

THE STUDY OF UPPER CRITICAL FIELD
CALCULATION OF
SUPERCONDUCTING MAGNESIUM
DIBORIDE

By
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**A THESIS PRESENTED TO
THE SCHOOL OF GRADUATE STUDIES
ADDIS ABABA UNIVERSITY
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF
MASTER OF SCIENCE in PHYSICS
ADDIS ABABA, ETHIOPIA
JULY 2006**

ADDIS ABABA UNIVERSITY

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Date: **July 2006**

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Title: **the study of upper critical field calculation of superconducting magnesium diboride**

Department: **Department of Physics**

Degree: **M.Sc.** Convocation: **July** Year: **2006**

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**This Work is Dedicated to
my father Dulla Berry**

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Acknowledgements

I would like to express my gratitude to my advisor pro. P. Singh for his consistent advice, valuable comments, suggestions, friendly encouragement, proof reading of my thesis and giving me valuable comments throughout my work.

I would also like to thank my family for their day to day encouragement and financial support. Specially, my heartily thanks are extended to Ato Akmel Abagaro for his financial support and for brotherly encouragement. This work as well as my graduate study as a whole couldn't have been completed with out the help of Akmel Abagaro .

Finally, I like to acknowledge my friends Derese Gugsu, Mesfin Asfaw, Gebru Tadese and Paulos who have helped me with moral and material support.

Abstract

Magnesium diboride(MgB₂) has joined the class of high T_c superconductors following the discovery of superconductivity in this compound in 2001 below $T_c \approx 40k$. A large part of the excitement is due to the vast amount of unusual properties originating from the involvement in superconductivity of two sets of bands that are of a very different nature. Because of the different dimensionality of the two sets of bands, this "two band superconductivity" leads to a complex behavior of the anisotropic superconducting state properties as a function of magnetic field and temperature. The purpose of this thesis is to study the upper critical field (H_{c2}) of two-band s-wave superconducting magnesium diboride(MgB₂) in the vicinity of T_c using a two-band Ginzburg-Landau(GL) theory. The analytical formula of $H_{c2}(T)$ involving anisotropy of order parameter and anisotropy of effective-mass are found. The parameters of the upper critical field in ab-plane(H_{c2}^{ab}) and c-axis (H_{c2}^c) can be found by fitting to the experimental data. In addition to this we have considered the linearized two band Eilenberger equations to calculate the upper critical field of superconducting magnesium diboride. Finally by taking the ratio of the upper critical field (the fields in ab-plane and c-axis) we tried to show the anisotropy property of superconducting magnesium diboride. We observe that the ratio of the two fields strongly depends on temperature. So, this ratio of upper critical field is in the range of experimental result and temperature dependent.

Key words: S-wave superconductor,anisotropy two-band superconductors,Ginzburg-Landau approach,Eilenberger equations,Magnesium diboride .

Chapter 1

General introduction to superconductivity

1.1 Transition to the superconducting state

Superconductivity was first discovered in 1911 by the Dutch physicist, Heike Kamerlingh Onnes. That is major advances in low-temperature refrigeration were made in the late nineteenth century. Onnes dedicated his scientific career to exploring extremely cold refrigeration. On July 10, 1908, he successfully liquified helium by cooling it to 452 degrees below zero Fahrenheit (4 kelvin or 4K). Onnes produced only a few milliliters of liquid helium that day, but this was to be the new beginnings of his explorations in temperature regions previously unreachable. Liquid helium enabled him to cool other materials closer to absolute zero (0K), the coldest temperature imaginable. In 1911, Onnes began to investigate the electrical properties of metals in extremely cold temperatures. It had been known for many years that the resistance of metals fell when cooled below room temperature but it was not known what limiting value the resistance would approach, if the temperature were reduced to very close to 0K.

