THE STUDY OF THE COEXISTENCE OF FERROMAGNETISM AND SUPERCONDUCTIVITY IN ZRZN2

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The undersigned hereby certify that they have read and recommend to the Faculty of Science for acceptance a senior project entitled " **The study of the coexistence of ferromagnetism and superconductivity in ZrZn2**" by **Paulos Taddesse Master of Science**.

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This Work is Dedicated to
My Mother Gudaynesh Kebede ,
my wife Adile Ayele and my
children

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Abstract

We study the possibility of the coexistence of ferromagnetism and superconductivity in a compound $ZrZn_2$. In the first case we derive the triplet equal spin pairing gap equation as a function of exchange splitting V_c. We have also shown that the splitting gap equation can be used to estimate the superconducting temperature,T_{sc}, of $ZrZn_2$in two aspects: $V_c = 0$ and $V_c \neq 0$. Here, we first report that the gap equation allows us the phase transition from A state (paramagnetic state) to A_1 or A_2 superconducting states. Additionally, for $V_c = 0$, we find that $T_{sc} = 0.37k$ and for $V_c \neq 0$ we also obtain that $T_{sc} = 0.4k$ for up-up pairing and $T_{sc} = 0.34k$ for down-down pairing respectively. Here we predict that the highest value of T_{sc} is related to the majority spin pairing state, and the smallest value of T_{sc} is related to the minority spin pairing state.

On the other hand, we report the phase diagram showing the ferromagnetic T_f and the superconducting T_{sc} temperatures as a function of pressure in $ZrZn_2$. It is found that both temperatures decrease with increasing pressure and they vanish simultaneously at the critical pressure P_c. Her we report that as the pressure increases more and more spins are fluctuated from their common directions, this effect reduces the transition temperatures of $ZrZn_2$, we suggest that the same electrons are responsible for both ferromagnetism and superconductivity in $ZrZn_2$. We compare our results with the theoretical models and with experimental observations in $ZrZn_2$.

Introduction

Superconductivity is a phenomena occurring in a certain materials at low temperature, characterized by the complete absence of electrical resistance and the exclusion of the interior magnetic field (the Meissner effect). This phenomena was first discovered in 1911 by Kammerligh Onnes [1,2,3] who observed an enormous drop in the d.c resistance of mercury at 4.2 K. After the discovery of the sudden drop in resistivity in Hg at liquid He temperature, many other materials were subsequently found to show a similar transition at a varies of temperature. Onnes's original data are shown in fig.(1).

The fundamental ideal behind all of superconductor's unique properties is that superconductivity is a quantum mechanical phenomenon on a microscopic scale created when the motion of individual electrons are correlated. According to the theory developed by J. Bardeen, L. Cooper, and R. Schrieffer (BCS theory), this correlation takes place when two electrons couple to form cooper pairs. The electrical charge carriers in a superconductor to be cooper pairs with a mass m^* and a charge q^* twice those of the normal electrons.

The average distance between the two electrons in a Cooper pair is known as the coherence length, ξ. Both the coherence length and the binding energy of two electrons in a Cooper pair,2Δ [4], depend upon the particular superconducting materials. Typically, the coherence is many times larger than the interatomic spacing of a solid, and so we should not think of cooper pairs as tightly bound electron molecules.

If we prevent the cooper pairs from forming by ensuring that all the electrons are at an energy greater than the binding energy, we can destroy the superconducting phenomenon. This can be accomplished, for example, with a thermal energy. In fact, according to the BCS theory, the critical temperature T_c, associated with energy is

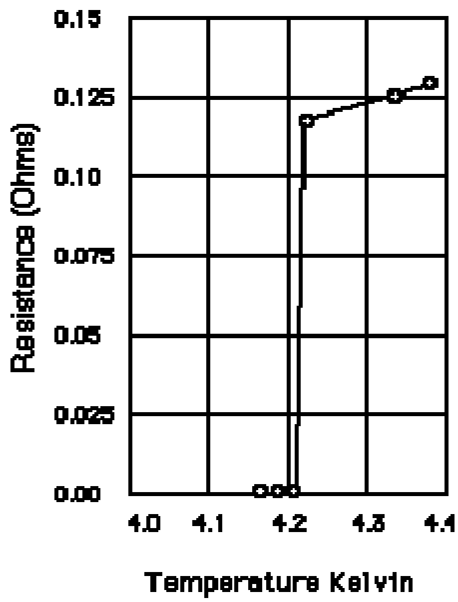

Figure 1: *Experimental data by H.K. Onnes in1911 which first showed the transition from the resistivity state to superconducting state .*

$\frac{2\Delta}{K_B T_c} \approx 3.5$. For low T_c (conventional) superconductors, 2Δ is typically on the order of 1 mev, and we see that these materials must be kept below the temperature of about 10 k to exhibit their unique behavior. The second way of increasing the energy of the electrons is electrically deriving them. In other words, if the critical current density, J_c, of a superconductor is exceeded , the electrons have sufficient kinetic energy to prevent the formation of Cooper pairs. The necessary kinetic energy can also be generated through the induced currents created by an external magnetic field. As a result, if a superconductor is placed in a magnetic field larger than its critical field, it will return to its normal state.

Another important proof of superconductivity is perfect diamagnetism. In 1933 two German physicists, Meissner and Ochenfeld [5], found that superconductors expel magnetic fields: if a superconductor is in its normal state is put in a magnetic field, and the temperature is lowered below the critical temperature (where a material becomes a superconductor) the magnetic field is expelled (this is shown in fig.(2)). The way in which this process takes place divides the superconducting materials into two types: type *I* and type *II*. fig.(3) shows the H-T phase diagram of the two types. In type *I* materials (in the first Fig.3) the magnetic field is totally excluded from the material up to a critical field H_c, and above H_c the magnetic field penetrates completely into the sample the normal electrical resistance is restored. Thus, below H_c, the material is its superconducting state (Meissner state), and above H_c, the material is in its normal state. In type *II* materials (in the second Fig. 3), the perfect superconducting state with a total expulsion of the magnetic field exists up to a lower critical field H_{c_1}. At field above the the upper critical field H_{c_2}, the magnetic field penetrates completely, and the material is its normal state. In the intermediate region between H_{c_1} and H_{c_2} there is a mixed state at which the magnetic field penetrates into the superconductor in the form of quantized flux line, or vortices.

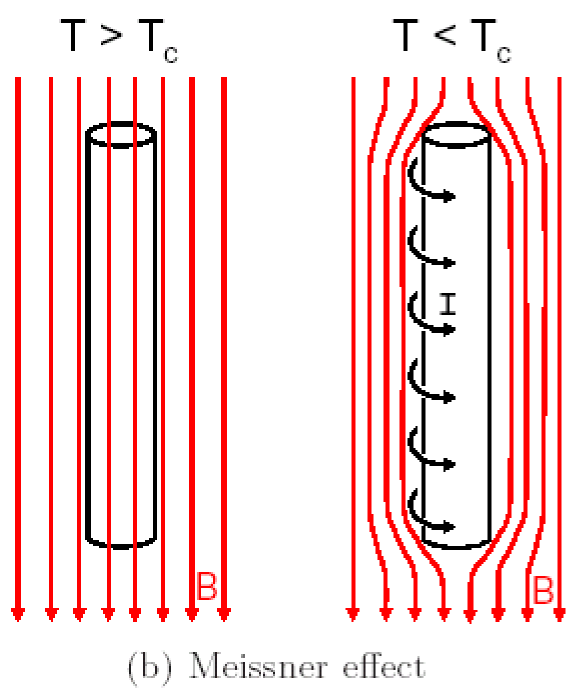

Figure 2: *A superconductor in the Meissner state.*

Superconductinity and magnetism are often thought of as antagonistic phenomena. This feature can be exploited to, for example, if one place a magnet that produces a field smaller than the critical field near above the superconductor, then the

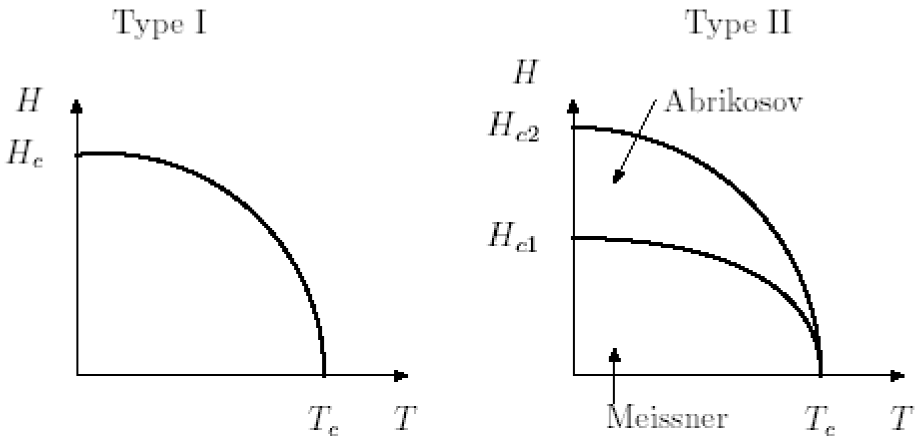

Figure 3: *H-T phase diagram of type I and type II superconductors.*

magnetic field will levitate above the superconductor see fig.(4). The magnetic field levitates because the superconductor will not allow the magnetic field to penetrate into its interior. This phenomena is called the Meissner effect. The strength of a magnetic field required to completely eradicate superconductivity is known as critical field. If the applied field is large enough, the superconductor material reverts back to the normal resistivity state.

This traditional view of antagonism between superconductivity and magnetism has come under threat recently. The discovery of unconventional superconductivity caused an explosive growth of activities in varies fields of condensed-matter physics research. So the recent discovery of three compounds which are ferromagnetic and superconductive at the same time came as a surprise to many physists. Even more surprisingly it appears that the same electrons are responsible for both the superconductivity and the ferromagnetism. These materials are UGe_2, URhGe, and $ZrZn_2$, the last of which we will study in this thesis.

The appearance of spin waves in ferromagnets at low temperature is one of the most basic physical quantum characteristics of spin systems. It was shown that

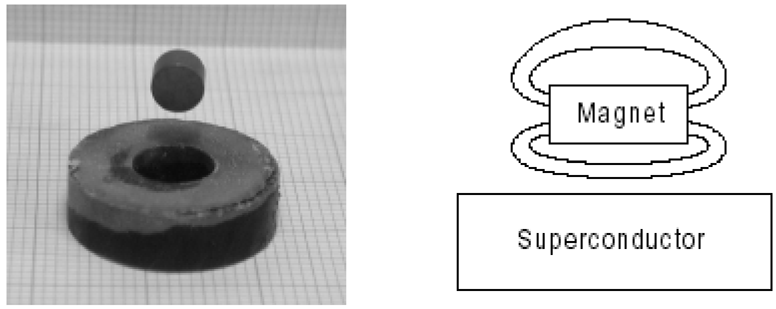

Figure 4: *A magnet levitating over a superconductor.*

if the magnetic moment of any given atom in the ferromagnet is deviated from its normal direction, a spin wave will propagate through the crystal. It is clear that the spin wave energy must be equal to the excitation energy of the crystal required to cause the change in the orientation of the atomic spin.

From the point of view of quantization of spin waves, a magnon is a collective excitation of electrons' spin structure in a crystal lattice. The concept of a magnon was introduced in 1930 by Felix Bloch in order to explain the reduction of the spontaneous magnetization in a ferromagnet. At absolute zero temperature, a ferromagnet reaches the state of lowest energy, in which all of the atomic spins or magnetic moments point in the same direction [6]. As the temperature increases, more and more spins deviate randomly from the common direction, thus increasing the internal energy and reducing the net magnetization. If one views the perfectly magnetized state at zero temperature of ferromagnet, the low temperature state with a view spins out of alignment can be viewed as a gas of quasi particles (electrons), in this case magnons. A brief outline of this thesis is as follows:

• Before we study the complex phenomena that is the coexistence of ferromagnetism and superconductivity in a compound $ZrZn$, we review some of the basic body theory of other work in chapter 1. In particular the phenomena of ferromagnetism, ferromagnetic curie temperature, and spin waves in ferromagnets are described in the first section of chapter 1. Further, in the second section of this chapter, we review the normal state, the ferromagnetic state, the superconducting state properties of our parameter $ZrZn_2$, and then we discuss the properties of other ferromagnetic superconductors.

• We also discuss an extended Hubbard model and Ginzburg-Landau theory for ferromagnetic superconductor in chapter 2.

• In chapter 3, first we derive the triplet equal spin pairing gap equation for the ferromgnetic superconductor $ZrZz_2$. Next using the simplified gap equation, we estimate the transition temperature of $ZrZn_2$ in different aspects. Further, we find out the phase diagram showing T_c and T_{sc} as a function of pressure in $ZrZn_2$.

• We draw our results and discussion in chapter 4.

• Finally, we deduce our results and suggest some direction for further work in chapter 5.

Chapter 1

Review Of Literature

The recent discovery of the coexistence of ferromagnetism and superconductivity in $ZrZn_2$ has led to renewed interest in the relation ship between ferromagnetism and superconductivity. In traditional type I superconductors, electron with opposite spins form cooper pairs with no net momentum or spin. Recall, this is also known as s-singlet superconductivity. This new ferromagnetic superconductivity-known as triplet superconductivity, occurs when electrons like spins join to form cooper pairs with a net one unit of spin. In this case the ferromagnetic spin fluctuations (spin waves) lead to spin triplet pairing [7].

Spin waves are low-lying collective excitations that occur in magnetic lattices with continuous symmetry, they are also called magnons [8]. Bloch introduced spin waves in order to explain the experimental observation that the magnetization of a ferro-magnet (a system which has a large number of atoms or electrons align their spins in the same directions) decreased when its temperature was raised from the absolute zero. This decrease arises from the fact that at higher temperature there will be some misalignment which will be caused by thermal activation, where as at zero degree kelvin the magnetic moment associated with each ion is oriented parallel to all other moments.

1.1 Spin Waves in Ferromagnets

Historically,the term ferromagnet was used for any material that would exhibit spontaneous magnetization: a net magnetic moment in the absence of an external magnetic field. This general definition still is use. The properties of ferromagnetism is due to the direct influence two effects from quantum mechanics: spin and Pauli exclusion principle. Moreover, only atoms with partially filled shells (e.g unpaired spins) can experience a net magnetic moment in the absence of an external magnetic field.

Ferromagnetic materials show ferromagnetic behavior only bellow a critical temperature called the curie temperature, above which the material has normal paramagnetic behavior. As the temperature of the ferromagnetic materials increase, the thermal exclusion of spin waves reduces a ferromagnet's spontaneous magnetism. In this section we shall review some important concepts of ferromagnetsm, curie temperature and spin waves.

1.1.1 Ferromagnetism

In the simplest type of magnetically ordered crystals i.e ferromagnets such as Fe, Ni, Co and Dy, the mean magnetic moments of all the atoms have the same orientation provided that the temperature of the ferromagnet does not exceed a critical value, i.e. the curie temperature. For this reason ferromagnets have spontaneous magnetic moments [9], that is non-zero macroscopic, even in the absence of an external magnetic field.

