the upper critical magnetic field it becomes normal state. Compound superconductors like [23] Nb_3Al , Nb_3Sn , and $PbMoS$ exhibit type II superconductivity.

1.4 Ferromagnetic superconductor Metals

Ferromagnetic superconductor metals are metals that superconduct in the ferromagnetic state under certain restricted conditions. Basically ferromagnetism and superconductivity are thought to be mutually repulsive [24] because superconductors as described by the (BCS) theory of superconductivity are characterized by superconductivity cooper- pairs (pairs of two fermions of opposite spin and opposite momenta) which is different from the case of ferromagnets described by parallel spins. Even when superconductivity has been thought as arising from magnetic mediation of paired electrons, it was believed that superconductivity occurs in the paramagnetic phase [10]. It has been believed that the conduction electrons in a metal can not be both ferromagnetically ordered and superconducting [25]. After the suggestion of coexistence

of ferromagnetism and superconductivity by Ginzburg [7] and experimental investigation made by Matthias et al. [26], as a theoretical development, Anderson and Suhl [27] discussed a possible coexistence phase where the FM is modified to long period modulated spin structure. This modified interaction is mediated by SC pairs. Similar to this idea, Blount Varma proposed magnetic spiral coexisting with SC to gain electromagnetic dipole interaction between localized moments. The above efforts led to unexpected discovery of heavy fermion ferromagnetic superconductor UGe_2 in which the 5f electrons of the U atom are responsible for both the ferromagnetism and superconductivity [8], and seem to be difficult to understand in terms of these theories so far proposed which assumes that two groups of electrons are distinguishable and clearly separated spatially, that FM comes from the well localized electrons while SC pairs are formed by conduction electrons. Ferromagnetic metals are characterized by the fact that their electronic energy bands are split by the exchange interaction between the electrons so that the spin up bands have different energies from the spin down bands. UGe_2 , $URhGe_2$, and $ZrZn_2$ are the currently found ferromagnetic superconductor metals at low temperature. The superconductivity critical temperatures for them are 0.8K [8], 0.25K [9], 0.29K [10], respectively.

1.5 Coexistence of antiferromagnetism and superconductivity

Coexistence between antiferromagnetism and superconductivity is rather easy to realize compared to ferromagnetism and actually observed in several compounds because

the antiferromagnetic moments spatially averaged over the superconducting coherence length vanish and on the average the magnetic moments in these compounds have almost no effect on the cooper pairs as the exchange interaction is zero. The coexistence was observed in heavy fermion systems like CeP, $CeIn_3$ and especially in high temperature superconductors such as $GdBa_2Cu_3O_7$ with spontaneous antiferromagnetic ordering of Gd moments, La_2CuO_4 , and in RMo_6S_8 (R=Tb, Dy, and Er) [43].

1.6 The Structure of $ZrZn_2$

The weak itinerant ferromagnetic metal $ZrZn_2$ characterized by weak magnetic moment ($0.12\mu_B$ - $0.23\mu_B$ per f.u) crystalizes into a cubic laves type $MgCu_2$ exhibiting a number of interesting phenomena including the much weaker ferromagnetism [28] (referred there). The structure is a very closely packed with 71% of the volume is filled by touching spheres. The lattice constant of $ZrZn_2$ is $a=7.393\text{\AA}$ [10]. The Zr atoms occupy the position of a diamond lattice, and the Zn forms a network of a corner [29] (referred there) sharing tetrahedra. In the structure a Zr atom is surrounded by 4 Zr atoms and 12 Zn neighbors. The position of the 4 Zr atoms is at 6.001 a.u and that of the Zn atoms is at 5.745 a.u. Since the metallic radius of Zn is 16% smaller than that of Zr, Zn and Zr do not form strong bonds. On the other hand, Zr does not form directional bonds, so four Zr-Zr bonds in $ZrZn_2$ do not provide strong bonding either. At the same time Zn has eight neighbors at a distance of 4.9 a.u noticeably less than in Zn metal.

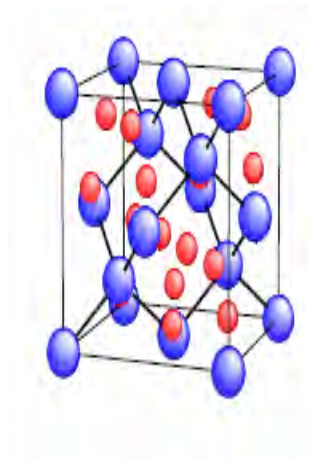


Figure 1.3: The structure of $ZrZn_2$. The larger sphere stands for Zr

1.7 Susceptibility

The AC magnetic measurements, in which an AC field is applied to a sample and the resulting AC moment is measured is important tool for characterizing many materials.

The differential [10] (AC susceptibility) given by

$$\chi = \frac{dM}{dH}$$

is the quantity of interest in AC magnetometry, where M is magnetization of a sample. When higher frequencies of AC is used the magnetization of the sample may be lag behind the derive field, thus the AC magnetic susceptibility measurement yields two quantities: the magnitude of susceptibility χ and the phase shift φ relative to the drive signal. Alternatively we can think of the susceptibility as having an in-phase, or χ' and an out-of-phase ,or imaginary component χ'' . In ferromagnets, a nonzero imaginary susceptibility can indicate irreversible domain wall movement or absorption due to a permanent moment. The AC, the imaginary component, and real

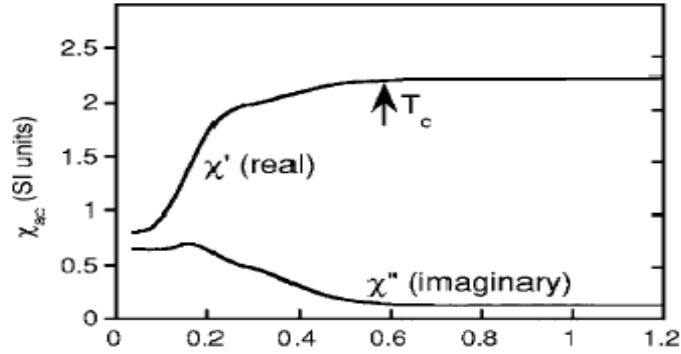


Figure 1.4: The temperature dependence of the Ac. susceptibility of $ZrZn_2$ taken from ref.[30]

component susceptibility measurement of $ZrZn_2$ [30] as a function of temperature is as shown in the figure. And it was found that both the imaginary component susceptibility (χ'') and the real component (χ') are large in the temperature range of $0.6K < T < 1.2K$ due to the alignment of the ferromagnetic domains inside it. The real part of the susceptibility begins to drop above the critical temperature. It was also shown by C. Pfliederer et al. that the ac susceptibility [10], has large component that is due to ferromagnetic domain alignment at low fields.