Some scientists, such as William Kelvin, believed that electrons flowing through a conductor would come to a complete halt as the temperature approached absolute zero. Other scientists, including Onnes, felt that a cold wire's resistance, allowing for better conduction of electricity. At some very low temperature point, scientists felt that there could be a leveling off as the resistance reached some ill-defined minimum value allowing the current to flow with little or no resistance.

Onnes passed a current through a very pure mercury wire and measured its resistance as he steadily lowered the temperature. Much to his surprise there was leveling off of resistance, let alone the stopping of electrons as suggested by kelvin. At 4.2k the resistance suddenly vanished. Current was flowing through the mercury wire and nothing was stopping it, the resistance was zero. According to Onnes as shown in fig.1.1 " mercury has passed into a new state, which on account of its extraordinary electrical properties may be called the superconductive state". The experiment left no doubt about the disappearance of the resistance of mercury wire. Kammerlingh Onnes called this newly discovered state, superconductivity.

Onnes recognized the importance of his discovery to the scientific community as well as its commercial potential. An electrical conductor with no resistance could carry current any distance with no losses. In one of onnes experiments he started a current flowing with out significant current loss. Onnes found that the superconductor exhibited what he called persistant currents, electric currents that continued flow with out an electric potential driving them. Onnes was awarded the nobel prize in 1913 for his discovery of this resistance less state. The temperature at which a material passes from a normal state to a superconducting state

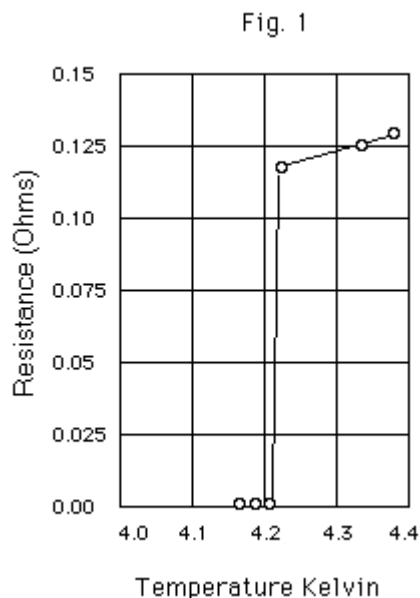


Figure 1.1: *The behavior of transition from normal to superconducting state in the first superconductor reported(Hg) by Onnes, with $T_c=4.2k$.*

is called a superconducting transition temperature (critical temperature) T_c of that material.

1.2 Developments in superconductivity over years

Superconductivity as we have seen in the above section was discovered by Kammerlingh Onnes in 1911 in mercury at a transition temperature of 4.2k. Kammerlingh noted that the superconducting state could be destroyed by applying a large magnetic field, but a current induced in a closed conducting loop of wire persists for a long time.

By 1933 Walter Meissner and R.O Chsenfeld discovered that superconductors are more than a perfect conductor of electricity, they also have an interesting magnetic property of excluding a magnetic field. A superconductor will not allow a magnetic field to penetrate its interior. It causes currents to flow that generate a magnetic field inside the superconductor that just balances the field that would have otherwise penetrated the material. This effect, called the Meissner effect, causes a phenomenon that is a very popular demonstration of superconductivity.

After Kammerlingh from 1911 up to 1957 there was no theory to explain superconductivity phenomenon. But in 1957 scientists began to unlock the mysteries of superconductors. Three American physicists at the University of Illinois, John Bardeen, Leon Cooper, and Robert Schrieffer, developed a model that has since stood as a good mental picture of why superconductors behave as they do. The model is expressed in terms of advanced ideas of quantum mechanics, but the main idea of the model suggests that electrons in a superconductor condense into a quantum ground state and travel together collectively and coherently. Their theory of superconductivity is known as the BCS theory. The theory explains superconductivity of most superconducting materials at temperatures close to absolute zero.

The phenomenological description of superconducting flow was pointed in 1935 by London. Accordingly, superconductivity is a quantum phenomenon on a macroscopic scale with the lowest energy state separated by finite interval from the excited states and hence diamagnetism is a fundamental property of a superconductor.