There are actually two sources of magnetization in metals [10]: localized magnetic moments and the "sea" of conduction electrons. Local magnetization occurs in rare-earth materials (such as gudolinium) and actinides (such as neptunium) due to the incomplete filling of electrons in the inner atomic shells. This leads to a well defined magnetic moments at every fixed atomic size, which in turn produces a long range magnetic coupling due to the exchange of conduction electrons. The second type magnetization arises from the magnetic moments of the conduction electrons themselves. In a metal electrons are itinerant, that is they are free to move from one atomic size to another, and they tend to align their magnetic moments in the direction of an applied field. This is also occurs in UGe_2, $URhGe_2$ and $ZrZn_2$.

At absolute zero temperature a ferromagnet reaches the state of lowest energy, in which all of the atomic spins point in the same directions. As the temperature increase, more and more spins deviate randomly from the common direction, thus increasing the internal energy and reducing the net magnetization. All the spins arrangements is plotted in Fig.(1.1).

1.1.2 Ferromagnetic Curie Temperature

The curie temperature T_c is the temperature below which there is the spontaneous magnetization M in the absence of an external applied magnetic field, and above which the material is paramagnetic (is the tendency of the atomic dipoles to align with an external magnetic field and they have non-spontaneous magnetic moments) [11]. In the disorder state, above the Curie temperature, thermal energy overrides any interaction between the local magnetic moments of ions. Below the curie temperature, these interaction are predominant and cause the local moments to order or align, so that there is a net spontaneous magnetization.

In ferromagnetic case, as the temperature T increases from absolute zero, the spontaneous magnetization decreases from M_0, its value at T=0 k [11]. The Curie temperature can be altered by changing composition, pressure, and other thermodynamic parameters. The curie temperature itself is a critical point, where the magnetic susceptibility is infinite and, although there is no net magnetization, domain like spin correlation at all length scales.

Materials	$T_c(k)$
$ZrZn_2$	28.5
UGe_2	52
URhGe	9.2
Fe	1043
Co	1388
Ni	627
Dy	85
$CrBr_3$	37
Gd	293

Table 1: the measured values of $T_c(k)$ for different compounds and elements

1.1.3 Spin Waves (Magnon) in Ferromagnets

The concept of spin waves (magnon) was introduced in 1930 by Felix Bloch [8,9,10] in order to explain the reduction of the spontaneous magnetization in a ferromagnet. At absolute zero temperature, a ferromagnet reaches a state of lowest energy, in which all of the atomic spin (magnetic moments) point in the same direction. As the temperature increases, more and more spins deviate randomly from their common directions, thus increase the internal energy and reducing the net magnetization. The spin deviation will not be static but it will travel through the lattice. Thus the spin deviation may be considered to be associated with all the ions in the crystal and it will form a collective excitation. These collective excitations, which are what we call spin waves, are the lowest type of magnetic excitation. If spin reversals are within the range of the exchange interaction, their over all energy is less than if they were apart. This gives rise to an attractive interaction for spin waves. On the other hand at low temperature, the magnons exchange excited in the ferromagent are mainly the long wave length magnons.

If we let all the spins share the reversal, as shown in the fig.(1.2), each spin is titled by the same angle and is processing at the same angular rate ω about the direction of the total magnetization of the system. The difference in direction of neighboring spins give the spin wave a characteristic wavelength λ [11], over which the spin direction changes by one cycle, and constitutes a departure from parallel spin alignment favored by the so-called exchange force between the spins. The elementary excitations of a spin system have a wave like form and are called magnons , which are boson modes of the spin lattice that correspond roughly to the phonon excitations of the nuclear lattice . A magnon can be viewed as a quantized spin waves and they carry a fixed amount of energy and lattice momentum.

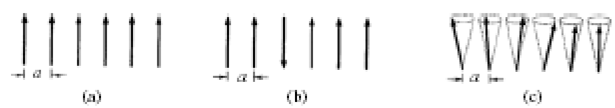

Figure 1.1: *Classical picture of the ground state of a simple ferromagnet; all spins are parallel. (b) A possible excitation; one spin is reversed. (c) The low-lying elementary excitations are spin waves. The ends of the spin vectors precess on the surfaces of cones, with successive spins advanced in phase by a constant angle [12] .*

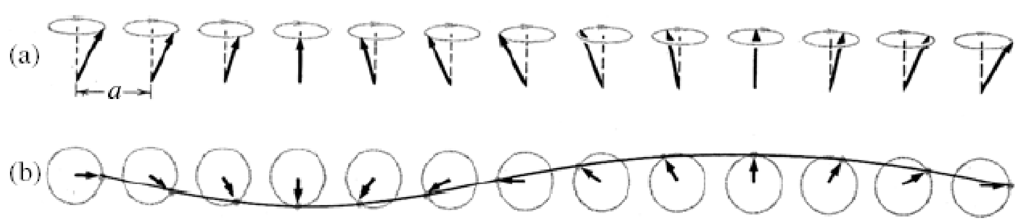

Figure 1.2: *A spin wave on a line of spins. (a) The spins viewed in perspective. (b) Spins viewed from above, showing one wavelength. The wave is drawn through the ends of the spin vectors [12].*

The energy of an elementary excitation caused with the spin wave can be obtained by multiplying its frequency $\omega(\overrightarrow{k})$ by $\hbar$, where $\overrightarrow{k}$ is a vector of spin wave. This energy is [8]:

$$\varepsilon(\overrightarrow{k}) = \hbar\omega(\overrightarrow{k}) \tag{1.1}$$

If the excitation energy $E(\overrightarrow{k})$ of the ferromagnet is small, it can be written as the sum of the energy of the individual spin waves propagating through it or, in other words, the sum of the magnon energy [8],

$$E(\overrightarrow{k}) = \sum_k \hbar\omega(\overrightarrow{k})n(\overrightarrow{k}) \tag{1.2}$$

were $n(\overrightarrow{k})$ is the number of magnons with a wave vector k, and the summation is evaluated over all k.

One important difference between phonons and magnons lies in their dispersion relation. The dispersion relation of phonon is to the first ordered linear in a wave vector k: $\omega(\overrightarrow{k})$= ck, where c is the velocity of sound. A ferro-magnon has a parabolic dispersion relation: $\omega = Ak^2$ [9], where A represents spin wave stiffness.

1.2 The Ferromagnetic Superconductor $ZrZn_2$

Very recently ferromagnetic superconductivity has been observed in $ZrZn_2$ [13,14]. The superconductivity is confined to the ferromagnetic phase. In this compound electrons with spins pointing in the same direction team up with each other to form pairing with one unit of spin, resulting in so called triplet superconductivity. In contrast, conventional superconductivity also known as s-wave singlet superconductivity which occurs when electrons with opposite spins bind together to form cooper pairs with zero momentum and spin. In this section we will review the properties of normal state, the ferromagnetic state and the superconducting state of $ZrZn_2$. Further we include other ferromagnetic superconductors.

1.2.1 The Normal State Properties of $ZrZn_2$

As noted by authors [15], the compound $ZrZn_2$ was first investigated by Matthias and Bozorth in the 1950_s, who discovered that it was ferromagnetic despite being made from nonmagnetic, superconducting constituents (Zr and Zn). $ZrZn_2$ occurs in a C15 cubic Laves crystal structure [15,16,] shown in fig.(1.3), with a lattice constant $a = 7.393A^o$ [17]. From fig.(1.3), the Zr atoms are represented by larger spheres while the Zn atoms are denoted by smaller spheres. In the compound $ZrZn_2$, the Zr atoms form a tetrahedrally coordinated diamond structure [15], and the Zn forms a net work of corner-sharing tetrahedra. As noted by the authors of [14,18], each Zr is surrounded by 12 Zn neighbors, forming a truncated tetrahedron at a distance (at T = 50k) 5.745 a.u and 4 Zr at 6.001a.u. The latter approximately corresponds to the bond length in Zr metal. Since the metallic radius of Zn is 16 percent smaller than that of Zr, Zr and Zn do not form strong bonds [14]. On the other hand, Zr, unlike carbon, does not form highly directional bond. So 4 Zr-Zr bonds in $ZrZn_2$ do not provide strong bonding either. This makes Zr "rattling" rather soft. At the same time, Zn has 8 neighbors at a distance 4.9 a.u, noticeably less than in Zn metal. Correspondingly, one expect that Zn bond-stretching vibrations should be relatively hard.

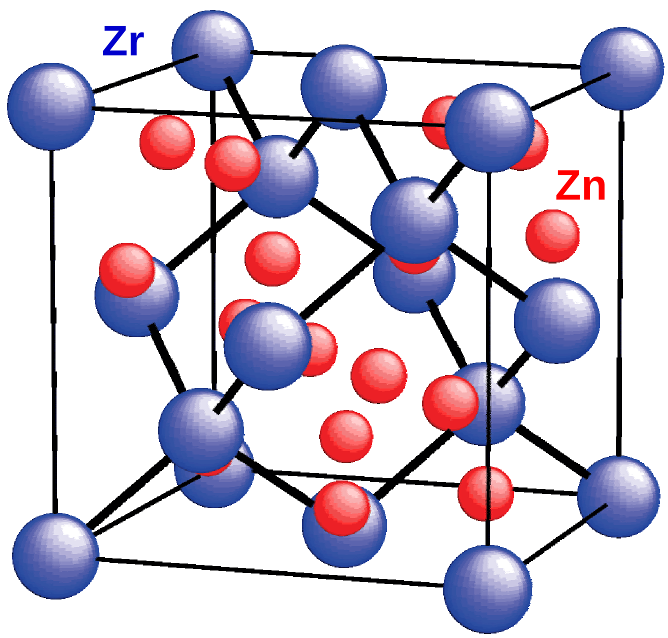

Figure 1.3: *The C15 structure of $ZrZn_2$ from reference [19].*

In [18],the authors showed that the density of states at the fermi level is dominated by the Zr atoms with the contribution density of state due to the Zn atoms being about 0.6Ry below the fermi level [17]. However, the presence of the Zn does substantially alter the density of states as they play the role of empty spheres which changes the crystal structure of the Zr. In fact, the density of states in the region of the fermi level calculated for Zr in a diamond structure with the appropriate lattice spacing for

$ZrZn_2$ is remarkably similar to that of $ZrZn_2$ itself.

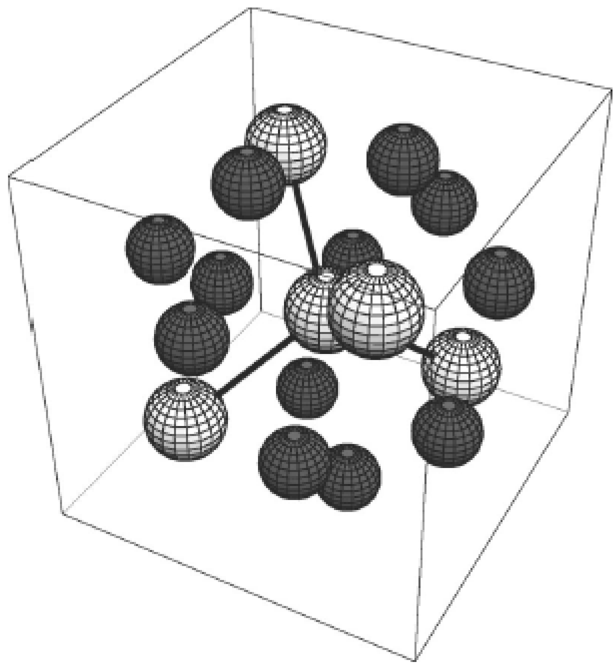

Figure 1.4: *A local invironment of a Zr atom in the C15 cubic laves structures, Zr atoms:large spheres, Zn atoms:small dark spheres[18] .*

In the normal state, at ambient pressure, resistivity of $ZrZn_2$ shows a T^2 temperature dependence. However, under pressure, but still in the normal state, this power law changes [20] to $T^{1.6}$ near P_c which has been attributed to the influence of spin waves.

1.2.2 The Ferromagnetic Properties of $ZrZn_2$

In [14,15], the authors showed that the two components of $ZrZn_2$ are non-magnetic. Its magnetic property is driven from Zr 4d orbitals, which have a significant direct overlap. and in this state ferromagnetism develops below the curie temperature $T_{sc} = 28.5k$ [21]. $ZrZn_2$ is a prototypical example of a weak itinerant (stoner) ferromagnet [6] or it is strongly unsaturated compound. This is due to very small magnetic moments (values from $0.17\mu_B$) [21,22] have been reported. These do not saturate even at magnetic field up to 35T [14], indicating softness of the magnetic moment amplitude and suggesting existence of soft longitudinal spin fluctuations. In contrast, strong ferromagnets such as Fe and Ni show a negligible increase of the ordered moment with field after a single domain is found. The unsaturated behavior of $ZrZn_2$ indicates a large longitudinal spin fluctuations. Further evidence for the existence of strong spin fluctuations in $ZrZn_2$ is provided by the remarkably large effective mass of its quasi particles. The most remarkable magnetic property of $ZrZn_2$ is the effect of

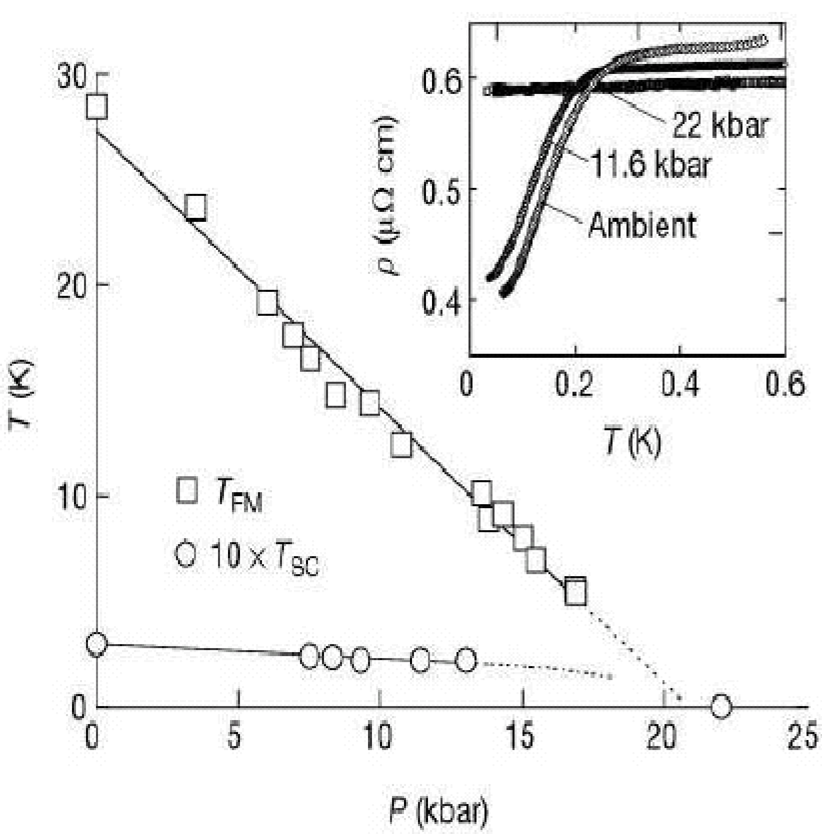

Figure 1.5: *The temperature pressure phase diagram of* $ZrZn_2$ *taken from [15].*

a magnetic field on the ordered momentum Fig. (1.6) show the magnetization of $ZrZn_2$ as a function of magnetic field. At T = 1.75 K a relatively small field $\mu_o H = 0.05T$ is required to form a single ferromagnetic domain. On further increasing the field, the ordered moment is rapidly increased with a field of 6T causing a 50 percent increase in the ordered momentum, which is unsaturated up to 35 T, the highest field measured. This behavior contrasts strongly with the elemental ferromagnets Fe, Ni, and Co, in which, after a single domain is formed, field applied parallel to the easy axis have only a small effect on their ordered momentum.