1.8 Ferromagnetism due to itinerant electrons

In a ferromagnet, all of the spins line up in the same direction, thereby breaking the spin-rotational invariance to the subgroup of rotations about this direction while preserving the discrete translational symmetry of the lattice. This can occur in a metal, and insulator, or a superconductor while in antiferromagnet, neighboring spins are oppositely directed, thereby breaking spin-rotational invariance to the subgroup of rotations about the preferred direction and breaking the lattice translational symmetry to the subgroup of translations by an even number of lattice sites.

The treatment of ferromagnetism in terms of exchange interaction between localized magnetic moments is not suitable for ferromagnetic metals, such as the 3d transition metals Fe, Co, and Ni [31], where the electrons responsible for the magnetism are itinerant and form a band: narrow, of delocalized states. And the exchange energy can be assumed simply to add to the energy of Bloch states, there by causing a displacement in energy of electron states having a given spin direction from those with the opposite spin direction. The exchange interaction acts as an internal magnetic field, causing a displacement of the density of states of electrons (in this case, d-electrons) with different spin direction, in an analogous fashion to the displacement caused by an external field in the case of paramagnetism of conduction electrons.

In $ZrZn_2$ the weak itinerant magnetism of magnetic moment discovered in 1958 by Mathias and Borth [32] is responsible by the Zr 4d electrons. Its occurrence is unusual because neither elemental Zr nor Zn is magnetically ordered. The low curie temperature and small magnetic moments of $ZrZn_2$ as Ni_3Al , $MnSi$, and Si_3In

under ambient pressure it makes it one of few examples of weak itinerant ferromagnetism.

The other most remarkable magnetic property of $ZrZn_2$ is the effect of a magnetic field on the ordered moments. At $T=1.75K$ a relatively small field of 0.05T was required to form a single ferromagnetic domain. On further increase of the field, the ordered moment is rapidly increased with a field of 6T causing a 50% increase in the ordered moment, which is unsaturated up to 35T, the highest field measured [10]. This behavior contrasts strongly with the elemental ferromagnets Fe, Ni, and Co in which after a single domain is formed, applied fields have only small effect on the ordered moment.

1.9 Source of superconductivity in $ZrZn_2$

The magnetic moment in it is unsaturated even at a magnetic field of 35T, which indicates that there is soft magnetic moment amplitude in it. This suggests the existence of longitudinal spin fluctuation which is supposed to be the cause of superconductivity in ferromagnetic metals. As proposed by Fay and Appel [18] the spin fluctuation mediated triplet superconductivity coexists with weak itinerant ferromagnetism. In view of the strong longitudinal spin fluctuation viewed in $ZrZn_2$ and its proximity into a quantum critical point (QCP) it has been proposed as a good candidate for magnetically mediated superconductivity. Similarly to that of UGe_2 the 4d electrons of Zr atoms are responsible for the dual purpose in $ZrZn_2$. This thought is strongly supported by the fact that the superconductivity and ferromagnetism in it disappears at the same value of critical pressure under the application of hydraulic pressure [10].

M. B. Walker and K. V. Samokin developed a model [33] in which the superconductivity in the ferromagnetic state of $ZrZn_2$ is stabilized by an exchange type interaction between the magnetic moments of triplet state cooper pairs and the ferromagnetic magnetization density, in which they give as a reason for the occurrence of superconductivity in it only in the ferromagnetic phase. They also mentioned that the spin fluctuation mechanism can provide an alternative explanation of the result they got.

1.10 Mechanism of pairing in $ZrZn_2$

Karchev et al [34] studied the coexistence of weak itinerant ferromagnetism with s-pairing (singlet pairing) by a model assuming that the same band electrons produce both phenomena. In their model, the long range ferromagnetic order is not resulted from an indirect exchange coupling between the localized spins, but is a consequence of a spontaneous broken spin rotation symmetry of those itinerant electrons that participate in the cooper pair formation. In 1964 Doniach and, Berk and Schrieffer in 1966 showed that in the paramagnetic phase the, phonon -induced s-wave superconductivity in exchange enhanced transition metals is suppressed by ferromagnetic spin fluctuation in the neighborhood of the curie temperature. At the same time a theory of superconductivity coexisting with long range ferromagnetic order was developed by Larkin and Ovchinnikov, and by Fulde and Ferrell for magnetic impurity induced ferromagnetism in metals known as (LOFF) state. The s-wave superconductivity state in ferromagnetic phase is un usual and is a generalization of of (LOFF) [35], R. Shen, Z. M. Zheng et.al [36] developed a model with both an attractive interaction and an exchange coupling between the itinerant electrons to study the coexistence

of spin singlet superconductivity and ferromagnetism. In their model the electrons responsible for ferromagnetism and superconductivity are the same and the exchange energy between the two spin sub bands is determined self consistently, and they found that coexistence of the two phenomenon and spin singlet pairing is not possible if the electrons responsible for both phenomenon are from the same band. They proposed that triplet pairing is most probable for these cases although there is a possibility of coexistence if the superconductivity and the ferromagnetism are caused by different electrons and others showed that only p-pairing (triplet pairing) superconductivity could coexist with the itinerant ferromagnetism similar to the case of A_1 phase of superfluid 3He . Apple and Fay proposed that spin triplet of pure sample of $ZrZn_2$ with a possible mechanism of pairing C. Pfeidere, M. Uhlarz et al. [10] found that superconductivity in $ZrZn_2$ occurs only in the ferromagnetic phase which may arise where the cooper pairs are in a parallel spin (triplet) states .

1.10.1 s-pairing

s-pairing is pairing of two fermions with opposite spin of opposite momenta. Its spin quantum number S is 0. The spin wave function corresponding to singlet pairing fermions has the form

$$\chi_{\alpha\beta} = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

in which the singlet fermions wave function is of the form $|\uparrow\rangle$ for up spin and $|\downarrow\rangle$ for down spin [37]. The wave function in the S-pairing is antisymmetric.

1.10.2 p-pairing

The best known example of triplet pairing is not a superconductor rather a superfluid is ${}^3\text{He}$ in which the condensate states of spin triplet is atomic cooper pairs [21]. In ${}^3\text{He}$ the He atoms are strongly repulsive at a short distance and becomes attractive only for interatomic separation of $r \sim r_0 \sim 3A^0$. Unlike to the singlet pairing for triplet pairing the spin quantum number S is 1. The spin wave function of triplet (p-pairing) can have either of the the three cases below [37].

a) $|\uparrow\uparrow\rangle$ for spin up pairing in which $S_z=1$.

b) $|\downarrow\downarrow\rangle$ for spin down pairing in which $S_z=-1$.

c) $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ for spin up-down pairing in which $S_z=0$. In triplet pairing the wave function is symmetric under particle permutation. As described above in section (1.4) that a metallic ferromagnet is characterized by the fact that the bands of the up pairing and the down pairing have different energies. And because of the curie temperature 28.5K [38] for $ZrZn_2$ is much higher than its superconductivity critical temperature, in addition of the large spin splitting of the fermi surface may suppress the last $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ type of pairing. More over the superconductivity occurs only in the ferromagnetic phase showing that electrons of parallel spins are favored in the pair formation [10]. Hence in our case we will consider only the other cases equal spin pairing (ESP) of triplet pairing.