In 1986, George Bednorz and Alex Muller, working at IBM in Zurich Switzerland, were experimenting with a particular class of metal oxide ceramics called perovskites. Bednorz and Muller surveyed hundreds of different oxide compounds. Working with ceramics of Lanthanum, Barium, copper, and oxygen they found indications of superconductivity at 35k, a

startling 12k above the old record for a superconductor of Nb_3Ge ($T_c \sim 23k$). So, this started a new era in superconductivity.

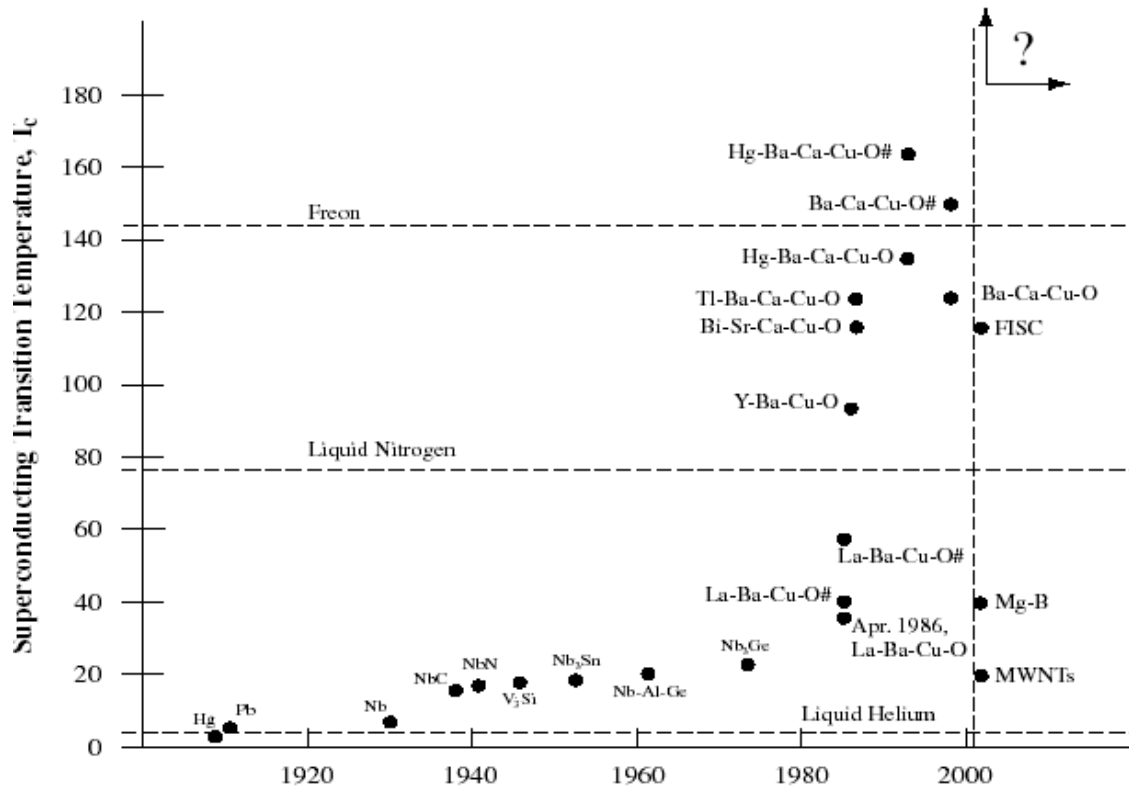


Figure 1.2: *developments in superconductivity over years.*

1.3 Effect of magnetic field on superconductor

It was not until 1933 that physicists became aware of the other property of superconductors that is about perfect diamagnetism. This was when Meissner and Oschenfeld discovered that a superconducting material cooled below its critical temperature in a magnetic field excluded the magnetic flux. This effect has now become known as the Meissner effect fig.1.2. The limit of external magnetic field strength at which a superconductor can exclude the field is known as the critical field strength, H_c .