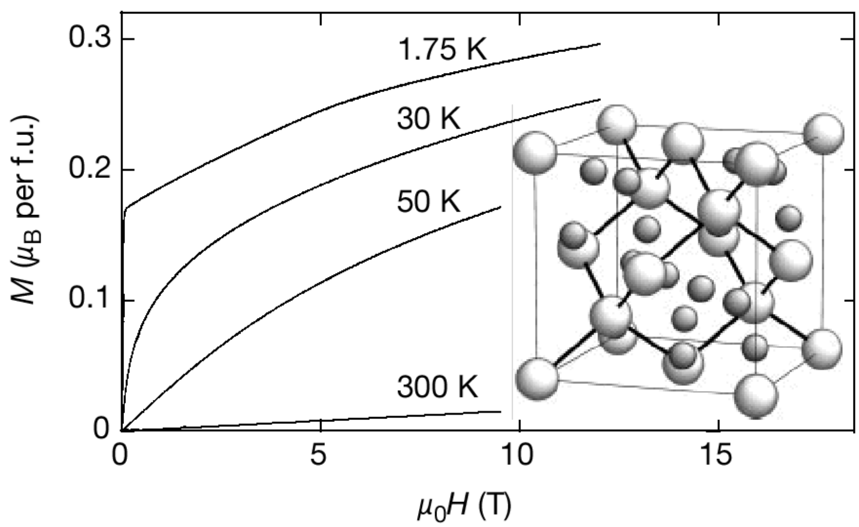

Figure 1.6: *magnetization curve of $ZrZn_2$ taken from [15].*

At ambient pressure $ZrZn_2$ is a ferromagnet with curie temperature of 28.5 K [14]. This temperature drops approximately linearly with pressure, starting at P=0 and decreasing to 4K at P=16 K bar up to 20K bar [7], see fig.(1.5). This effect shows that the ferromagnetism $ZrZn_2$ is extremely sensitive to pressure. Recent experiments on the samples studied here have shown that the pressure of P_c= 16.5 K bar causes the ferromagnetism to disappear with a first order transition.

1.2.3 The Properties of $ZrZn_2$ in its Superconducting State

$ZrZn_2$ is a weak ferromagnet whose superconductivity was previously unknown. When theorists began to investigate magnetically induced pairing in the 1960s and 1970s, $ZrZn_2$ looked like an ideal system in which to hunt for the phenomenon.

Recently, the observation of superconductivity in $ZrZn_2$ has renewed the interest on the coexistence of ferromagnetism and superconductivity to occur [23]. One needs both some sorts of attraction between quasi particles [24], which can be provided by magnetic fluctuation and low temperature. Since the magnetic fluctuation become large near continuous magnetic phase transition, ideal candidates for this phenomenon would seem to be itinerant ferromagnets with a low curie temperature. The combined requirements of low temperatures, high purity, and vicinity to a continuous ferromagnetic transition severely restricts the number of materials where ferromagnetically induced superconductivity might be observed.

The coexistence of ferromagnetism and superconductivity are believed to be caused by itinerant electrons in the same 4d electrons in the same band [15,16]. Since superconductivity in the presence of ferromagnetism is likely to be of spin triplet type, magnetic-fluctuation induced pairing is the possible mechanism. However, two aspects of the experiments are not reconcilable with previous theories of superconductivity in ferromagnets. First the magnetization is observed to be of the first order , so that there are no divergent fluctuations as the transition is approached. Second, the superconducting state is found only on the ferromagnetic side of the phase boundary.

Some authors and collaborators have shown that the critical temperature for $ZrZn_2$ superconductivity mediated by spin fluctuation is generally much higher in Heisenberg ferromagnetic phase than in paramagnetic one, due to the coupling of the magnons to the longitudinal magnetic susceptibility. In addition the superconducting critical temperature of $ZrZn_2$ at ambient pressure is $T_{sc} = 0.29k$ [25].

The exchange of spin fluctuation can lead to an effective four fermion theory. It describes the interaction of the components of spin 1 composite fields $(|\uparrow\uparrow\rangle, \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle)$ which have a projection of spin 1,0 and -1 respectively [23], and the interaction of the spin singlet composite fields $\frac{1}{\sqrt{2}}|\uparrow\downarrow - \downarrow\uparrow\rangle$. This appropriate linear combinations can be tabulated as follows [2]:

States	S	S_z
$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$	0	0
$|\uparrow\uparrow\rangle$	1	1
$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$	1	0
$|\downarrow\downarrow\rangle$	1	-1

Note that from the above table the one state with S = 0 (known as the singlet state) changes sign when the spins of the two electrons are interchanged, while the three states with S = 1 (known as the triplet states)

In [15], the authors noted that the superconductivity in $ZrZn_2$ has a number of remarkable feature.

•This type of superconductivity is very sensitive to non magnetic disorder, so that very clean samples are also required. Unconventional or non-s- wave forms of superconductivity generally require the superconducting coherence length $\xi = 290A^o$ to be some what smaller than the electronic mean free path l_o [15]. Thus in view of its sensitivity in $ZrZn_2$ to the quality of the sample, the superconductivity in $ZrZn_2$ is likely to be unconventional.

• There is no superconducting anomaly in specific heat. If we interpret this literally, it meas that the superconducting state strongly gapless with large portion of the fermi surface, or even all of it surviving in superconducting state. The zero field superconducting transition in $ZrZn_2$ is fundamentally difference to that in a conventional superconductor, because it occurs in the presence of ferromagnetism.

•The superconductivity in $ZrZn_2$ observed only within the ferromagnetic phase.

The superconductivity nature of $ZrZn_2$ has not yet been studied widely. This is due to superconductivity in $ZrZn_2$ is easily destroyed by disorder. Very little is known about its superconducting state. Indeed to the best of our knowledge only two groups have reported the observation of superconductivity in $ZrZn_2$. Only Pfleiderer et al have studied the dependence of the superconducting critical temperature (T_{sc}) on pressure (see fig.(1.5)). They found that the transition temperature did not superconductor (they were able to go as cold as 15mk) for P=22K bar$>P_c$. However, they did not report any result for pressure in the range 18kbar $<$ P<22kbar. It is also noted that the resistivity of $ZrZn_2$ did not fall all the way to zero. Although, a drop of $>$ 35 percent was observed, see fig. (1.5). This must call into doubt the quality of the sample.

A magnetic field destroys singlet superconductivity by the orbital effect or the paramagnetic effect. The orbital effect is a manifestation of the Lorentz forces since the electrons have opposite momenta, these forces act in opposite directions, pulling them apart. The paramagnetic effect occurs when the applied field attempts to align the spins of both electrons along the magnetic field. However, the paramagnetic effect does not destroy triplet superconductivity because the pairs already have their spins aligned. This means that only the orbital effect can destroy triplet superconductivity.

1.2.4 Other Ferromagnetic Superconductors

We now focus on systems in which the same electrons are simultaneously involved in both superconductivity and magnetism, other than $ZrZn_2$ only two examples which are currently known, they are uranium germanium (UGe_2) and uranium rhodium germanium (URhGe).

Very recently ferromagnet superconductivity has been also observed in UGe_2 and URhGe [25,27]. The superconductivity and the ferromagnetism are believed to arise due to the same band electrons similar to $ZrZn_2$. However, in UGe_2, and $URhGe$, the 5f electrons of U atoms both superconductivity and ferromgnetic order [28,29].

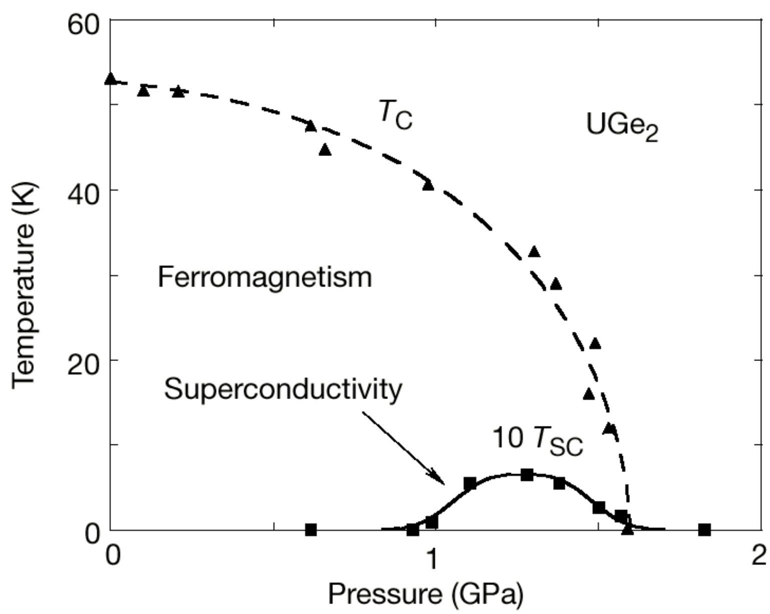

Figure 1.7: *The phase diagram of UGe_2 taken from [30].*

The phase diagram of UGe_2 as shown in fig.(1.7) is dissimilar to that of $ZrZn_2$. UGe_2 is a ferromagnt with a curie temperature of 54K at ambient pressure. With applied pressure the curie temperature decreases not linear as in $ZrZn_2$. Ferromagnetism is not observed above the critical pressure of 16 K bar. On the other hand, superconductivity is not observed at ambient pressure in UGe_2, but it appears at 10K bar which is dissimilar to $ZrZn_2$. As a function of pressure, the superconducting critical temperature rises to a maximum at 12K bar and then falls to zero again at approximately the critical pressure.

At ambient pressure URhGe is a ferromagnet with a curie temperature of 9.5 K and superconductor at superconducting temperature of 0.25 K [25]. It has many similar properties to the high pressure UGe_2.

In summary, the various experimental quantities of these three important materials is shown below;

	$T_c(k)$	$T_{sc}(k)$	$P_c(kbar)$	$\Delta C/C$	$H_{c_2}(T)$	$\xi(A^0)$	$M(\mu_B/f.u$
$Zrzn_2$	28.5	0.29	21	-	0.4	290	0.17
UGe_2	53	0.8	17	0.2-0.3	1.9	130	1.4
$URhGe$	9.5	0.25	-	0.3-0.4	0.71	180	0.42

table 2; Comparison of 3 superconducting ferromagnets , from [28].

Chapter 2

Mathematical Techniques

In this chapter we will review an extended Hubbard model which is used for our further study in order to calculate the linearized gap equation of triplet equal spin pairing state and the general Ginzburg-Landau (LG) free energy function to investigate the ferromagnetic and the superconducting phase in a ferromagnetic superconductor $ZrZn_2$.

2.1 Hubbard Model

In 1963 Hubbard in a series of papers developed a model for electron correlations in narrow energy bands. Although Gutzwiller and Kanamori considered similar models at about the same time, this paradigm of condensed matter physics is universally known as the Hubbard model. In his original paper Hubbard postulates a Hamiltonian for the electrons in a band and then, by introducing the Wannier functions, derives his Hamiltonian. However, from the perspective of tight binding theory which is the perspective we predominantly take in this thesis the correct thing to do is to postulate the Hubbard Hamiltonian and proceed from there. We will therefore take the later approach. Within the tight binding approximation it is natural to consider a lattice of 'sites'. Each site represents a single orbital of a single atom which can accommodate, at most, two electrons (one of each spin.)

The canonical one band Hubbard Hamiltonian is [31];

$$\hat{H} = -\sum_{ij\sigma} t_{ij}\hat{C}^{+}_{i\sigma}\hat{C}_{j\sigma} + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{2.1}$$

In (2.5), the first term (the kinetic term) therefore hops fermions from one lattice site i to another site j with a matrix element t_{ij}, and the second term is a product fermionic number operators of opposite spins, and hence this term is zero when there is zero or one fermion on a site, and gives an energy penalty U for having two fermions on the same site [31]. The particle number operator, $\hat{n}_{i\sigma} = \hat{C}^{+}_{i\sigma}\hat{C}_{i\sigma}$, counts the number of electrons with spin σ on site i, and clearly only take the values 0 or 1.

From eq. (2.1), $\hat{C}^{+}_{i}$ increases the number of particles, $\hat{n}_{i}$, in the state by one, $\hat{C}^{+}_{i}$ is therefore known as a creation operator. Similarly $\hat{C}_{i}$ decreases, $\hat{n}_{i}$, by one and is therefore known as an annihilation operator. To fully specify their commutation relations. For fermions, the anti commutation relations are;

$$\{\hat{C}_i, \hat{C}^{+}_j\} = \hat{C}_i\hat{C}^{+}_j + \hat{C}^{+}_j\hat{C}_i = \delta_{ij} \tag{2.2}$$

$$\{\hat{C}^{+}_i, \hat{C}^{+}_j\} = \hat{C}^{+}_i\hat{C}^{+}_j + \hat{C}^{+}_j\hat{C}^{+}_i = 0 \tag{2.3}$$

$$\{\hat{C}_i, \hat{C}_j\} = \hat{C}_i\hat{C}_j + \hat{C}_j\hat{C}_i = 0 \tag{2.4}$$

To derive the Hartree- Fork approximation, we can write the interaction term of Hubbard Hamiltonian (2.1) in terms of the mean values of number operators as [31]:

$$\begin{aligned}\hat{H}_{int} &= U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\\ &= U\sum_i(\hat{C}^{+}_{i\uparrow}\hat{C}_{i\uparrow}\hat{C}^{+}_{i\downarrow}\hat{C}_{i\downarrow})\\ &= U\sum_i\{(\hat{C}^{+}_{i\uparrow}\hat{C}_{i\uparrow} - <\hat{C}^{+}_{i\uparrow}\hat{C}_{i\uparrow}> + <\hat{C}^{+}_{i\uparrow}\hat{C}_{i\uparrow}>)(\hat{C}^{+}_{i\downarrow}\hat{C}_{i\downarrow} - <\hat{C}^{+}_{i\downarrow}\hat{C}_{i\downarrow}> + <\hat{C}^{+}_{i\downarrow}\hat{C}_{i\downarrow}>)\}\end{aligned} \tag{2.5}$$

clearly, $<\hat{C}^{+}_{\sigma}\hat{C}_{\sigma}>$ is the mean of $\hat{n}_{i\sigma}$ and the fluctuations about the mean are given by $\hat{C}^+_{i\sigma}\hat{C}_{i\sigma} - < \hat{C}^+_{i\sigma}\hat{C}_{i\sigma} >$. Thus we find that,

$$\hat{H}_{int} = U\sum_i \{(\hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} - < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} >)(\hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} - < \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} >) + (\hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} - < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} >) < \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} >$$

$$+ < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} > (\hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} - < \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} >) + < C^+_{i\uparrow}\hat{C}_{i\uparrow} >< \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} >\} \quad (2.6)$$