1.11 Order Parameter in p-Pairing

In superconductors the cooper pairs formed in such a way that it enters into a state characterized by an energy gap (order parameter) of the superconductor. The energy

gap is zero at the critical temperature (T_c) and attains its maximum value at zero temperature [22]. In triplet pairing superconductivity, the order parameter has three components: $\Delta \uparrow\uparrow$ corresponding to the pairing of electrons in the spin-up band, $\Delta \downarrow\downarrow$ corresponding to the pairing of electrons in the spin-down band, and $\Delta \uparrow\downarrow$ corresponding to the pairing of one spin-up and one spin-down electron. The $\Delta \uparrow\downarrow$ component is expected to be very small for the same reason expressed in section (1.10.2) that inhibit the possibility of singlet superconductivity in a ferromagnet. And it can be written [39] as a matrix form as shown below.

$$\Delta_{\alpha\beta} = \begin{pmatrix} \Delta_{\uparrow\uparrow} & \Delta_{\uparrow\downarrow} \\ \Delta_{\downarrow\uparrow} & \Delta_{\downarrow\downarrow} \end{pmatrix} \quad (1.11.1)$$

where α and β stands for spin directions. And in general for p-wave superconductor the energy gap function $\Delta_\sigma(\mathbf{k})$ takes the form of $\sin(k_x a)$ or $\sin(k_y a)$ for lattice constant a [38]. For ferromagnetic superconductors the Magnetization is the other order parameter.

1.12 phase diagram of $ZrZn_2$

It has been known that for some time the ferromagnetism of $ZrZn_2$ is extremely sensitive to pressure [11]. And different people try to study this effect near the transition temperature. Recent advances have allowed for the investigation of the quantum critical region in weak ferromagnetic metals as well as in some heavy fermion compounds. When hydrostatic pressure is applied on a transition metal compounds such as MnSi, $ZrZn_2$, the curie temperature can be driven down to zero at a critical pressure [35]. And experiments on $ZrZn_2$ have shown that a pressure of $p_c=21$

Kbar cause the ferromagnetism to disappear with first order transition. And $ZrZn_2$ is close to a quantum critical point (QCP). So far experiments failed to find the phenomena in the paramagnetic phase of ferromagnetic compounds. Eventhough there is a theoretical supposition of the occurance in the case of $ZrZn_2$ which predicts even higher T_c .

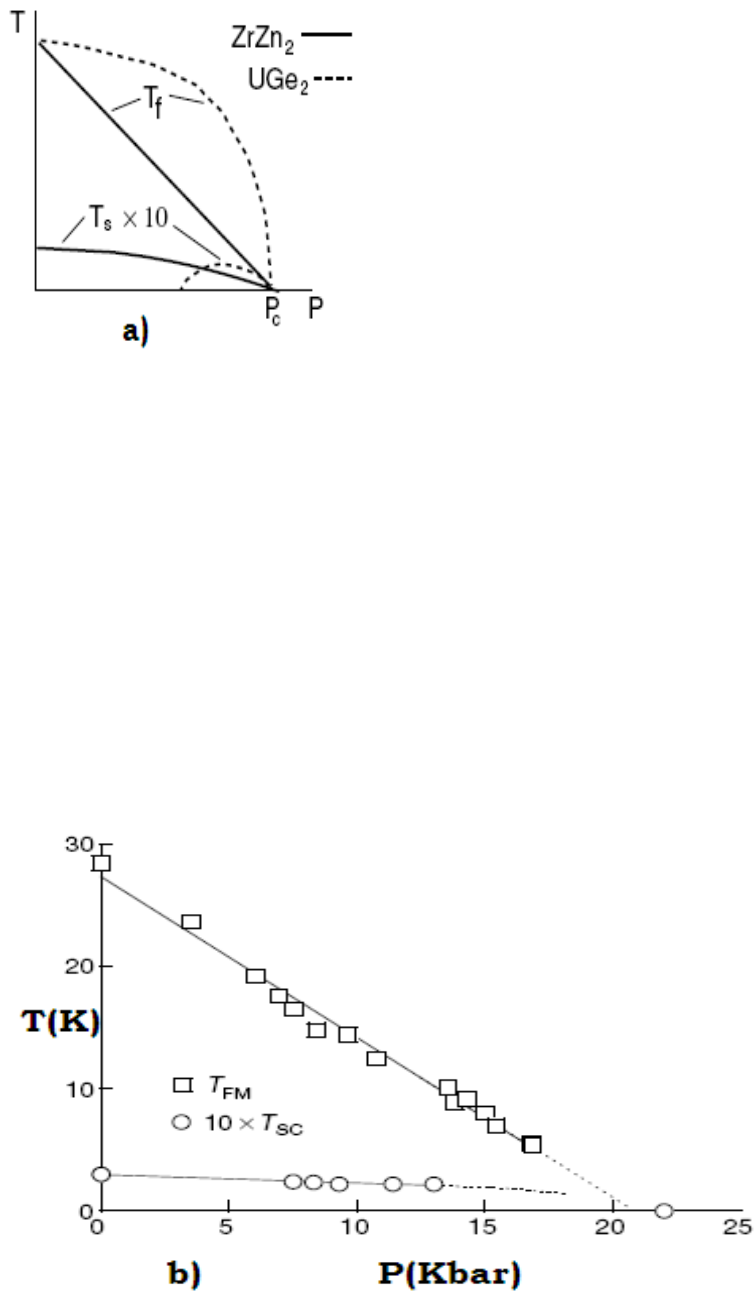


Figure 1.5: T versus pressure P where T_s is superconducting critical temperature and T_f is ferromagnetic critical temperature (a) Taken from ref [33] (b) Experimental result from ref [10]

Chapter 2

Mathematical Techniques

In the investigation of the problem we have used the mean field approximation of generalized BCS (Bardeen-Cooper-Sheifer) hamiltonian of ferromagnetic superconductors [39]. And we used green's function method zubarev [40]. We obtained the expression for critical temperature (T_c) for triplet pairing (of equal spin pairing case).

2.1 The Hamiltonian of Ferromagnetic Superconductors

The BCS Hamiltonian of two band Ferromagnetic Superconductors [39] is

$$\hat{H} = \sum_{k\sigma} \epsilon_{k\sigma} \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} + \frac{1}{2} \sum_{k,k'\sigma} V(k, k') \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \quad (2.1.1)$$

where $\hat{a}_{k\sigma}^\dagger$ is creation operator and $\hat{a}_{k\sigma}$ is annihilation operator of the fermions.

$$\epsilon_{k\sigma} = \epsilon_k - \mu_\sigma \quad (2.1.2)$$

with

$$\varepsilon_k = -t(\cos k_x + \cos k_y)$$

as the dispersion relation for fermions in two dimensional quasi particle system. And $\epsilon_{k\sigma}$ is the free energy of electrons with spin σ

$$\mu_{\uparrow} = \mu + \frac{1}{2}JM$$

for spin up pairing and

$$\mu_{\downarrow} = \mu - \frac{JM}{2}$$

for spin down pairing ; where μ is fermi energy

J is ferromagnetic exchange constant.

M is magnetization of the system and $V(k,k')$ is interaction potential between fermions.

And for p-wave pairing ferromagnetic superconductors [38]

$$V(k, k') = g[\cos(k_x - k'_x) + \cos(k_y - k'_y)] \quad (2.1.3)$$

with g the ferromagnetic coupling constant. The model hamiltonian is written as two interaction terms. The first term stands for spin spin magnetic interaction and the second term is electron electron interaction of the same spin. The magnetic coupling described by the constant J which mediates the ferromagnetic strength. The interaction strength is measured by the coupling interaction potential $V(k,k')$.

2.2 Green's Function Formalism

We have used Green's functions formalism [40] to study the problem. In quantum field theory they are also called propagators. It stands for the fact that it is used using the average behavior of one or two typical particles in stead of using the detailed

behavior of each particle in a system. There are different types of Green's functions. Among them we used the retarded double-time Green's functions given by

$$G(t, t') = \ll A(t), B(t') \gg$$

$$G(t, t') = -i\theta(t - t') \langle [A(t), B(t')] \rangle \quad (2.2.1)$$

where $\ll A(t), B(t') \gg$ is simple representation of the Green's functions and $\langle \dots \rangle$ stands for average value over the canonical ensemble for the operators. $\theta(t - t')$ is heaviside step function and $A(t), B(t')$ are operators in Heisenberg picture in which $A(t)$ is described as

$$A(t) = \exp iHtA(0) \exp iHt$$

taking \hbar as 1. And

$$\theta(t - t') = -\lim_{\epsilon \rightarrow 0} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-i\omega(t-t')}}{i\epsilon + \omega} d\omega$$

$$\begin{aligned} \theta(t - t') &= 1 \text{ for } t > t' \\ &= 0 \text{ for } t < t' \end{aligned}$$

$[A(t), B(t')]$ above stands for commutation for bosons and anticommutation for fermions.

Differentiating equation (2.2.1) and multiplying it by i both side

$$\begin{aligned} i \frac{dG(t, t')}{dt} &= i \frac{d}{dt} \ll A(t), B(t') \gg \\ &= \frac{d}{dt} \theta(t - t') \langle [A(t), B(t')] \rangle + -i\theta(t - t') \langle [\frac{dA(t)}{dt}, B(t')] \rangle \\ &= \frac{d}{dt} \theta(t - t') \langle [A(t), B(t')] \rangle + \ll i \frac{dA(t)}{dt}, B(t') \gg \end{aligned} \quad (2.2.2)$$

Lets consider the relation between heaviside step function $\theta(t)$ and Dirac delta function δ where

$$\theta(t) = \int_{-\infty}^t \delta(t)dt$$

hence $\frac{d\theta(t)}{dt} = \delta(t)$. Since the operators $A(t)$ and $B(t')$ satisfy Heisonberg equation of motion

$$i\frac{dA}{dt} = [A, \hat{H}] \quad (2.2.3)$$

taking $\hbar=1$ then equation (2.2.2) becomes

$$i\frac{dG(t, t')}{dt} = \delta(t - t') \langle [A(t), B(t')] \rangle + \ll [A, \hat{H}], B(t') \gg \quad (2.2.4)$$

In order to solve equation (2.2.4) lets use fourier transform of equation (2.2.2). Since we are dealing on retarded interaction we can use $G(t - t')$ in the place of $G(t, t')$ and lets represent $G(\omega)$ as the fourier transform of $G(t - t')$ in which

$$G(t - t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega) e^{-i\omega(t-t')} d\omega \quad (2.2.5)$$

and

$$G(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t-t')} G(t - t') dt \quad (2.2.6)$$

using the delta function

$$\delta(t - t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega(t-t')} d\omega \quad (2.2.7)$$

and using the fourier transform of $G(t)$

where

$$G(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega) e^{-i\omega t} d\omega$$

hence

$$\frac{dG}{dt} = -i\omega \times G(\omega)$$

equation (2.2.4) will take the form

$$\omega G(\omega) = \langle [A(t), B(t')] \rangle_{\omega} + \ll [A(t), \hat{H}], B(t') \gg_{\omega} \quad (2.2.8)$$

In simplified form equation (2.2.8) can be of the form

$$\omega \ll A, B \gg_{\omega} = \langle [A, B] \rangle_{\omega} + \ll [A, \hat{H}], B(t') \gg_{\omega} \quad (2.2.9)$$

This is equation of motion involving the fourier transform of the green function $\ll A, B \gg$, $\ll [A, \hat{H}], B(t') \gg_{\omega}$, and the thermal average $\langle [A, B] \rangle_{\omega}$ over the canonical ensemble, that is $\langle F \rangle = \frac{\text{Tre}^{-\beta H} F}{e^{-\beta H}}$ where $\beta = \frac{1}{k_B T}$ k_B is Boltzman constant.

The correlation function for fermions interms of green's function is given by

$$\langle B(t'), A(t) \rangle = \text{ilim}_{\varepsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{(G(\omega + i\varepsilon) - G(\omega - i\varepsilon))e^{i\omega(t-t')}}{e^{\beta\omega} + 1} \quad (2.2.10)$$

In our case we defined the following correlation for the order parameter of the superconductor

$$\Delta_{k\sigma} = \sum_{k',\sigma} V(k, k') \langle \hat{a}_{k'} \hat{a}_{-k'\sigma} \rangle \quad (2.2.11)$$

And from consistency condition of order parameter we have

$$\Delta_{k\sigma} = \sum_{k,n} \frac{V(k, k')}{\beta} \ll \hat{a}_{\dagger -k'\sigma}, \hat{a}_{\dagger k'\sigma} \gg \quad (2.2.12)$$

Chapter 3

Formulation of The Problem

In this chapter we have tried to get expression for critical temperature T_c using mean field mechanism on the generalized BCS hamiltonian of two band superconductors [39] with zero momentum pairing case.