So the first order in fluctuation, we have;

$$\hat{H}_{int} = U\sum_i \{(\hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} - < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} >) < \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} > + < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} > (\hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} - < \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} >)$$

$$+ < C^+_{i\uparrow}\hat{C}_{i\uparrow} >< \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} >\}$$

$$= U\sum_i \{< \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} > \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} + < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} > \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} - < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} >< \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} >\} \quad (2.7)$$

Ignoring the last term of the right side of equation (the constant term) (2.7), one can get the Hartree - Fork approximation;

$$\hat{H}_{int} = U\sum_i \{< \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} > \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} + < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} > \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow}\} \quad (2.8)$$

Therefore, eq. (2.1) is approximated by;

$$\hat{H} = -\sum_{ij\sigma} t_{ij}\hat{C}^+_{i\sigma}\hat{C}_{j\sigma} + U\sum_i \{< \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} > \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} + < \hat{C}^+_{i\uparrow}\hat{C}_{i\uparrow} > \hat{C}^+_{i\downarrow}\hat{C}_{i\downarrow} \quad (2.9)$$

As the Hamiltonian is an operator, we can of course write the Hamiltonian interims of the field operatures. For example, the single particle Hamiltonian, $\hat{H}_o$, is given by;

$$\hat{H}_o = \sum_\sigma \int d^3r\psi^+_\sigma(r)(\frac{-\hbar^2}{2m}\nabla^2 + V(r))\psi_\sigma(r) \quad (2.10)$$

where $\psi^+_\sigma(r)$ and $\psi_\sigma(r)$ are the field operators which are defined as :

$$\psi^+_\sigma(r) = \sum_\lambda \hat{C}^+_\lambda\phi^*_\lambda(r) \quad (2.11)$$

and

$$\psi_\sigma(r) = \sum_\lambda \hat{C}_\lambda\phi_\lambda(r) \quad (2.12)$$

Here $\phi_\sigma(r)$ is the wave function of a particle in state λ at position r, $\psi^+_\sigma(r)$ therefore creates a particle with spin σ at position r and $\psi_\sigma(r)$ annihilates a particle with spin σ at position r.

substituting (2.11) and (2.12) in to (2.10), we can find that;

$$\hat{H}_o = \sum_{k\sigma} \int d^3r \hat{C}^+_{k\sigma} \phi^*_{k\sigma}(r)(\frac{-\hbar^2}{2m}\nabla^2 + V(r))\phi_{k\sigma}(r)\hat{C}_{k\sigma} \tag{2.13}$$

Where we have identified k and σ as the state labels λ. Recall $\phi_{k\sigma}(r)$ is the solution of a single particle;

$$(\frac{-\hbar^2}{2m}\nabla^2 + V(r))\phi_{k\sigma}(r) = \varepsilon_{k\sigma}\phi_{k\sigma}(r) \tag{2.14}$$

Substituting this in to (2.3), we get that;

$$\hat{H}_o = \sum_{k\sigma} \varepsilon_{k\sigma}\hat{C}^+_{k\sigma}\hat{C}_{k\sigma} \tag{2.15}$$

We now introduce the lattice Fourier transformations

$$\hat{C}_{i\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{ik.R_i}\hat{C}_{k\sigma} \tag{2.16}$$

$$\hat{C}^+_{i\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{-ik.R_j}\hat{C}^+_{k\sigma} \tag{2.17}$$

Substituting these in to (2.15), we find that;

$$\hat{H}_o = \sum_{ij\sigma} t_{ij}\hat{C}^+_{i\sigma}\hat{C}_{j\sigma} \tag{2.18}$$

Where the hopping t_{ij}, must clearly be Fourier transformation of the state of energy, $\varepsilon_{k\sigma}$. Thus

$$\varepsilon_{k\sigma} = \sum_{ij} t_{ij}e^{ik.(R_i-R_j)} \tag{2.19}$$

We will now use the Hubbard model to study superconductivity. In real materials, interactions are not only on site. We can take account of this by introducing inter-site interaction constants, $U_{ij\sigma\sigma'}$, which will in general depend on the spin of the two electrons. These new interaction constants still describe two body interactions, so our generalized Hubbard Hamiltonian is

$$\hat{H} = -\sum_{ij\sigma} t_{ij} C^{+}_{i\sigma} C_{j\sigma} + \frac{1}{2} \sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'} \tag{2.20}$$

Where $C^{+}_{i\sigma}(C_{j\sigma})$ is the creation (annihilation) operators of electrons, the number operators $\hat{n}_{i\sigma} = C^{+}_{i\sigma} C_{i\sigma}$ and $\hat{n}_{j\sigma'} = C^{+}_{j\sigma'} C_{j\sigma'}$ and t_{ij} denotes the hopping integral.

It is simple to see that on site potentials (in eqn.(2.1)) cannot give triplet superconductivity. As only one electron of each spin can occupy each site the equal spin pairing (ESP) states will clearly not arise from on site potentials. However, one can see that no triplet states can arise from an on site potential as all triplet states must have odd parity and on site potentials cannot give a k dependent order parameter, which means that the order parameter is, trivially, even.

In general two new terms are introduced into the Schrodinger equation by a magnetic field: the minimal coupling term ($\hat{P} = -i\hbar\nabla \mapsto -i\hbar\nabla - \frac{e}{c}A$) and the Zeeman term ($\frac{1}{2}\mu_B \sigma H$). The vector potential enters via minimal coupling and thus only affects the kinetic minimal coupling and thus only effects the kinetic energy terms, t_{ij}. It can be shown [27,30,32] that in a magnetic field

$$t_{ij} \mapsto t_{ij} exp[\frac{-ie}{\hbar} \int_{R_i}^{R_j} A(r).dr] = t_{ij} e^{-iA_{ij}}$$

Thus the Hamiltonian for the Hubbard model generalized to include n^{th} nearest neighbor interactions in the presence of a magnetic field is

$$\hat{H} = -\sum_{ij\sigma} t_{ij} e^{-iA_{ij}} C^{+}_{i\sigma} C_{j\sigma} + \frac{1}{2} \sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'} + \mu_B \sum_{i\sigma\sigma'} C^{+}_{i\sigma} C_{i\sigma} (\sigma_{\sigma\sigma'}.H)$$

where the $\sigma_{\sigma\sigma'}$ are the components of the vector of Pauli matrices

$$\sigma = (\sigma_1, \sigma_2, \sigma_3)$$

The differences between singlet and triplet superconductors are caused by the spin of the Cooper pairs. Thus, the most interesting new physics observed in a triplet superconductor is likely to be due to the interaction of the Cooper pairs with a magnetic field via the Zeeman term. For weak Stoner ferromagnet $ZrZn_2$, the Zeeman term is likely to be the dominant interaction between ferromagnetism and superconductivity.

Neglecting the effect of the vector potential our Hamiltonian becomes

$$\hat{H} = -\sum_{ij\sigma} t_{ij} C^{+}_{i\sigma} C_{j\sigma} + \frac{1}{2} \sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'} + \mu_B \sum_{i\sigma\sigma'} C^{+}_{i\sigma} C_{i\sigma} (\sigma_{\sigma\sigma'}.H) \tag{2.21}$$

2.2 Ginzburg-Landau Theory

The Ginzburg-Landau (GL) theory [33,34] is based on Landau theory of second order phase transitions developed in 1937. This was a natural starting point, since in the absence of a magnetic field the transition into the superconducting state at a critical temperature T_{sc} is a second-order phase transition. Landau theory describes the transition from a disordered to an ordered state in terms of an order parameter, which is zero in the disordered phase and nonzero in the ordered phase.

In the Landau approach, the free energy of the low temperature phase can be written as a power series in the order parameter η:

$$F(\eta) = F_o + \frac{1}{2}\alpha(T)\eta^2 + \frac{1}{4}\beta\eta^4 + ... \tag{2.22}$$

where the parameters $\alpha(T)$ and β are Landau coefficients, and F_o is the free energy of the system for $\eta = 0$. Usually $F(\eta)$ is independent of the sign of η and therefore only contains terms with even powers of η. There are some cases, however, when $F(\eta) \neq F(-\eta)$, and then terms with odd powers of η must be included in (2.22). Eq. (2.22) represents an expansion of the free energy about a maximum value in the low temperature phase and is therefore expected to be valid only for small values of η, i.e., only close to the phase transition. According to Landau theory at high temperature $(T > T_c)$ there is a single minimum at $\eta = 0$. At low temperature $(T << T_c)$ the free energy has a maximum at $\eta = 0$ and minima at non-zero values of $\eta = \pm\eta_o$.

For the free energy of (2.22) to represent a phase transition, it is necessary that the value of α changes sign at the transition temperature. So that it is positive for temperature above the transition T_c and negative below. The simplest implementation of this condition is to assume that $\alpha = \alpha_o(T - T_c)$. It is also assume that we only need to consider the smallest number of terms in the expansion, so that we can write eq.

(2.22) as

$$F(\eta) = F_0 + \frac{1}{2}\alpha_o(T - T_c)\eta^2 + \frac{1}{4}\beta\eta^4 \tag{2.23}$$

where α_o and β are positive constants. The equilibrium condition $\frac{\partial F(\eta)}{\partial \eta} = 0$ applied to (2.23) leads to the prediction that $\eta = 0$ for $T > T_c$, that there is a continues (second order) phase transition at $T = T_c$, and that at lower temperature η is non-zero and has the temperature dependence:

$$\eta = \{\frac{\alpha_o(T_c - T)}{\beta}\}^{\frac{1}{2}} \tag{2.24}$$

In the theory of ferromagnetism, for example, the order parameter is the spontaneous magnetization (M).

On the other hand Ginzburg - Landau (GL) based on three fundamental assumptions:

1. There exist an order parameter ψ, which goes to zero at the transition.
2. The free energy may be expanded in powers of ψ.
3. The coefficients are regular functions of T.

The strength of superconductivity state can be described by an order parameter ψ which may be spatially varying. In the normal state ψ is zero. Then they assumed that near T_{sc} , the superconductivity is weak and ψ is small, the free energy of a superconductror can be expressed as a sum of a series of terms in increasing powers of $|\psi|^2$. Thus, free energy functional for superconductiving state at finite temperature in the presence of external field is given by

$$f_s = f_n + f_g + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + ... + \frac{H^2}{8\pi} \tag{2.25}$$

where f_n is the free energy of the normal state($\psi = 0$) , and f_g is the gradient term which can be expressed by;

$$f_g = \frac{1}{2m^*}|(-ih\nabla - \frac{e^*A}{c})\psi|^2 \tag{2.26}$$

and a stable superconducting state is obtained if β is a psitive constant and $\alpha = \alpha_o(T - T_s)$. From the gradiant term, H is the external magnetic field, c is the speed of light, A is the vector potentional, and $m^* = 2m_e$ and $e^* = 2e$.

In GL theory the absolute value is used here because ψ is allowed to a complex number with an amplitude ψ_o and a phase ϕ, $\psi = \psi_o e^{i\phi}$

Neglecting higher powers (by taking the fourth order of free energy) the total free energy for both superconductor and the magnetic field is given by;

$$F = \int d^3 r f_s \tag{2.27}$$

sustituting (2.25) in to (2.27), we find that

$$F = f_n + \int \frac{\hbar^2}{2m^*} |(\frac{\nabla}{i} - \frac{2e^*}{c} A)\psi(r)|^2 + \alpha|\psi(r)|^2 + \frac{\beta}{2}|\psi(r)|^4 + \frac{H^2}{8\pi})d^3 r \tag{2.28}$$

The condition for the minimum free energy state is again found by performing a final differentiation to minimize with respect to $\psi(r)$, upon doing so, one obtains the GL differential equations;

$$\frac{1}{2m*}(-i\hbar\nabla - \frac{2e^*}{c} A)^2 \psi + \alpha\psi + \beta|\psi|^2\psi = 0 \tag{2.29}$$

This leaves two coupled non-linear differential equations from which to determine $\psi(r)$.

Chapter 3

Formulation Of The Problem

In this chapter we first use our one Hubbard model (derived in chapter 2) to the ferromagnetic superconductor $ZrZn_2$. We then derive the gap equations for triplet equal spin pairing state in the presence of exchange splitting from our microscopic Hamiltonian. We further estimate the superconducting transition temperature of $ZrZn_2$ in different aspects. Then we use the Generalized-Landau (GL) theory to investigate the phase diagram showing the ferromagnetic (T_f) and superconducting (T_{sc}) transition temperature of $ZrZn_2$.

3.1 The Gap Equation for Ferromagnetic Superconductor

We consider superconductivity arising in one band Hubbard model with an effective, pairwise, nearest interaction $U_{ij\sigma\sigma'}$, acting between electrons at crystal sites, i,j with spins $\sigma = \pm 1$. Further, we derive the equal spin pairing gap equation for a ferromagnetic superconductor, which we study for $ZrZn_2$.

The complete hamiltonian for Hubbard model is given by:

$$\hat{H} = \hat{H}_o + \hat{H}_I + \hat{H}_z \tag{3.1}$$

Here

$$\hat{H}_0 = -\sum_{ij\sigma} t_{ij} \hat{C}^{+}_{i\sigma} \hat{C}_{j\sigma} \tag{3.2}$$

is the Hamiltonian of free or non-interacting electrons, $\hat{C}^{+}_{i\sigma}$ and $\hat{C}_{j\sigma}$ are the usual creation and annihilation operators for electrons on sites i and j respectively, t_{ij} is the hopping integral. $\varepsilon(k)$ the band energy. Moreover;

$$\hat{H}_I = \frac{1}{2}\sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'}\hat{n}_{i\sigma}\hat{n}_{j\sigma'} \tag{3.3}$$

is the interaction term of Hubbard Hamiltonian, the number operators $\hat{n}_{i\sigma} = \hat{C}^{+}_{i\sigma}\hat{C}_{i\sigma}$ and $\hat{n}_{j\sigma'} = \hat{C}^{+}_{j\sigma'}\hat{C}_{j\sigma'}$, and the factor of 1/2 to take ease of a double counting . Next:

$$\hat{H}_z = \sum_{i\sigma\sigma'} \hat{C}^{+}_{i\sigma}\hat{C}_{i\sigma}(\sigma_{\sigma\sigma'}.V_C) \tag{3.4}$$

is the Hamiltonian of Zeeman splitting with σ denotes the component of the vector of Pauli matrices and V_c the Zeeman splitting term.

Substituting equations (3.2), (3.3) and (3.4) into (3.1), we get:

$$\hat{H} = -\sum_{ij\sigma} t_{ij}\hat{C}^{+}_{i\sigma}\hat{C}_{j\sigma} + \frac{1}{2}\sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'}\hat{n}_{i\sigma}\hat{n}_{j\sigma'} + \sum_{i\sigma\sigma'} \hat{C}^{+}_{i\sigma}\hat{C}_{i\sigma}(\sigma_{\sigma\sigma'}.V_c) \tag{3.5}$$

we can modefy this Hamiltonian using Hartree- Fork approximation as:

$$\begin{aligned}
\hat{H}_I &= \sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'} n_{i\sigma} n_{j\sigma'} \\
&= \sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'} C^{+}_{i\sigma} C_{i\sigma} C^{+}_{j\sigma'} C_{j\sigma'} \\
&= -\sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'} C^{+}_{i\sigma} C^{+}_{j\sigma'} C_{i\sigma} C_{j\sigma'} \\
&= -\sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'} (C^{+}_{i\sigma} C^{+}_{j\sigma'} + < C^{+}_{i\sigma} C^{+}_{j\sigma'} > - < C^{+}_{i\sigma} C^{+}_{j\sigma'} >) \times \\
&(C_{i\sigma} C_{j\sigma'} + < C_{i\sigma} C_{j\sigma'} > - < C_{i\sigma} C_{j\sigma'} >)
\end{aligned} \tag{3.6}$$

So, the first order in the fluctuation we have:

$$\hat{H}_I = -\sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'}\{-(C^+_{i\sigma}C^+_{j\sigma'} + < C^+_{i\sigma}C^+_{j\sigma'} >) < C_{i\sigma}C_{j\sigma'} > - < C^+_{i\sigma}C^+_{j\sigma'} > (C_{i\sigma}C_{j\sigma'} + < C_{i\sigma}C_{j\sigma'} >)$$
$$+ < C^+_{i\sigma}C^+_{j\sigma'} >< C_{i\sigma}C_{j\sigma'} >\}$$
$$= \sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'}\{< C_{i\sigma}C_{j\sigma'} > C^+_{i\sigma}C^+_{j\sigma'} + < C^+_{i\sigma}C^+_{j\sigma'} > C_{i\sigma}C_{j\sigma'} + < C^+_{i\sigma}C^+_{j\sigma'} >< C_{i\sigma}C_{j\sigma'} >\} \tag{3.7}$$

Trasforming away the last term of right hand side of (3.6) which is a constant, we have:

$$\hat{H}_I = \sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'}\{< C_{i\sigma}C_{j\sigma'} > C^+_{i\sigma}C^+_{j\sigma'} + < C^+_{i\sigma}C^+_{j\sigma'} > C_{i\sigma}C_{j\sigma'}\} \tag{3.8}$$

Substituting (3.8) into (3.5), we get:

$$\hat{H} = -\sum_{ij\sigma} t_{ij}C^+_{i\sigma}C_{j\sigma} + \frac{1}{2}\sum_{ij\sigma\sigma'} U_{ij\sigma\sigma'}\{< C_{i\sigma}C_{j\sigma'} > C^+_{i\sigma}C^+_{j\sigma'} + < C^+_{i\sigma}C^+_{j\sigma'} > C_{i\sigma}C_{j\sigma'}\}$$
$$+ \sum_{i\sigma\sigma'} C^+_{i\sigma}C_{i\sigma}(\sigma_{\sigma\sigma'}.V_c) \tag{3.9}$$

Using the Hartree-Fork-Gorkov approximation, such that;

$$\Delta_{ij\sigma\sigma'} = -U_{ij\sigma\sigma'} < C_{i\sigma}C_{j\sigma'} > \tag{3.10}$$

$$\Delta^+_{ij\sigma\sigma'} = -U_{ij\sigma\sigma'} < C^+_{j\sigma'}C^+_{i\sigma} > \tag{3.11}$$

We express (3.9) as a form:

$$\hat{H} = -\sum_{ij\sigma} t_{ij}C^+_{i\sigma}C_{j\sigma} + \frac{1}{2}\sum_{ij\sigma\sigma'}\{-\Delta_{ij\sigma\sigma'}C^+_{i\sigma}C^+_{j\sigma'} + \Delta^+_{ij\sigma\sigma'}C_{i\sigma}C_{j\sigma'}\} + \sum_{i\sigma\sigma'} C^+_{i\sigma}C_{i\sigma}(\sigma_{\sigma\sigma'}.V_c)$$
$$= -\sum_{ij\sigma\sigma'}\{t_{ij}\delta_{\sigma\sigma'}C^+_{i\sigma}C_{j\sigma} + \frac{1}{2}\Delta_{ij\sigma\sigma'}C^+_{i\sigma}C^+_{j\sigma'} - \frac{1}{2}\Delta^+_{ij\sigma\sigma'}C_{i\sigma}C_{j\sigma'} - \delta_{ij}C^+_{i\sigma}C_{i\sigma}(\sigma_{\sigma\sigma'}.V_c)\} \tag{3.12}$$

For further simplification, we use Bogoliubov-Valatin transformations:

$$\hat{C}_{i\sigma} = \sum_{k\sigma'}\{u_{k\sigma\sigma'}(R_i)\hat{\gamma}_{k\sigma'} + v^*_{k\sigma\sigma'}(R_i)\hat{\gamma}^+_{k\sigma'}\} \tag{3.13}$$

and

$$\hat{C}_{j\sigma'} = \sum_{k'\sigma''} \{u_{k'\sigma'\sigma''}(R_j)\hat{\gamma}_{k'\sigma''} + v^*_{k'\sigma'\sigma''}(R_j)\hat{\gamma}^+_{k'\sigma''}\} \tag{3.14}$$

where v and u Bogoliubov coefficients to be determined,$\hat{\gamma}$ is fermions operator that satisfies

$$\{\hat{\gamma}^+_{k\sigma}, \hat{\gamma}_{k'\sigma'}\} = \delta(k-k')\delta_{\sigma\sigma'},$$

and

$$u_k(R_i)u^*_k(R_j) + v_k(R_i)v^*_k(R_j) = \delta_{ij}$$

Substituting (3.13) and (3.14) into (3.10) gives:

$$\begin{aligned}
\Delta_{ij\sigma\sigma'} &= -U_{ij\sigma\sigma'} < C_{i\sigma}C_{j\sigma'} > \\
&= -U_{ij\sigma\sigma'} < \sum_{k\sigma'}\{u_{k\sigma\sigma'}(R_i)\gamma_{k\sigma'} + v^*_{k\sigma\sigma'}(R_i)\gamma^+_{k\sigma'}\}, \sum_{k'\sigma''}\{u_{k'\sigma'\sigma''(R_j)}\gamma_{k'\sigma''} + v^*_{k'\sigma'\sigma''}(R_j)\gamma^+_{k'\sigma''} >\} \\
&= -U_{ij\sigma\sigma'} \sum_{k'\sigma''}\{u_{k'\sigma\sigma''}(R_i)v^*_{k'\sigma'\sigma''}(R_j) < \gamma_{k'\sigma''}, \gamma^+_{k'\sigma''} > +v^*_{k\sigma\sigma''}(R_i)u_{k'\sigma'\sigma''(R_j)} < \gamma+_{k'\sigma''}, \gamma_{k'\sigma''} > \\
&= -U_{ij\sigma\sigma'} \sum_{k'\sigma''}\{u_{k'\sigma\sigma''}(R_i)v^*_{k'\sigma'\sigma''}(R_j)(1-f(E_{k'\sigma''})) + v^*_{k'\sigma\sigma''}(R_i)u_{k'\sigma'\sigma''}(R_j)f(E_{k\prime\sigma})\}
\end{aligned} \tag{3.15}$$

Here,$< \hat{\gamma}_{k'\sigma''}, \hat{\gamma}^+_{k'\sigma''} >= 1-f(E_{k'\sigma})$ and $< \hat{\gamma}^+_{k'\sigma''}, \hat{\gamma}_{k'\sigma''} >= f(E_{k'\sigma})$ is a fermi function which is expressed by:

$$f(E_{k'\sigma}) = \frac{1}{exp(\beta E_{k'\sigma}) + 1}$$

and, the order parameter $\Delta_{ij\sigma\sigma'}$ is antisymmetric under the exchange of spin and coordinate label. That is:

$$\begin{aligned}\Delta_{ij\sigma\sigma'} &= -\Delta_{ji\sigma'\sigma} \\ &= U_{ij\sigma\sigma'}\sum_{k'\sigma''}\{u_{k'\sigma'\sigma''}(R_j)v^*_{k'\sigma\sigma''}(R_i)(1-f(E_{k'\sigma''})) + (v^*_{k'\sigma'\sigma''}(R_j)u_{k'\sigma\sigma''}(R_i)f(E_{k\prime\sigma''}))\}\end{aligned} \tag{3.16}$$

Subtracting (3.16) from (3.15), we obtain:

$$\Delta_{ij\sigma\sigma'} = -\frac{1}{2}U_{ij\sigma\sigma'}\sum_{k'\sigma''}\{u_{k'\sigma\sigma''}(R_i)v^*_{k'\sigma'\sigma''}(R_j) - v^*_{k'\sigma\sigma''}(R_i)u_{k'\sigma'\sigma''}(R_j)\}(1-2f(E_{k'\sigma''})) \tag{3.17}$$

We find that the order parameter $\Delta_{\sigma\sigma'}(k)$ shall be determined using Fourier transformation as:

$$\Delta_{\sigma\sigma'}(k) = -\frac{1}{2}\sum_{k'\sigma''}U_{\sigma\sigma'}(k-k')\{(u_{\sigma\sigma''}(-k')v^*_{\sigma'\sigma''}(-k') - v^*_{\sigma\sigma''}(k')u_{\sigma'\sigma''}(k'))(1-2f(E_{k'\sigma''}))\} \tag{3.18}$$

and, we can write the self consistency equation of (3.18) as:

$$\Delta_{\sigma\sigma}(k) = \sum_{k'\sigma}U_{\sigma\sigma}(k-k')u_{\sigma\sigma}(k')v^*_{\sigma\sigma}(k')(1-2f(E_{k'\sigma})) \tag{3.19}$$

where $U_{\sigma\sigma}(k-k')$ is the lattice Fourier transformation of $U_{ij\sigma\sigma'}$.

To determine the variables $u_{\sigma\sigma'}(k')$ and $v_{\sigma\sigma}(k')$, we use the following methods. We now choise our Bogoliubov-Valatin transformation to diagonalize the Hamiltonian or equivalently:

$$\hat{H}' = \sum_{k\sigma}E_{k\sigma}\hat{\gamma}^+_{k\sigma}\hat{\gamma}_{k\sigma} \tag{3.20}$$

where $E_{k\sigma}$ is a single particle unperturbed energy or it is a quasi particle spectrum.

Now from (3.12) and (3.13), we have

$$[\hat{H}, C_{i\sigma}] = [-\sum_{ij\sigma\sigma'}\{t_{ij}\delta_{\sigma\sigma'}C^{+}_{i\sigma}C_{j\sigma} + \frac{1}{2}\Delta_{ij\sigma\sigma'}C^{+}_{i\sigma}C^{+}_{j\sigma'} - \frac{1}{2}\Delta^{+}_{ij\sigma\sigma'}C_{i\sigma}C_{j\sigma'} - \delta_{ij}C^{+}_{i\sigma}C_{i\sigma}(\sigma_{\sigma\sigma'}.V_c)\}, C_{i\sigma}]$$

$$= -\sum_{ij\sigma\sigma'}(t_{ij}\delta_{\sigma\sigma'}\{C^{+}_{i\sigma}C_{j\sigma}, C_{i\sigma}\} + \frac{1}{2}\Delta_{ij\sigma\sigma'}\{C^{+}_{i\sigma}C^{+}_{j\sigma'}, C_{i\sigma}\} - \frac{1}{2}\Delta^{+}_{ij\sigma\sigma'}\{C_{i\sigma}C_{j\sigma'}, C_{i\sigma}\}$$

$$- \delta_{ij}(\sigma_{\sigma\sigma'}.V_c)\{C^{+}_{i\sigma}C_{i\sigma}, C_{i\sigma}\}$$

$$= \sum_{ij\sigma\sigma'}(t_{ij}\delta_{\sigma\sigma'}C_{j\sigma'} + \frac{1}{2}\Delta_{ij\sigma\sigma'}C^{+}_{j\sigma'} - C_{i\sigma}\delta_{ij}(\sigma_{\sigma\sigma'}.V_c))$$

$$= \sum_{ij\sigma\sigma'} t_{ij}\delta_{\sigma\sigma'}(\sum_{k'\sigma''} u_{k'\sigma'\sigma''}(R_j)\gamma_{k'\sigma''} + v^{*}_{k'\sigma'\sigma''}(R_j)\gamma^{+}_{k'\sigma''}) + \frac{1}{2}\Delta_{ij\sigma\sigma'}(\sum_{k'\sigma''} u^{*}_{k'\sigma'\sigma''}(R_j)\gamma^{+}_{k'\sigma''}$$

$$+ v_{k'\sigma'\sigma''}(R_j)\gamma_{k'\sigma''}) - \delta_{ij}(\sigma_{\sigma\sigma'}.V_c)(\sum_{k\sigma'} u_{k\sigma\sigma'}(R_i)\gamma_{k\sigma'} + v^{*}_{k\sigma\sigma'}(R_i)\gamma^{+}_{k\sigma'}$$

$$= \sum_{kj\sigma'\sigma''}\{(t_{ij}\delta_{\sigma\sigma'} - (\sigma_{\sigma\sigma'}.V_c))(u_{k\sigma'\sigma''}(R_j)\hat{\gamma}_{k\sigma''} + v^{*}_{k\sigma'\sigma''}(R_j)\hat{\gamma}^{+}_{k\sigma''})$$

$$- \Delta_{ij\sigma\sigma'}(u^{*}_{k\sigma'\sigma''}(R_j)\hat{\gamma}^{+}_{k\sigma''} + v_{k\sigma'\sigma''}(R_j)\hat{\gamma}_{k\sigma''})\} \tag{3.21}$$

And, from (3.20) and (3.13), we have,

$$[\hat{H}', C_{i\sigma}] = [\hat{H}', \sum_{k\sigma''}(u_{k\sigma\sigma''}(R_i)\hat{\gamma}_{k\sigma''} + v^{*}_{k\sigma\sigma''}(R_i)\hat{\gamma^{+}}_{k\sigma''}]$$

$$= \sum_{k\sigma''}(E_{k\sigma''}u_{k\sigma\sigma''}(R_i)\{\gamma^{+}_{k\sigma''}\gamma_{k\sigma''}, \gamma_{k\sigma''}\}$$

$$+ \sum_{k\sigma''} E_{k\sigma''}v^{*}_{k\sigma\sigma''}(R_i)\{\gamma^{+}_{k\sigma''}\gamma_{k\sigma''}, \gamma^{+}_{k\sigma''}\}$$

$$= \sum_{k\sigma''}(-E_{k\sigma''}u_{k\sigma\sigma''}(R_i)\hat{\gamma}_{k\sigma''} + E_{k\sigma''}v^{*}_{k\sigma\sigma''}(R_i)\hat{\gamma}^{+}_{k\sigma''}) \tag{3.22}$$