3.1 Mean Field Hamiltonian

The model hamiltonian for p-wave ferromagnetic superconductor is similar to the s-wave superconductor. Lets start from the generalized BCS hamiltonian of two band(one up pairing the other down pairing) ferromagnetic superconductor of the form

$$\hat{H} = \sum_{k\sigma} \epsilon_{k\sigma} \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} + \frac{1}{2} \sum_{kk'\sigma} V(k, k') \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \quad (3.1.1)$$

To arrive at the effective mean field hamiltonian one needs to perform a mean field transformation on the second term in equation (3.1.1). This term is composed of four fermion interaction which is difficult to work with, and it would be convenient to make it quadratic in the fermion operator. To do this we can take two of this operators and define

$$\hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger = \langle \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \rangle + (\hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger - \langle \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \rangle) \quad (3.1.2)$$

and

$$\hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} = \langle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \rangle + (\hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} - \langle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \rangle) \quad (3.1.3)$$

which is obviously true and can be interpreted as for example the operator $\hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger$ equal to its average $\langle \dots \rangle$ plus the fluctuation about its average, denoted by the term in parentheses. Upon multiplication of equation (3.1.2) with (3.1.3), terms that are quadratic in fluctuation can be dropped because they can be considered as small, especially [41] for systems with many particles as in superconductors. Hence

$$\begin{aligned} \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} &= \langle \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \rangle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} + \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \langle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \rangle \\ &- \langle \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \rangle \langle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \rangle \end{aligned} \quad (3.1.4)$$

Plugging equations (3.1.4) in equation (3.1.1) the hamiltonian will become

$$\begin{aligned} \hat{H} &= \sum_{k\sigma} \epsilon_{k\sigma} \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} + \frac{1}{2} \sum_{k\sigma} V(k, k') \langle \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \rangle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \\ &+ \sum_{k\sigma} V(k, k') \langle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \rangle \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger - \frac{1}{2} \sum_{k\sigma} V(k, k') (\langle \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger \rangle) \langle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \rangle \end{aligned}$$

The full effective hamiltonian will be

$$\begin{aligned} \hat{H} &= \sum_{k\sigma} \epsilon_{k\sigma} \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} + \frac{1}{2} \sum_{k\sigma} (\Delta_{k\sigma}^* \hat{a}_{-k\sigma} \hat{a}_{k\sigma} + \Delta_{k\sigma} \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger) \\ &- \frac{1}{2} \sum_{k\sigma} \frac{|\Delta_{k\sigma}|^2}{V(k, k')} \end{aligned} \quad (3.1.5)$$

where

$$\Delta_{k\sigma}^* = \sum_{k'\sigma} V(k, k') \langle \hat{a}_{-k'\sigma} \hat{a}_{k'\sigma}^\dagger \rangle \quad (3.1.6)$$

and

$$\Delta_{k\sigma} = \sum_{k'\sigma} V(k, k') \langle \hat{a}_{k'\sigma} \hat{a}_{-k'\sigma} \rangle \quad (3.1.7)$$

is the superconductivity order parameter, or energy gap. This mean field theory transformation is used very often in many-body problems, especially in superconductors. Here the energy gap is assumed momentum (k) dependent.

3.2 Equation of Motion of parallel Spin pairing (ESP)

In this section we will use the relation for three operators A, B, and C.

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

and

$$\{\hat{a}_{k\sigma}^\dagger, \hat{a}_{k'\alpha}^\dagger\} = 0$$

$$\{\hat{a}_{k\sigma}, \hat{a}_{k'\alpha}\} = 0$$

$$\{\hat{a}_{k\sigma}^\dagger, \hat{a}_{k'\alpha}\} = \delta_{k,k'} \delta_{\sigma,\alpha}$$

To obtain equation of motion for the ESP pairing lets start from the green functions of the form of equation (2.2.9)

$$\omega \ll \hat{a}_{k\alpha}, \hat{a}_{k'\alpha}^\dagger \gg_\omega = \delta_{kk'} + \ll [\hat{a}_{k\alpha}, \hat{H}], \hat{a}_{k'\alpha}^\dagger \gg_\omega \quad (3.2.1)$$

And then computing the commutation $[\hat{a}_{k\alpha}, \hat{H}]$. The commutation with the first term of \hat{H} using anticommutation relation for fermions is

$$\begin{aligned}
[\hat{a}_{k\alpha}, \sum_{p\sigma} \epsilon_{p\sigma} \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma}] &= \sum_{p\sigma} \epsilon_{p\sigma} \hat{a}_{p\sigma} \delta_{k,p} \delta_{\alpha,\sigma} \\
&= \epsilon_{k\alpha} \hat{a}_{k\alpha}
\end{aligned} \tag{3.2.2}$$

and

$$\begin{aligned}
[\hat{a}_{k\alpha}, \frac{1}{2} \sum_{k\sigma} (\Delta_{p\sigma}^* \hat{a}_{p\sigma} \hat{a}_{-p\sigma} + \Delta_{p\sigma} \hat{a}_{-p\sigma}^\dagger \hat{a}_{p\sigma}^\dagger)] &= [a_{k\alpha}, \frac{1}{2} \sum_{p\sigma} \Delta_{p\sigma} \hat{a}_{-p\sigma}^\dagger \hat{a}_{p\sigma}^\dagger] \\
&= \frac{1}{2} \sum_{p\sigma} \Delta_{p\sigma} [\hat{a}_{k\alpha}, \hat{a}_{-p\sigma}^\dagger \hat{a}_{p\sigma}^\dagger] \\
&= \frac{1}{2} \sum_{p\sigma} \Delta_{p\sigma} \hat{a}_{p\sigma}^\dagger \{\hat{a}_{k\alpha}, \hat{a}_{-p\sigma}^\dagger\} - \frac{1}{2} \sum_{p\sigma} \Delta_{p\sigma} \hat{a}_{-p\sigma}^\dagger \{\hat{a}_{k\alpha}, \hat{a}_{p\sigma}^\dagger\} \\
&= \frac{1}{2} \sum_{p\sigma} \Delta_{p\sigma} \hat{a}_{p\sigma}^\dagger \delta_{k,-p} \delta_{\alpha\sigma} - \frac{1}{2} \sum_{p\sigma} \Delta_{p\sigma} \hat{a}_{-p\sigma}^\dagger \delta_{k,p} \delta_{\alpha\sigma} \\
&= \frac{1}{2} (\Delta - k\alpha - \Delta_{k\alpha}) \hat{a}_{-k\alpha}^\dagger
\end{aligned} \tag{3.2.3}$$

Then plugging equation (3.2.3) and (3.2.2) in equation (3.2.1) and taking $k = k'$ we will get

$$(\omega - \epsilon_{k\alpha}) \ll \hat{a}_{k\alpha}, \hat{a}_{k\alpha}^\dagger \gg_\omega = 1 + \frac{1}{2} (\Delta - k\alpha - \Delta_{k\alpha}) \ll \hat{a}_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \gg_\omega \tag{3.2.4}$$

Now lets solve the last term of equation (3.2.4) using green's function of the form of equation (3.2.1)

$$\omega \ll \hat{a}_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \gg_\omega = \delta_{k,-k} + \ll [\hat{a}_{-k\alpha}^\dagger, \hat{H}], \hat{a}_{k\alpha}^\dagger \gg \tag{3.2.5}$$