Equating coefficients of $\hat{\gamma}_{k\sigma''}$from (3.21) and (3.22), we get,

$$\sum_{j\sigma''}\{(t_{ij}\delta_{\sigma'\sigma''} + (\sigma_{\sigma'\sigma''}.V_c))u_{k\sigma''\sigma}(R_j) + \Delta_{ij\sigma'\sigma''}v_{k\sigma''\sigma}(R_j)\} = E_{k\sigma}u_{k\sigma'\sigma}(R_i) \tag{3.23}$$

Similarly equating of $\hat{\gamma}^{+}_{k\sigma''}$ gives,

$$\sum_{j\sigma''}(-t_{ij}\delta_{\sigma'\sigma''} - (\sigma^{*}_{\sigma\sigma''}.V_c))v_{k\sigma''\sigma}(R_j) - \Delta^{*}_{ij\sigma'\sigma''}u_{k\sigma''\sigma}(R_j) = E_{k\sigma}v_{k\sigma'\sigma}(R_i) \tag{3.24}$$

Here, (3.23) and (3.24) are the spin generalized Bogoliubov- de Gennes equations in real space. Using Fourier transformation, we express them as a form:

$$\sum_{\sigma''}(\varepsilon_k\delta_{\sigma'\sigma''} + (\sigma_{\sigma'\sigma''}.V_c))u_{k\sigma''\sigma} + \Delta_{\sigma'\sigma''}(k)v_{k\sigma''\sigma} = E_{k\sigma}u_{k\sigma'\sigma} \tag{3.25}$$

$$\sum_{\sigma''}(-\varepsilon_k\delta_{\sigma'\sigma''} - (\sigma^{*}_{\sigma'\sigma''}.V_c))v_{k\sigma''\sigma} - \Delta^{*}_{\sigma'\sigma''}(k)u_{k\sigma''\sigma} = E_{k\sigma}v_{k\sigma'\sigma} \tag{3.26}$$

We shall now consider Pseudo-Spinor notations using $V_c = V_{c_1} + V_{c_2} + V_{c_3}$ as,

$$\begin{pmatrix} \xi(k) & \Delta_k \\ -\Delta^{*}_{-k} & -\xi(k) \end{pmatrix} \begin{pmatrix} u_\sigma(k) \\ v_\sigma(k) \end{pmatrix} = E_\sigma(k) \begin{pmatrix} u_\sigma(k) \\ v_\sigma(k) \end{pmatrix}$$

where:

$$\xi(k) = \begin{pmatrix} \varepsilon_k + V_{c_3} & V_{c_1} - iV_{c_2} \\ V_{c_1} + iV_{c_2} & \varepsilon_k - V_{c_3} \end{pmatrix}$$

$$\Delta_k = \begin{pmatrix} \Delta_{\uparrow\uparrow}(k) & \Delta_{\uparrow\downarrow}(k) \\ \Delta_{\downarrow\uparrow}(k) & \Delta_{\downarrow\downarrow}(k) \end{pmatrix}$$

$$u_\sigma(k) = \begin{pmatrix} u_{\uparrow\sigma}(k) \\ u_{\downarrow\sigma}(k) \end{pmatrix}$$

$$v_\sigma(k) = \begin{pmatrix} v_{\uparrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix}$$

$$-\xi(k) = \begin{pmatrix} -\varepsilon_{-k} - V_{c_3} & -V_{c_1} - iV_{c_2} \\ -V_{c_1} + iV_{c_2} & -\varepsilon_{-k} + V_{c_3} \end{pmatrix}$$

$$-\Delta^*_{-k} = \begin{pmatrix} -\Delta^*_{\uparrow\uparrow}(-k) & -\Delta^*_{\uparrow\downarrow}(k) \\ -\Delta^*_{\downarrow\uparrow}(-k) & -\Delta^*_{\downarrow\downarrow}(-k) \end{pmatrix}$$

Using this notation, we can write (3.25) and (3.26) in their more familiar matrix form (which is called Bogoliubov-de Genness (BdG) equation) as:

$$\begin{pmatrix} \varepsilon_k + V_{c_3} & V_{c_1} - iV_{c_2} & \Delta_{\uparrow\uparrow}(k) & \Delta_{\uparrow\downarrow}(k) \\ V_{c_1} + iV_{c_2} & \varepsilon_k - V_{c_3} & \Delta_{\downarrow\uparrow}(k) & \Delta_{\downarrow\downarrow}(k) \\ -\Delta^*_{\uparrow\uparrow}(-k) & -\Delta^*_{\uparrow\downarrow}(k) & -\varepsilon_{-k} - V_{c_3} & -V_{c_1} - iV_{c_2} \\ -\Delta^*_{\downarrow\uparrow}(-k) & -\Delta^*_{\downarrow\downarrow}(-k) & -V_{c_1} + iV_{c_2} & -\varepsilon_{-k} + V_{c_3} \end{pmatrix} \begin{pmatrix} u_{\uparrow\sigma}(k) \\ u_{\downarrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix} = E_{\sigma(K)} \begin{pmatrix} u_{\uparrow\sigma}(k) \\ u_{\downarrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix} \tag{3.27}$$

But, in our study, the triplet vector d(k) is perpendicular to V_c (i.e d(k) is parallel to $\hat{x}$, the magnetic field is parallel to $\hat{z}$) . This implies that d(k).V_c = 0. In this case, for V_c = (0,0,-V_c), we shall express (3.27) as a form:

$$\begin{pmatrix} \varepsilon_k - V_c & 0 & \Delta_{\uparrow\uparrow}(k) & 0 \\ 0 & \varepsilon_k + V_c & o & \Delta_{\downarrow\downarrow}(k) \\ -\Delta^*_{\uparrow\uparrow}(-k) & 0 & -\varepsilon_{-k} + V_c & o \\ o & -\Delta^*_{\downarrow\downarrow}(-k) & 0 & -\varepsilon_{-k} - V_c \end{pmatrix} \begin{pmatrix} u_{\uparrow\sigma}(k) \\ u_{\downarrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix} = E_{\sigma(K)} \begin{pmatrix} u_{\uparrow\sigma}(k) \\ u_{\downarrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix} \tag{3.28}$$

we can now easily separate (3.28) in to a pair of equation for up electrons $|\uparrow\uparrow\rangle$ as:

$$\begin{pmatrix} \varepsilon_k - V_c & \Delta_{\uparrow\uparrow}(k) \\ -\Delta^*_{\uparrow\uparrow}(-k) & -\varepsilon_{-k} + V_c \end{pmatrix} \begin{pmatrix} u_{\uparrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \end{pmatrix} = E_{\sigma(K)} \begin{pmatrix} u_{\uparrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \end{pmatrix}$$

Similarly, for down electrons $|\downarrow\downarrow\rangle$:

$$\begin{pmatrix} \varepsilon_k + V_c & \Delta_{\downarrow\downarrow}(k) \\ -\Delta^*_{\downarrow\downarrow}(-k) & -\varepsilon_{-k} - V_c \end{pmatrix} \begin{pmatrix} u_{\downarrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix} = E_{\sigma(K)} \begin{pmatrix} u_{\downarrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix}$$

Therefore, from equation (3.28), we get:

$$u_{\sigma\sigma}(k) = \sqrt{\frac{E_\sigma(K) + (\varepsilon(k) - \sigma V_c)}{2E_\sigma(k)}}$$

and

$$v^*_{\sigma\sigma}(k) = \frac{-\Delta_{\sigma\sigma}}{\sqrt{2E_\sigma(K)(E_\sigma(K) + (\varepsilon(k) - \sigma V_c))}}$$

with,

$$E_\sigma(k) = \sqrt{(\varepsilon(k) - \sigma V_c)^2 + |\Delta_{\sigma\sigma}(k)|^2}$$

Substituting these results in to (3.19) , we now arive at the gap equation of triplet equal spin pairing of ferromagnetic superconductor state;

$$\Delta_{\sigma\sigma}(k) = -\sum_{k'} \frac{U_{\sigma\sigma}(k-k')\Delta_{\sigma\sigma}(k')}{2E_\sigma(k')}(1 - 2f(E_\sigma(k')) \tag{3.29}$$

To proceed further, we replace $f(E_\sigma(k')$ by $\frac{1}{\exp(\beta E_\sigma(k'))+1}$. Using (3.29), we find that:

$$\begin{aligned}\Delta_{\sigma\sigma}(k) &= -\sum_{k'} \frac{U_{\sigma\sigma}(k-k')\Delta_{\sigma\sigma}(k')}{2E_\sigma(k')}(1 - \frac{2}{\exp(\beta E_\sigma(k')) + 1}) \\ &= -\sum_{k'} \frac{U_{\sigma\sigma}(k-k')\Delta_{\sigma\sigma}(k')}{2E_\sigma(k')}(\frac{\exp(\beta E_\sigma(k'))}{\exp(\beta E_\sigma(k')) + 1} - \frac{1}{\exp(\beta E_\sigma(k')) + 1}) \\ &= \sum_{k'} \frac{U_{\sigma\sigma}(k-k')\Delta_{\sigma\sigma}(k')}{2E_\sigma(k')} tanh(\frac{\beta E_\sigma(k')}{2}) \end{aligned} \tag{3.30}$$

As T $\rightarrow T_{sc}$ from below, $|\Delta_{\sigma\sigma}(k)| \rightarrow 0$ and hence $E_\sigma(K) \rightarrow \varepsilon(k) - \sigma V_c$, and we obtain the linearized gap equation as:

$$\Delta_{\sigma\sigma}(k) = \sum_{k'} \frac{U_{\sigma\sigma}(k-k')\Delta_{\sigma\sigma}(k')}{2(\varepsilon(k') - \sigma V_c)} tanh(\frac{\varepsilon(k') - \sigma V_c}{2K_B T_{sc}}) \tag{3.31}$$

3.1.1 The Superconducting Transition Temperature T_{sc}

The linearized gap equation (3.31) can be used to predict the critical temperature T_{sc} of $ZrZn_2$. In this point of view, some simplifying assumptions are made to solve the equation. In this sub section we shall be interested to derive and to calculate the numerical values of T_{sc} in two cases: $V_c = 0$ and $V_c \neq 0$.

First, for zero exchange splitting (i.e. $V_c = 0$), the mathematical form of equation (3.31) is changed as a form:

$$\Delta_{\sigma\sigma}(k) = \sum_{k'} \frac{U_{\sigma\sigma}(k-k')\Delta_{\sigma\sigma}(k')}{2\varepsilon(k')} tanh(\frac{\varepsilon(k')}{2K_B T_{sc}}) \tag{3.32}$$

For further simplification, it is often assume that the potential U(k-k') is constant, i.e. U(k-k')=U, which results in a constant gap $\Delta(k) = \Delta$. This considerably simplifies the problem since a factor Δ can be removed from both sides in eqn.(3.32). With this assumption (3.32) becomes,

$$1 = U \sum_{k'} \frac{1}{2\varepsilon_{k'}} \tanh(\frac{\varepsilon_{k'}}{2K_B T_{sc}}) \tag{3.33}$$

Further, we assume the sperical Fermi surface, we replace the summation over k in (3.33) with an integration in the form:

$$\begin{aligned} 1 &= U \int_0^{\hbar w_c} \frac{d^3k}{(2\pi)^3 \varepsilon_{k'}} \tanh(\frac{\varepsilon_{k'}}{2K_B T_{sc}}) \\ &= U \int_0^{\hbar w_c} \frac{m}{2\pi^2 \hbar^2} \frac{d\varepsilon_{k'}}{\varepsilon_{k'}} \tanh(\frac{\varepsilon_{k'}}{2K_B T_{sc}}) \\ &= UD(E_f) \int_0^{\hbar w_c} \frac{d\varepsilon_k}{\varepsilon_{k'}} \tanh(\frac{\varepsilon_{k'}}{2K_B T_{sc}}) \end{aligned} \tag{3.34}$$

This equation can be reduced as a form

$$\begin{aligned} \frac{1}{\lambda} &= \int_0^{\frac{\hbar\omega_c}{2K_B T_{sc}}} \frac{\tanh x}{x} dx \\ &= (\ln(x) \tanh x)|_0^{\frac{\hbar\omega_c}{2K_B T_{sc}}} - \int_0^{\frac{\hbar\omega_c}{2K_B T_{sc}}} \frac{\ln(x)}{\cosh^2(x)} dx \end{aligned} \tag{3.35}$$

Where $\lambda = UD(E_f)$ and $x = \frac{\varepsilon_{k'}}{2k_B T_{sc}}$

Here, for low temperature, we can replace $\tanh(\frac{\hbar\omega_c}{2K_BT_{SC}})$ by unity and extend the upper limit of the integral to infinity to obtain:

$$\begin{aligned}\frac{1}{\lambda} &= \ln(\frac{\hbar\omega_c}{2K_BT_{sc}}) - \int_0^\infty \frac{\ln(x)}{\cosh^2(x)}dx \\ &= \ln(\frac{\hbar\omega_c}{K_BT_{sc}}) - \ln(\frac{\pi}{4\gamma}) \\ &= \ln(\frac{2\gamma}{\pi}\frac{\hbar\omega_c}{K_BT_{sc}}) \end{aligned} \tag{3.36}$$

This gives us;

$$T_{sc} = \frac{2\gamma}{\pi}\frac{\hbar\omega_c}{K_B}e^{-\frac{1}{UD(E_f)}} \tag{3.37}$$

Where, γ denotes the Euler's constant $\gamma = 1.78$, ω_c is the cut of frequency and the dimensionless parameter λ is interaction coupling constant.