Lets compute the commutation $[\hat{a}_{-k\alpha}^\dagger, \hat{H}]$. The commutation with the first term of the full hamiltonian \hat{H} is

$$\begin{aligned}
[\hat{a}_{-k\alpha}^\dagger, \sum_{p\sigma} \epsilon_{p\sigma} \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma}] &= - \sum_{p\sigma} \epsilon_{p\sigma} \hat{a}_{p\sigma}^\dagger \delta_{-k,p} \delta_{\alpha\sigma} \\
&= -\epsilon_{-k\alpha} \hat{a}_{-k\alpha}^\dagger
\end{aligned} \tag{3.2.6}$$

and the commutation with the second term is

$$\begin{aligned}
[\hat{a}_{-k\alpha}^\dagger, \frac{1}{2} \sum_{k\sigma} (\Delta_{p\sigma}^* \hat{a}_{p\sigma} \hat{a}_{-p\sigma} + \Delta_{p\sigma} \hat{a}_{-p\sigma}^\dagger \hat{a}_{p\sigma}^\dagger)] &= \frac{1}{2} \sum_{k\sigma} \Delta_{p\sigma}^* [\hat{a}_{-k\alpha}^\dagger, \hat{a}_{p\sigma} \hat{a}_{-p\sigma}] \\
&= \frac{1}{2} \sum_{k\sigma} \Delta_{p\sigma}^* \hat{a}_{p\sigma} \{ \hat{a}_{-k\alpha}^\dagger, \hat{a}_{p\sigma} \} - \frac{1}{2} \sum_{k\sigma} \Delta_{p\sigma}^* \hat{a}_{-p\sigma} \{ \hat{a}_{-k\alpha}^\dagger, \hat{a}_{-p\sigma} \} \\
&= \frac{1}{2} \sum_{k\sigma} \Delta_{p\sigma}^* \hat{a}_{-p\sigma} \delta_{-k,p} \delta_{\alpha\sigma} - \frac{1}{2} \sum_{k\sigma} \Delta_{p\sigma}^* \hat{a}_{-p\sigma} \delta_{-k,-p} \delta_{\alpha\sigma} \\
&= \frac{1}{2} (\Delta_{-k\alpha}^* - \Delta_{k\alpha}^*) \hat{a}_{k\alpha}
\end{aligned} \tag{3.2.7}$$

The commutation with the 3rd term of \hat{H} is zero. Then plugging equations (3.2.6) and (3.2.7) in (3.2.5)

$$\omega \ll a_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \gg_\omega = \ll -\epsilon_{-k\alpha} \hat{a}_{k\alpha}, \hat{a}_{k\alpha}^\dagger \gg_\omega + \frac{1}{2} (\Delta_{-k\uparrow}^* - \Delta_{k\alpha}^*) \ll \hat{a}_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \gg_\omega$$

then

$$\ll \hat{a}_{k\alpha}, \hat{a}_{k\alpha}^\dagger \gg_\omega = \frac{2(\omega + \epsilon_{-k\alpha})}{(\Delta_{-k\alpha}^* - \Delta_{k\alpha}^*)} \ll a_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \gg_\omega \tag{3.2.8}$$

Hence plugging equations (3.2.8) in (3.2.4) and simplifying it we will get

$$\ll a_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \gg = \frac{2(\Delta_{-k\alpha}^* - \Delta_{k\alpha}^*)}{4(\omega + \epsilon_{-k\alpha})(\omega - \epsilon_{k\alpha}) - (\Delta_{-k\uparrow}^* - \Delta_{k\alpha}^*)(\Delta_{-k\alpha} - \Delta_{k\alpha})} \tag{3.2.9}$$

for ferromagnetic superconductors the order parameter [38] can be expressed as

$$\Delta_{k\alpha} = \Delta_\alpha \sin k_x \quad (3.2.10)$$

hence

$$\begin{aligned} \Delta_{-k\alpha} &= -\Delta_\alpha \sin k_x \\ \Delta_{-k\alpha} &= -\Delta_{k\alpha} \end{aligned} \quad (3.2.11)$$

$$\begin{aligned} \Delta_{k\alpha}^* &= \Delta_\alpha \sin k_x \\ \Delta_{k\alpha}^* &= \Delta_{k\alpha} \end{aligned} \quad (3.2.12)$$

from equation (2.1.2) we can see that ϵ_k is even function of k . Hence

$$\epsilon_{-k\alpha} = \epsilon_{k\alpha} \quad (3.2.13)$$

using equations (3.2.11-13) equation (3.2.9) becomes

$$\begin{aligned} \langle\langle \hat{a}_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \rangle\rangle &= \frac{4(\Delta_{k\alpha})}{4(\omega^2 - \epsilon_{k\alpha}^2) - (2\Delta_{k\alpha})^2} \\ &= -\frac{\Delta_\alpha \sin k_x}{(\omega^2 - \epsilon_{k\alpha}^2) - (\Delta_\alpha \sin k_x)^2} \\ \langle\langle \hat{a}_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \rangle\rangle &= \frac{\Delta_\alpha \sin k_x}{(-\omega^2 + \epsilon_{k\alpha}^2) + (\Delta_\alpha \sin k_x)^2} \end{aligned} \quad (3.2.14)$$

But by the self consistency condition of order parameter

$$\Delta_{k\sigma} = \sum_{k',n} \frac{V(k, k')}{\beta} \langle\langle \hat{a}_{-k\alpha}^\dagger, \hat{a}_{k\alpha}^\dagger \rangle\rangle \quad (3.2.15)$$

hence

$$\Delta_{k\alpha} = \sum_{k',n} \frac{g[\cos(k_x - k'_x) + \cos(k_y - k'_y)] \Delta_\alpha \sin k'_x}{\beta[\epsilon_{k\alpha}^2 + \Delta_\alpha \sin k'_x - \omega^2]}$$

$$\begin{aligned}\Delta_\alpha \sin k_x &= \sum_{k',n} \frac{g[\cos(k_x - k'_x) + \cos(k_y - k'_y)] \Delta_\alpha \sin k'_x}{\beta[\epsilon_{k\alpha}^2 + (\Delta_\alpha \sin k'_x)^2 - \omega^2]} \\ \sin k_x &= \sum_{k',n} \frac{g[\cos(k_x - k'_x) + \cos(k_y - k'_y)] \sin k'_x}{\beta[\epsilon_{k\alpha}^2 + (\Delta_\alpha \sin k'_x)^2 - \omega^2]}\end{aligned}\quad (3.2.16)$$

using the mathematical relation

$$\sum_n \frac{1}{\pi^2(2n+1)^2 + x^2} = \frac{\tanh \frac{x}{2}}{2x}$$

in our case $x = \beta E_{k\alpha}$ and using the following substitutions :

$$\omega = i\omega_n \quad (3.2.17)$$

for Matsubara frequency of fermions. Where

$$\omega_n = \frac{\pi}{\beta}(2n+1) \quad (3.2.18)$$

and

$$E_{k\alpha}^2 = \epsilon_{k\alpha}^2 + (\Delta_\alpha \sin k_x)^2 \quad (3.2.19)$$

equation (3.2.16) will be reduced to

$$\begin{aligned}\sin k_x &= \sum_{k',n} \frac{g[\cos(k_x - k'_x) + \cos(k_y - k'_y)] \sin k'_x}{\beta(E_{k'\alpha}^2 + \omega_n^2)} \\ &= \sum_{k',n} \frac{g\beta[\cos(k_x - k'_x) + \cos(k_y - k'_y)] \sin k'_x}{(\beta^2 E_{k'\alpha}^2 + (2n+1)^2 \pi^2)} \\ &= \sum_{k'} \frac{g[\cos(k_x - k'_x) + \cos(k_y - k'_y)] \sin k'_x \tanh(\frac{E_{k'\alpha}}{2k_B T})}{2E_{k'\alpha}}\end{aligned}\quad (3.2.20)$$

for maximum value of

$\sin k_x$, k_x is $\frac{\pi}{2}$ and ignoring the interaction along the y

$$\begin{aligned}
1 &= g \sum_{k'} \frac{\cos(\frac{\pi}{2} - k'_x) \sin k'_x \tanh \frac{E_{k'_\alpha}}{2k_B T}}{2E_{k'_\alpha}} \\
1 &= g \sum_{k'} \frac{\sin k'_x \tanh \frac{E_{k'_\alpha}}{2k_B T} \sin k'_x}{2E_{k'_\alpha}} \\
\frac{1}{g} &= \sum_k \frac{\sin^2 k_x \tanh \frac{E_{k_\alpha}}{2k_B T}}{2E_{k_\alpha}} \tag{3.2.21}
\end{aligned}$$

where

$$\begin{aligned}
\epsilon_{k_\alpha} &= -t(\cos k_x + \cos k_x) - \mu \pm \frac{JM}{2} \\
&= -t\left(1 - \frac{k_x^2}{2} + 1 - \frac{k_y^2}{2}\right) - \mu \pm \frac{JM}{2} \\
\epsilon_{k_\alpha} &= t\left(\frac{k_x^2 + k_y^2}{2}\right) - 2t - \mu \pm \frac{JM}{2} \tag{3.2.22}
\end{aligned}$$

the above expression was found by linearization. And in \pm above we will take + for the up pairing and - for down pairing

3.3 Critical Temperature T_c for ESP pairing

The critical temperature T_c of a superconductor is the temperature above which it comes to the normal state and at this point the energy gap is zero. Applying this condition to equation (3.2.19) we can get $E_{k_\downarrow} = \epsilon_{k_\downarrow}$ using this relation, and equation (3.2.22) lets integrate equation (3.2.21) on the first Brillouin zone using polar coordinate system for the spin down pairing case.

$k_x=r\cos\theta$, $k_y=r\sin\theta$ and then $k_x^2+k_y^2=r^2$

$$\begin{aligned}
\frac{1}{g} &= \left(\frac{1}{2\pi}\right)^2 N(0) \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{k_x^2 \tanh\left(\frac{t(k_x^2+k_y^2-4)-2\mu-JM}{4k_B T_c}\right)}{t(k_x^2+k_y^2-4)-2\mu-JM} dk_x dk_y \\
&= \frac{N(0)}{4\pi^2} \int_0^{2\pi} \int_0^R \frac{r^2 \cos^2\theta \tanh\left(\frac{t(r^2-4)+b}{4k_B T_c}\right)}{t(r^2-4)+b} r dr d\theta \\
&= \frac{N(0)}{4\pi} \int_0^R \frac{r^2 \tanh\left(\frac{t(r^2-4)+b}{4k_B T_c}\right)}{t(r^2-4)+b} r dr
\end{aligned} \tag{3.3.1}$$

where

$N(0)$ is density of states

$b = -2\mu - JM$, here the area of the first brillouin zone is

$(2\pi)^2 = 4\pi^2$ and in polar coordinate it is

$= \pi R^2$. Then from this we can get

$R = \sqrt[2]{2\pi}$. To use integration by substitution: let

$u = \frac{t(r^2-4)+b}{4k_B T_c}$ then

$r dr = \frac{2k_B T_c}{t} du$

$r^2 = \frac{4k_B T_c u - b}{t} + 4$ and the limit of integration for u will be from

$\frac{b-4t}{4k_B T_c}$ to $\frac{t(4\pi-4)+b}{4k_B T_c}$

then equation (3.3.1) becomes

$$\begin{aligned}
\frac{1}{g} &= \frac{N(0)}{4\pi} \int_{\frac{b-4t}{4k_B T_c}}^{\frac{t(4\pi-4)+b}{4k_B T_c}} \frac{(\frac{4k_B T_c u - b}{t} + 4) \tanh u}{4k_B T_c u} 2k_B T_c du \\
&= \frac{N(0)}{8\pi} \int_{\frac{b-4t}{4k_B T_c}}^{\frac{t(4\pi-4)+b}{4k_B T_c}} \frac{(\frac{4k_B T_c u - b}{t} + 4) \tanh u}{u} du \\
&= \frac{N(0)}{8\pi} \int_{\frac{b-4t}{4k_B T_c}}^{\frac{t(4\pi-4)+b}{4k_B T_c}} \left(\frac{4k_B T_c}{t}\right) \tanh u du \\
&+ \frac{N(0)}{8\pi} b \int_{\frac{b-4t}{4k_B T_c}}^{\frac{t(4\pi-4)+b}{4k_B T_c}} (4t - b) \frac{\tanh u}{ut} du
\end{aligned} \tag{3.3.2}$$

taking the condition $t(4\pi - 4) + b > 0$ and $b - 4t < 0$ the limit for the first term of the integration can be taken as from $-\infty$ to ∞ because $4k_B T_c$ is very small. Then the first term

$\frac{N(0)}{8\pi} \int_{-\infty}^{\infty} \left(\frac{4k_B T_c}{t}\right) \tanh u du = 0$ since $\tanh u$ is odd function. Then

$$\begin{aligned}
\frac{1}{g} &= \frac{N(0)}{8\pi} \left(\frac{4t - b}{t}\right) \left(2 \int_0^{\frac{t(4\pi-4)+b}{4k_B T_c}} \frac{\tanh u}{u} du\right) \\
&= \frac{N(0)}{4\pi} \left(\frac{4t - b}{t}\right) (\tanh u \ln u \Big|_0^{\frac{t(4\pi-4)+b}{4k_B T_c}} - \int_0^{\infty} \sec^2 u \ln u du) \\
&= \frac{N(0)}{4\pi} \left(\frac{4t - b}{t}\right) (\ln(\frac{t(4\pi - 4) + b}{4k_B T_c}) - \ln 0.44) \\
\frac{1}{g} &= \frac{N(0)}{4\pi} \left(\frac{4t - b}{t}\right) \ln\left(\frac{t(4\pi - 4) + b}{(0.44)4k_B T_c}\right)
\end{aligned} \tag{3.3.3}$$