To solve (3.37) numerically, we fixed U= 0.88 t from [35], where t=0.12 ev, we use the calculated $D(E_f) = 1.69ev^{-1}$ which is almost in agreement with calculation of [17] and $\frac{\hbar\omega_c}{K_B} = 90k, from[17]$. Substituting these into (3.37), we obtain that;

$$T_{sc} = 0.37k \tag{3.38}$$

Next, for the case of $V_C \neq 0$, we can write (3.34) as a form:

$$1 = U\int_0^{\hbar\omega_c} D_\sigma(\varepsilon_{k'} + \sigma V_c)\frac{d\varepsilon_{k'}}{(\varepsilon_{k'} - \sigma V_c)}\tanh(\frac{\varepsilon_{k'} - \sigma V_c}{2K_BT_{sc}^\sigma}) \tag{3.39}$$

Here, the density of state, D,is dependent on $V_c = \frac{1}{2}\mu_B\sigma H$. expanding $D(\varepsilon_{k'} + \sigma V_c)$ in Tayler Series [36] for small values of magnetic field H, about the Fermi energy and neglecting higher derivative terms, we obtain that:

$$D(\varepsilon_{k'} + \sigma V_c) = D(\varepsilon_{k'})|_{E_f} + \sigma V_c\frac{dD(\varepsilon_{k'})}{d\varepsilon_{k'}}|_{E_f}$$

By substituting this into (3,39), we obtai that:

$$1 = U[D_\sigma(\varepsilon_{k'})|_{E_f} + \sigma V_c\frac{dD\varepsilon_{k'})}{dE_f}|_{E_f}]\int_0^{\hbar\omega_c}\frac{d\varepsilon_{k'}}{(\varepsilon_{k'} - \sigma V_c)}\tanh(\frac{\varepsilon_{k'} - \sigma V_c}{2K_BT_{sc}^\sigma}) \tag{3.40}$$

This can be reduced as a form:

$$\frac{1}{\lambda^{\uparrow,\downarrow}} = \int_{\frac{-\sigma V_c}{2K_B T_{sc}}}^{\frac{\hbar\omega_c - \sigma v_c}{2K_B T_{sc}}} \frac{\tanh x}{x} dx \tag{3.41}$$

Where $x = \frac{\varepsilon_{k'} - \sigma V_c}{2K_B T_{sc}}$ and $\lambda^{\uparrow,\downarrow} = U(D_\sigma(\varepsilon_{k'})|_{E_f} \pm V_c \frac{dD(\varepsilon_{k'})}{d\varepsilon_{k'}})|_{E_f}$. But, for small magnetic field we take the lower limit of integration as zero. So, eq.(3.41) takes the form:

$$\frac{1}{\lambda^{\uparrow,\downarrow}} = \int_{0}^{\frac{\hbar\omega_c - \sigma v_c}{2K_B T_{sc}}} \frac{\tanh x}{x} dx \tag{3.42}$$

Next, following the same way of integration as we have done for the case $V_c = 0$, we therefore get the following form of;

$$\frac{1}{\lambda^{\uparrow,\downarrow}} = \ln\{\frac{2\gamma}{\pi}(\frac{\hbar\omega_c - \sigma V_c}{2K_B T_{sc}^\sigma})\} \tag{3.43}$$

This can be rewritten as:

$$-\frac{1}{\lambda^{\uparrow,\downarrow}} = \ln\{\frac{\pi}{2\gamma}(\frac{2K_B T_{sc}^\sigma}{\hbar\omega_c - \sigma V_c})\}$$

This gives us:

$$T_{sc}^\sigma = \frac{2\gamma}{\pi}(\frac{\hbar\omega_c - \sigma V_c}{K_B})e^{-\frac{1}{\lambda^{\uparrow,\downarrow}}} \tag{3.44}$$

We assume that for small magnetic field H, $\sigma V_c \approx 0$, so we arrive at;

$$T_{sc}^{\uparrow,\downarrow} = \frac{2\gamma}{\pi}(\frac{\hbar\omega_c}{K_B})e^{-\frac{1}{U\{D_\sigma(\varepsilon_{k'})|_{E_f} \pm V_c \frac{dD\varepsilon_{k'}}{d\varepsilon_{k'}}|_{E_f}\}}} \tag{3.45}$$

Next, using the final result (3.45), we are interested to estimate T_{sc} numerically for both $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ states. To do this , first we assume that $\frac{dD(\varepsilon_{k'})}{d\varepsilon_{k'}}|_{E_f} = 1$, Next, we use a fixed value of $V_c = 0.02ev$ and we assume that the calculated value $D(E_f) = 1.69ev^{-1}$ is the same for both states. In this approach, we get that

$$T_{sc}^{\uparrow} = 0.4k \tag{3.46}$$

and, for down-down pairing

$$T_{sc}^{\downarrow} = 0.34k \tag{3.47}$$

3.2 Phase Diagram of $ZrZn_2$

It has been known for some time that the ferromagnetism in $ZrZn_2$ is rapidly suppressed under pressure. This, and the prediction that superconductivity is controlled by a quantum critical which leads us to perform high pressure studies. In this section we shall be interested to study the effect of pressure on ferromagnetic superconducting transition temperatures: T_f and T_{sc}, in a compound $ZrZn_2$ using Ginzburg-Landau theory.

A phase transition can be characterized by a parameter called the order parameter, which contains all the information about the degree of the order. In the Landau theory we assumed that near T_f the ferromagnetic property is weak and M is small, as a result the free energy of the ferromagnetic state can be written as a power series:

$$F(M) = F_0 + \frac{1}{2}a_f(T)M^2 + \frac{1}{4}b_f(T)M^4 + ... \tag{3.48}$$

where the parameters b_f and b_f are the Landau coefficients (experimental quantities determained near T_f), M is the ferromagnetic ordered parameter (ferromagnetic magnetiztion) and F_0 denotes the free energy of the system at M = 0.

Equation (3.48) represents an expression of the free energy about the value in the low temperature phase and is therefore expected to be valid only for small values of M, i.e. very close to the phase transition. And F(M) is independent of the sign of M and therefore only contains with even power of M.

Moreover, in equation (3.48), it is necessary that the value of, a_f, changes sign at the transition temperature of ferromagnet, T_f, so that it is positive for $T > T_f$ and negative for $T < T_f$. The simplest implication of this condition is to assume that,

$$a_f(T) = \alpha_f(T - T_f) \tag{3.49}$$

Here, T_f, is assumed to depend on the pressure P, and it is also asummed that we only need to concider the smallest numberof terms in the eqation, so that using (3.49), we can write (3.48) as:

$$F(M) = F_0 + \frac{1}{2}\alpha_f(T - T_f(p))M^2 + \frac{1}{4}b_f(T)M^4 \tag{3.50}$$

Where α is positive constants, we show latter that for equilibrum condition, the free energy has a turning point when $\frac{\partial F(M)}{\partial M} = 0$. It follows from this condition that we have from (3.50) as:

$$\frac{\partial F(M)}{\partial M} = \frac{\partial}{\partial M}(F_0 + \frac{1}{2}\alpha_f(T - T_f(p))M^2 + \frac{1}{4}b_f(T)M^4) = o$$

Hence we find that, the order parameter M as:

$$M = (\frac{\alpha_f}{b_f})^{1/2}(T_f(P) - T)^{1/2} \tag{3.51}$$

For further simplicity, we consider the total Ginzburg-Landau free energy:

$$F(\psi, M) = Vf(\psi, M) \tag{3.52}$$

Where $\psi = \{\psi_j, j = 1, 2, 3, \}$ is the three dimentional superconducting complex parameter, V, is the volume of the system, and $f(\psi, M)$ is the free energy of a spin triplet ferromagnetic superconductor. We use latter that the free energy, $f(\psi, M)$, can be written as [37]:

$$f(\psi, M) = f_s(\psi) + f_F(M) + f_{sF}(\psi, M) + \frac{B^2}{8\pi} - B.M \tag{3.53}$$

Where, $B = (H + 4\pi M) = \nabla \times A$ is the magnetic induction, H, denotes the external magnetic field, and $A = \{A_j, j = 1, 2, 3, \}$ is the magnetic vector potential with $\nabla.A = 0$. The last two terms in the right hand side of (3.53) are magnetic energy which includes both diamagnetic and paramagnetic effect in the superconductor.
In eqn.(3.53), the first term $f_s(\psi)$ describes the superconductivity free energy for H =

M = 0. It can be written in the form

$$f_s(\psi) = f_g(\psi) + a_s|\psi|^2 + \frac{b_s}{2}|\psi|^4 + \frac{u_s}{2}|\psi^2|^2 + \frac{v_s}{2}\sum_{j=1}^{3}|\psi|^4 \tag{3.54}$$

Here, it is assumed that:

$$a_s = \alpha_s(T - T_{sc}(p)) \tag{3.55}$$

Moreover, $b_s > 0$, the quantities u_s and v_s describe anisotopy of the spin triplet cooper pair and the crystal an isotropy respectivily, and we denote the gradient term $f_g(\psi)$ which is the kinetic energy term in the form;

$$f_g(\psi) = \frac{1}{2m^*}|(-ih\nabla - \frac{e^* A_j}{c})\psi|^2 \tag{3.56}$$

The charge e^* is a 2e (or e^* = 2e, e is the charge of free electron), and the mass m^* is twice that of the mass of un paired electrons, i.e. m^* = 2m, and, c, denotes the speed of light.

The second term in eqn. (3.53) is the free energy of ferromagnetic term for ψ = 0. It can be written generally as:

$$f_F(M) = c_f \sum_{j=1}^{3}|\nabla_j M_j|^2 + a_f M^2 + \frac{b_f}{2}M^4 \tag{3.57}$$

Where, $\nabla_i = \frac{\partial}{\partial x_j}$ and $b_f > 0$. Recall that a_f is assumed to be;

$$a_f = \alpha_f(T - T_f(p)) \tag{3.58}$$

Where $\alpha_f > 0$.

The third term $f_{SF}(\psi, M)$ in (3.53) denotes the free energy due to coupling of superconductivity and ferromagnetic system. And it can be written as:

$$f_{SF}(\psi, M) = i\gamma_0 M.(\psi \times \psi^*) + \eta M^2|\psi|^2 \tag{3.59}$$

where, the γ_0 term ensures the triggering of the superconductivity by ferromagnetic order $(\gamma_0 > 0)$, and η denotes the coupling parameter.

In eqn.(3.59), γ_0 can be represented in the form $\gamma_0 = 4\pi J$, where $J > 0$ is the ferromagnetic exchange parameter, and we show latter (3.59) as:

$$f_{SF}(\psi, M) = 4\pi J.S + \eta M^2 |\psi|^2 \tag{3.60}$$

where $S = i\psi^* \times \psi$ is called spin exchange parameter.

For further simplification we consider a homogeneous system with constant order parameters, ψ and M, i.e. M and ψ do not depend on the spatial vector x $\in$ V, where V is the volume of the system. Following this, in (3.53), the free energy $f(\psi, M)$ of spin triplet ferromagnetic superconductor can be written as:

$$f(\psi, M) = a_s|\psi|^2 + \frac{b_s}{2}|\psi|^2 + \frac{u_s}{2}|\psi^2|^2 + \frac{v_s}{2}\sum_{j=1}^{3}|\psi_j|^4 + a_f M^2 + \frac{b_f}{2}M^4 + 4\pi J \cdot S + \eta M^2 \psi \cdot \psi^* \tag{3.61}$$

Next, in order to reduce the number of parameters, we shall use the following notations [38]:

$$b = b_s + u_s + v_s \tag{3.62}$$

And the order parameters and the other quantities are redefined as [38]:

$$b^{1/4}\psi_j = \phi_j e^{i\theta_j}, M = b_f^{1/4} M_z, r = \frac{a_s}{\sqrt{b}}, t = \frac{a_f}{\sqrt{b_f}}, w = \frac{u_s}{b}, v = \frac{v_s}{b}, \gamma = \frac{\gamma_0}{b^{1/2} b_f^{1/4}}, \gamma_1 = \frac{\eta}{(b_f)^{1/2}} \tag{3.63}$$

where M_z is magnetization in the z direction and ϕ is the phase angle.

For further simplicity we shall concider the Walker- Samokhin (who studied Landau theory for a magnetic state and Ginzburg-Landau theory for the superconducting state simultaneously) model [38]. In this case the coupling between the order parametrs ψ and M is taken into account ($\gamma > 0$, γ_1 =0) and the anisotropies (w=v=0) are ignored.

Taking equations (3.55)and (3.58), we can write r and t in equ. (3.63) as a form;

$$r(T) = \frac{\alpha_s}{\sqrt{b}}\{T - T_{sc}(p)\} \tag{3.64}$$

and

$$t(T) = \frac{\alpha_f}{\sqrt{b_f}}\{T - T_f(P)\} \tag{3.65}$$

According to Walker-Samokhins' model, the equilibrium ferromagnetic-ferromagnetic superconductor (FR-FS) phase transition can be expressed by the respective equilibrium phase temperature T_{eq} is defined by the equations $r_{eq} = r(T_{eq})$ where $r_{eq} = \gamma|t|^{\frac{1}{2}}$ and $r(T_{eq}) = \frac{\alpha_s}{\sqrt{b}}(T_{eq} - T_{sc})$, and with the help of the relation M_{eq}= $M(T_{eq})$. This limits the possible values of the parameters of the theory. For example, for critical temperature $T_0 = T_{eq}$ of FM-FS phase, from eqns.(3.55) and (3.63), we can find that;

$$\begin{aligned} r_{eq} &= r(T_{eq}) \\ &= \gamma|t|^{\frac{1}{2}} \\ &= \frac{a_s}{\sqrt{b}} \\ &= \frac{\alpha_s}{\sqrt{b}}(T_{eq} - T_{sc}(p)) \end{aligned} \tag{3.66}$$

Using(3.63), we can express (3.66);

$$\frac{\gamma_0}{b^{\frac{1}{2}} b_f^{\frac{1}{4}}}|\frac{a_f}{\sqrt{b_f}}|^{\frac{1}{2}} = \frac{\alpha_s}{\sqrt{b}}(T_0 - T_{sc}(p))$$

recalling that $\gamma_0 = 4\pi J$, then we can express this equation in the form

$$4\pi J(\frac{a_f}{b_f})^{\frac{1}{2}} = \alpha_s(T_0 - T_{sc}(p))$$

This is equivalent to;

$$
\begin{aligned}
T_{sc}(p) &= T_0 - \frac{4\pi J}{\alpha_s}(\frac{a_f}{b_f})^{\frac{1}{2}} \\
&= T_0 + \frac{4\pi JM}{\alpha_s}
\end{aligned} \tag{3.67}
$$

For $T \sim T_{sc}$, we can write (3.51) as:

$$
M = (\frac{\alpha_f}{b_f})^{\frac{1}{2}}(T_f(P) - T_{sc}(P))^{\frac{1}{2}}
$$

Substituting this into (3.38), we obtain that;

$$
T_{sc}(P) = T_0 + T^{*1/2}[T_f(p) - T_{sc}(P)]^{1/2} \tag{3.68}
$$

Where T_0 is the superconducting transition temperature in paramagnetic state and

$$
T^* = (\frac{\alpha_f}{b_f})(\frac{4\pi J}{\alpha_s})^2
$$

For simplicity, we assume that $T_{sc} \gg T_0$. Furthermore, for P very close to P_c, $T_0 = 0$, $T_{sc} \approx T_f(p)$ and $T_f(p) \ll T^*$, under this condition and using power expansion, we arrive at the pressure dependence of the ferromagnetic transition temperature (T_f) of $ZrZn_2$ is;

$$
T_f(P) = T_f(0)(1 - \frac{P}{P_c}) \tag{3.69}
$$

On the other hand, except for pressure P very close to critical pressure P_c, $T_f(p) \gg T_{sc}(P)$, and applying Binomial expansion and using (3.69), we get that the pressure dependence of the ferromagnetic superconductor transition temperature (T_{sc}) for $ZrZn_2$ is:

$$
T_{sc}(P) = T_{sc}(0)(1 - \frac{P}{P_c})^{1/2} \tag{3.70}
$$

Chapter 4

Results and Discussion

In this section we study the properties of the gap energy equations for equal spin pairing state in the presence of exchange splitting in both analytically and graphically, and from the calculated gap equation, we estimate the critical temperature of $ZrZn_2$ for $V_c = 0$ and $V_c \neq 0$. Further, we also discuss the pressure dependence of the ferromagnetic critical temperature T_f and the superconducting transition temperature T_{sc} of $ZrZn_2$ in both analytically and graphically.

In the first section of the preceding chapter, we have derived the gap equation (3.29) for superconductivity in coexistence with ferromagnetism for $ZrZn_2$. We have trite triplet state with equal spin pairing, we used this gap equation to study the behavior of this state as a function of exchange splitting. The derived gap equation shows a special quality. That is there is a complete separation of spin up and spin down system in the presence of exchange splitting and the absence of opposite spin pairing or spin flip process.

We linearized our gap equation for spin up-up pairing $|\uparrow\uparrow\rangle$, the derived gap equation (3.31) takes the form:

$$\Delta_{\uparrow\uparrow}(k) = \sum_{k'} U_{\uparrow\uparrow}(k-k') tanh(\frac{\varepsilon(k') - \uparrow V_c}{2K_B T_{sc}})$$

but

$$\Delta_{\downarrow\downarrow}(k) = \Delta_{\uparrow\downarrow}(k) = 0$$

Similarly for spin down-down pairing $|\downarrow\downarrow\rangle$, (3.31) is reduced to:

$$\Delta_{\downarrow\downarrow}(k) = \sum_{k'} U_{\downarrow\downarrow}(k-k') tanh(\frac{\varepsilon(k') - \downarrow V_c}{2K_B T_{sc}})$$

but

$$\Delta_{\uparrow\uparrow}(k) = \Delta_{\uparrow\downarrow}(k) = 0$$

Our gap equations are identical with what is obtained by the authors in [35,39,40].

From the calculated gap equation (3,31), we have also estimated T_{sc} of $ZrZn_2$ in two cases: $V_c = 0$ and $V_c \neq 0$ using eqns.(3.36) and (3.44) respectively. We find that $T_{sc} = 0.37k$ for $V_c = 0$ and in the second case, $T_{sc} = 0.4k$ for $|\uparrow\uparrow\rangle$pairing and $T_{sc} = 0.34k$ for $|\downarrow\downarrow\rangle$ pairing respectively. Comparing these results we thus predict that the maximum value of T_{sc} corresponds to the majority spin pairing (i,e.$|\uparrow\uparrow\rangle$) and the minimum value corresponds to minority spin pairing (i.e.$|\downarrow\downarrow\rangle$). The solution we have expected here is almost the same as those predicted in[41,42].

The result of our numerical calculations are shown in figs.(4.1) and (4.2). In fig.(4.1), we have plotted the transition temperature for $|\uparrow\uparrow\rangle$ pairing on the positive V_c scale and $|\downarrow\downarrow\rangle$ pairing on the negative V_c scale. This plot shows that, T_{sc} is actually increased by exchange splitting, which will imply spin triplet pairing.

The second Fig.(4.2) shows that, T_{sc} for both $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ pairing on the same graph and it shows that for any given exchange splitting V_c, there are two transition temperatures corresponding to the two separate spin components of the equal spin pairing. The higher transition temperature is the transition to the A_1 phase which represents superconductivity in only up-up pairing $|\uparrow\uparrow\rangle$. In this case the exchange splitting V_c increases the T_{sc}. The A_1 phase has zero pairing amplitude in the $|\downarrow\downarrow\rangle$ and $\frac{1}{2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ states and so only has finite pairing in the $|\downarrow\downarrow\rangle$ state. However, the lower transition temperature is a transition to the A_2 phase which represents superconductivity down-down pairing $|\downarrow\downarrow\rangle$. In this case we have pairing in the $|\downarrow\downarrow\rangle$ but none in $|\uparrow\uparrow\rangle$ or $\frac{1}{2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ channels. On the other hand, the A phase, which

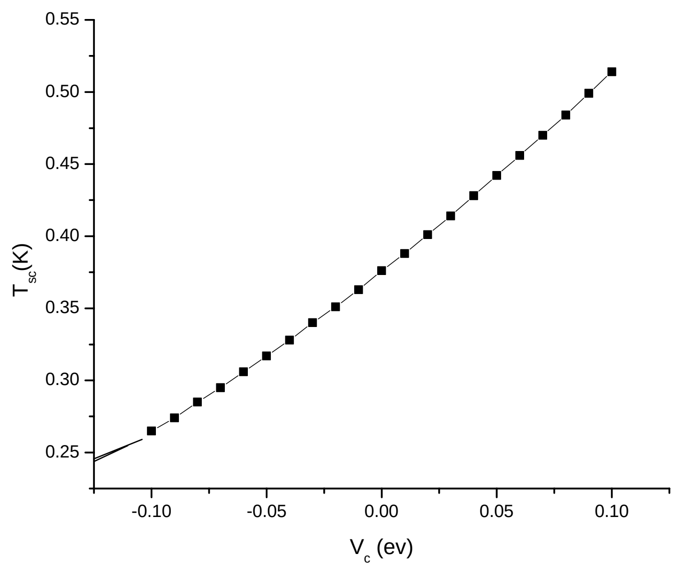

Figure 4.1: *The transition temperature T_{sc} versus exchange splitting V_c for $ZrZn_2$.*

is stable in zero exchange splitting has the same transition temperature in both the $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ pairing states. Then the phase A (the paramagnetic phase) of the equal spin pairing state will turn into phase A_1 (with only spin up pairing $|\uparrow\uparrow\rangle$) and phase A_2 (with only spin down pairing $|\downarrow\downarrow\rangle$),respectively. Therefore, the coexistence of ferromagnetism and superconductivity gives rise to phase transition from A to A_1 or A_2.

Our diagrams shown in figs.(4.1) and (4.2) are almost similar to what is obtained by authors of [35,39]. Particularly, the phase diagram shown in fig.(4.2) is the same as the experiment result of Remeijer et al [39] fort he $A_1 - A_2$ splitting of ^3He in magnetic field. Their experiment result is;

$$\frac{T_{sc}^{A_1} - T_{sc}^{A_2}}{T_{sc}^{A}} = \tilde{a}(\frac{\mu_n B}{K_B T_F}) + \tilde{b}(\frac{\mu_n B}{K_B T_F})^2$$

where μ_n is the nuclear magneton for ^3He, K_F is the Fermi energy, and $\tilde{a} = 36.3 \pm 0.91$ and $\tilde{b} = 522 \pm 17$

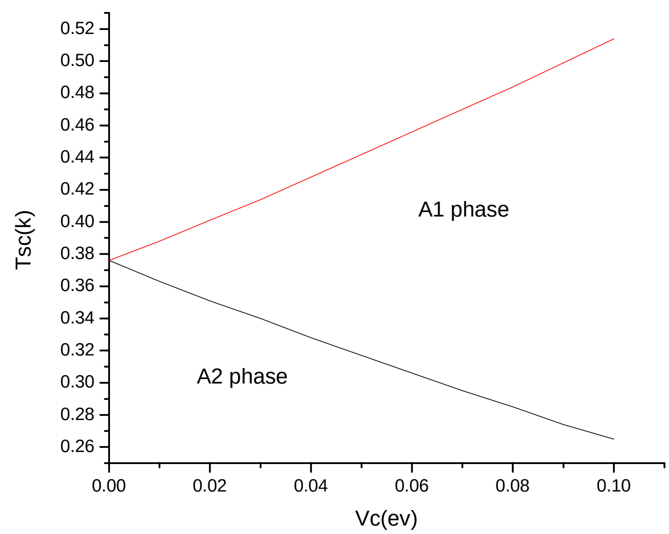

Figure 4.2: *The phase diagram showing T_{sc} for both A_1 and A_2 phases over a range of V_c.*

In the second section of the preceding chapter, we have studied the phase diagram showing ferromagnetic (T_f) and superconducting (T_{sc}) transition temperatures as a function of pressure of $ZrZn_2$. To do this we used mainly the Ginzburg-Landau free energy theory in three dimension. Our first result, i.e. eqn.(3.69) clearly show that T_f of our parameter $ZrZn_2$ is a linear function of pressure. And it shows that the ferromagnetism in $ZrZn_2$ is rapidly suppressed under pressure. Further, this parameter vanishes at the critical pressure P_C.

The other interesting part of our result, i.e. eqn.(3.70) surprisingly show that the superconductivity of $ZrZn_2$ occurs in the ferromagnetic phase. Moreover, it shows that T_{sc} vanishes at P_c. Our critical temperature calculations are very similar to what is obtained by the authors in [35,40].

The result of our calculations are shown in fig.(4.3). In this we have sketched behavior of the transition temperature of $ZrZn_2$ as a function of pressure. To draw this we have fixed experimental values of P_c=21k bar [32], $T_f(0) = 28.5k$ [25],and $T_{sc}(0) = 0.29k$[25] respectively. It is clearly seen from the graph that,

• at ambient pressure (P=0), $ZrZn_2$ has maximum T_f and T_{sc}. But, at this pressure the phase transition temperature (T_f) to the ferromagnertic state is much higher than the phase transition temperature (T_{sc}) from ferromagnetic to a mixed state of coexistence of ferromagnetism and superconductivity.

• the ferromagnetic critical temperature drops rapidly by further increasing of pressure. On the other hand, the superconducting critical temperature drops slowly with increasing pressure.

• superconductivity and ferromagnetism properties of $ZrZn_2$ are vanished at crit ical pressure P_c. From this we note that the vanishing of T_f and T_{sc} at P_c indicates that the coexistence of ferromagnetism and superconductivity in $ZrZn_2$

In this study we also point out that as the pressure increases, more and more spins are inverted (fluctuated) from their common direction, this effect increases the internal energy of the system and reduces the ferromagnetic and superconducting critical temperatures. From this we note that the decline of these critical temperatures of $ZrZn_2$ with pressure could be a simple consequence of P-wave (magnon) pairing. This is an indication of the hole quantum spin fluctuation. Finally, our diagram shown in fig(4.3) is similar to that of the phase diagram of $ZrZn_2$ taken from Pfleiderer et al [15] shown in fig.(1.5). When we compare our graph with the graph of the authors in [15], in our case T_f(p) is exactly zero at P_c, but for Pfleiderer et al graph, $T_f(P)$ is not shown exactly zero at P_c.

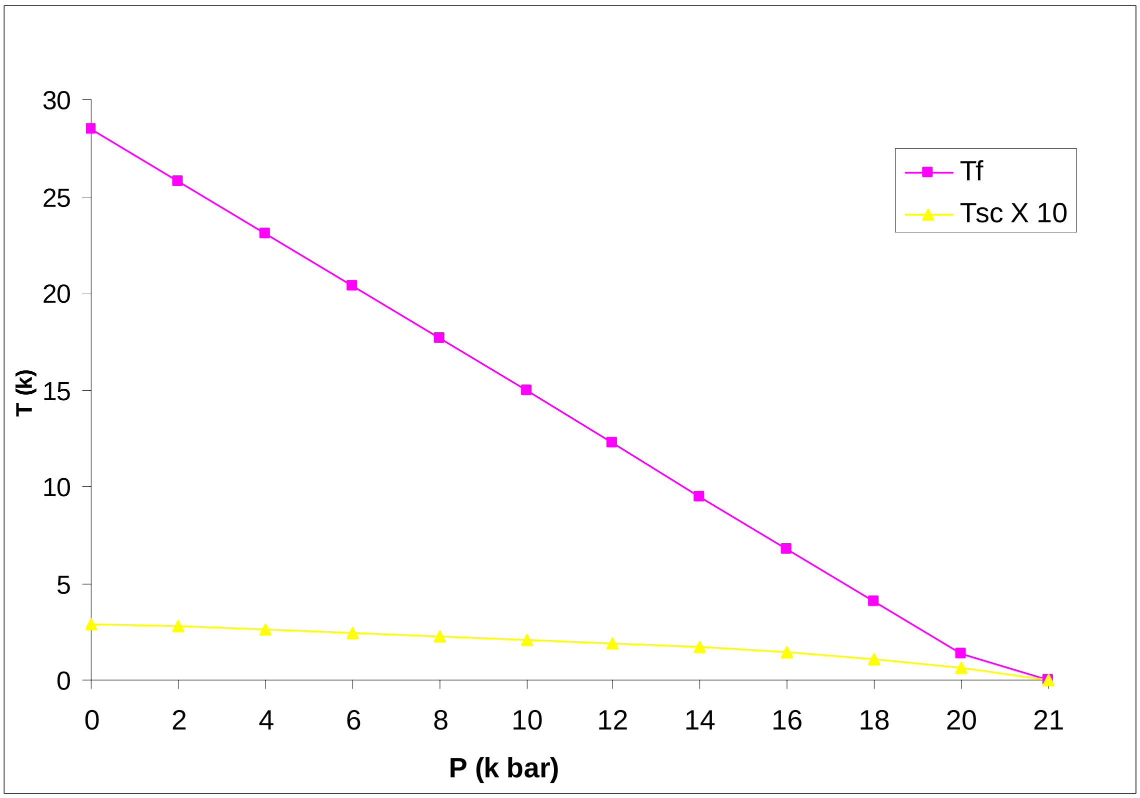

Figure 4.3: *The phase diagram showing the ferromagnetic (T_f) and superconducting (T_{sc}) transition temperatures as a function of pressure..*

Chapter 5

Conclusion

In the present work we have investigated the coexistence of ferromagnetism and superconductivity in $ZrZn_2$. This system is more more interesting than conventional superconductors with spin singlet pairing as it shown triplet superconducting pairing coexisting with ferrromagnetism.

In section (3.1) we derived the gap equation for equal spin pairing, i.e. $|\uparrow\uparrow\rangle or |\downarrow\downarrow\rangle$ in ferromagnetic superconductor $ZrZn_2$ using one band Hubbard model in three dimension which includes the nearest neighbor interaction and the effect of the Zeeman term. In this work we neglect the effect of the vector potential. Further in sub section (3.1.1), we estimated the T_{sc} of $ZrZn_2$ in different aspects (i.e. $V_c = 0$ and $V_c \neq 0$). Here it is found that the transition temperature T_{sc} for majority spin states $|\uparrow\uparrow\rangle$ is higher than that of the minority spin states $|\downarrow\downarrow\rangle$

It is also shown that the exchange splitting separates the two spins states in to two subsystems. Here,it should be noted that the spectrum of one spin state is entirely independent of the order parameter of the spin state.

We have also shown that the equal spin triplet state shows different behavior our in an exchange splitting:

• In the first case the superconducting temperature is increased by exchange split ting.

• In the second case, as we have seen in the discussion part, the A_1 phase have finite pairing in spin up-up, i.e $|\uparrow\uparrow\rangle$ state only. On the other hand the A_2 phase has a finite pairing in the spin down-down state i.e $|\downarrow\downarrow\rangle$. We further obtained that phase

A has the same transition temperature in both spin pairing states. Besides to this phase A is turned into phase A_1 or A_2 respectively.

We therefore, noted that the coexistence of ferromagnetism and superconductivity in $ZrZn_2$ gives rise to phase transition from A to A_1 or A_2.

In section (3.2) we have shown that the variation of the superconducting transition temperature T_{sc} and the ferromagnetic transition temperature T_f of $ZrZn_2$ with pressure. As we have mentioned in chapter four both T_f and T_{sc} of $ZrZn_2$ decrease with increasing the pressure and they vanish at P_c simultaneously. We therefore, deduce that pressure has a strong effect on the ferromagnetic and superconducting phase properties of $ZrZn_2$.Here we also point out that as the pressure increases more and more spins are inverted from their common direction, this effect reduce the transition temperatures. From this we conclude that spin fluctuations reduces the degeneration of the ground state of the system. Further we tried to show that the superconducting properties of $ZrZn_2$ is observed in the ferromagnetic phase.

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