The second integration above is found from its equal value $-\ln(\frac{4\gamma}{\pi})$ with $\gamma \simeq 1.78107$ being the Euler constant[42]. After a certain rearrangement we will get

$$4k_B T_c = \left(\frac{t(4\pi - 4) + b}{0.44}\right) e^{\frac{-4\pi t}{gN(0)(4t-b)}} \tag{3.3.4}$$

Then after substituting the value of b the expression of T_c for the spin down pairing will be

$$T_{c\downarrow} = \frac{t(4\pi - 4) - 2\mu - JM}{1.516 \times 10^{-4}} e^{\frac{4\pi t}{gN(0)(-JM-4t-2\mu)}} \quad (3.3.5)$$

For the spin up pairing the expression of T_c is similar to that of spin down except substituting of JM in the place of -JM, hence

$$T_{c\uparrow} = \frac{t(4\pi - 4) - 2\mu + JM}{1.516 \times 10^{-4}} e^{\frac{4\pi t}{gN(0)(JM-4t-2\mu)}} \quad (3.3.6)$$

Chapter 4

Results and Discussions

In chapter two we used green function formalism important in many particle system especially in superconductivity. We take a model hamiltonian for two band superconductors as we only consider triplet pairing (ESP) which can have two bands one spin up band and the other spin down band. Only spin triplet case was taken because the superconducting state lie only in the ferromagnetic phase [10] hence parallel spin electrons favored to participate in pair formation. On the other hand the curie temperature of the ferromagnetic metal is 28.5K which is much greater than its superconducting temperature 0.29K then the spin singlet pairing is improbable as it is far from the paramagnetic phase suitable for spin singlet pairing.

Since ferromagnetic state is characterized by magnetization we found expression of superconducting critical temperature for triplet pairing(ESP) interms of the order parameter magnetization. Starting from a model Hamiltonian

$$\hat{H} = \sum_{k\sigma} \epsilon_{k\sigma} \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} + \frac{1}{2} \sum_{k\sigma} (\Delta_{k\sigma}^* \hat{a}_{-k\sigma} \hat{a}_{k\sigma} + \Delta_{k\sigma} \hat{a}_{-k\sigma}^\dagger \hat{a}_{k\sigma}^\dagger) - \frac{1}{2} \sum_{k\sigma} \frac{|\Delta_{k\sigma}|^2}{V(k, k')},$$

for a triplet superconductor an expression for the critical temperature has been obtained. The critical temperature for the down pairing is

$$T_{c\downarrow} = \frac{t(4\pi - 4) - 2\mu - JM}{1.516 \times 10^{-4}} e^{\frac{4\pi t}{gN(0)(-JM-4t-2\mu)}}$$

and for the up pairing

$$T_{c\uparrow} = \frac{t(4\pi - 4) - 2\mu + JM}{1.516 \times 10^{-4}} e^{\frac{4\pi t}{gN(0)(JM-4t-2\mu)}}$$

The graphs of the two critical temperatures are as shown below. In drawing the graphs we used 1eV for t , 2.4eV for the fermi energy, 0.126 for $gN(0)$, and $0.08 \frac{eV}{\mu_B}$ for J . The value of the fermi energy was chosen considering the value of fermi energy of most metals ≤ 5 eV, for $gN(0)$ the value is taken because for different superconductors the experimental values are ≤ 0.3 most of them have in the order of 0.18 [23] and the value of J is chosen considering the experimental value of the exchange integral of order of 70meV for UGe_2 [8] with the same property of $ZrZn_2$ and considering the value magnetization of $ZrZn_2$.

The graph of the down pairing of fig 4.3 is similar to the graph of T_c versus J in [38]. Since M increases as J increases the effect of M on T_c is similar to J . Hence the graph is consistent. As we can see from the graph T_c of the down pairing it increases firstly then decrease this shows that the T_c increases until the magnetization approaches saturation and then decreases after saturation is achieved [33]. Since the $T_{c\downarrow}$ increases with the increase in magnetization it is indicative of the coexistence of superconductivity and, for the $T_{c\uparrow}$ channel the electrons in the spin up band do not affecting pair and that is why $T_{c\uparrow}$ decreases fast.

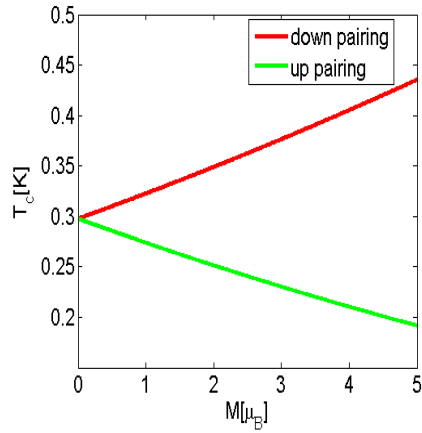


Figure 4.1: Critical temperature T_c versus magnetization for lower range of magnetization

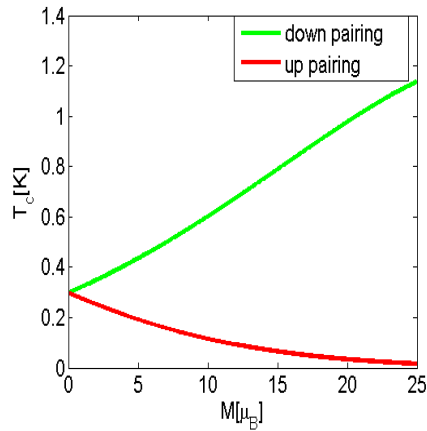


Figure 4.2: Critical temperature T_c versus magnetization for larger range of magnetization

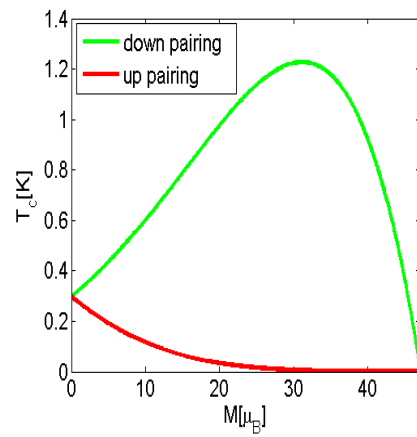


Figure 4.3: Critical temperature T_c versus magnetization for even larger range of magnetization

Chapter 5

Conclusion

On the basis of our study we conclude the coexistence of triplet superconductivity and ferromagnetism is as a possibility and that only the down pairing electrons participate in the pair formation as $T_{c\downarrow}$ is increasing and the $T_{c\uparrow}$ is decreasing. Since spin up electrons and spin down electrons differ by exchange energy we can conclude that the value of the energy of electrons affect the pair formation.

We saw that the superconducting critical temperature for the spin down pairing increases for a certain value of magnetization and then decreases shows that the coexistence phase is possible up to certain value of magnetization. It appears that spin fluctuation may be involved in the pairing of the electrons although the mechanism of the superconductivity and ferromagnetism is yet to be established.

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Declaration

I hereby declare that this thesis is my original work and has not been presented for a degree in any other university. All sources of material used for the thesis have been duly acknowledged.

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