Another property discovered by Onnes, shortly after his observation of the disappearance of resistance below T_c , is that small magnetic fields destroy superconductivity. This critical field (H_c) is a function of the temperature given approximately by Tuyn's law

$$H_c = H_0 \left(1 - \left(\frac{T}{T_c}\right)^2\right). \quad (1.1)$$

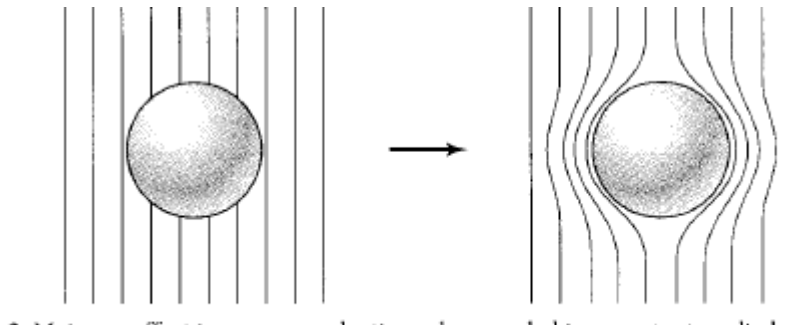


Figure 1.3: *Meissener effect.*

Onnes has recognized that a superconducting state can again be changed to normal state by passing exclusive current through the wire. He then recognized that the magnetic field induced by this current is making the wire to come back to its normal conducting state.

1.4 BCS theory and its contribution

The BCS theory successfully shows that electrons can be attracted to one another through interactions with the crystalline lattice. This occurs despite the fact that electrons have the same charge. When the atoms of the lattice oscillate the electron pair is alternatively pulled together and pushed apart without collision. The electron pairing is favorable because it has the effect of putting the material into a lower energy state. When electrons are linked together in pairs, they move through the superconductor in an orderly fashion. In general the transition of a material to the superconducting state in BCS theory is due to an effective attraction between pairs of electrons of opposite spin and momentum.

All in all there are two main ingredients in the microscopic theory of superconductivity developed by Berdeen, Cooper, and Schrieffer. The first is an effective attraction interaction

between two electrons that have opposite momenta and opposite spins, which leads to the formation of the so called "Cooper pairs" as shown in fig.1.4. The second is the condensation of the cooper pairs into a single coherent quantum state which is called the "superconducting condensate". This is the state responsible for all the manifestations of superconducting behavior[1].

The BCS theory explains superconductivity at temperatures close to absolute zero. Cooper realized that atomic lattice vibrations were directly responsible for unifying entire current. They forced the electrons to pair up into teams that could pass all of the obstacles which caused resistance in the conductor. Below the superconducting transition temperature, T_c (in superconducting state), the electron pairs form a condensate, a macroscopically occupied single quantum state, which flows with no resistance and acts to screen out modest external magnetic fields, thus bringing about the perfect diamagnetism measured in the Meissner effect. At low temperatures, it requires a finite amount of energy,

$$\Delta \approx 1.75K_B T_C, \quad (1.2)$$

to split up of the pairs in the condensate , this is the energy gap.

To conclude this part we can explain the phenomenon of BCS the electron may be thought of as a car racing down a high way. As it speeds along, the car cleaves the air in front of it. Trailing behind the car is a vacuum, a vacancy in the atmosphere quickly filled by in rushing air into this vacuum. The rear car is, effectively, attracted to the one in front. As the negatively charged electrons pass through the crystal lattice of a material they draw the surrounding positive ion cores toward them. As the distorted lattice returns to this normal state another electron passing near by will be attracted to the positive lattice in much the same way that a tailgater is drawn forward by the leading car. The electrons in the superconducting state are like an array of rapidly moving vehicles. Vacuum regions between cars locks them all into an ordered array as does the condensation of electrons into a macroscopic, quantum ground state. Random gusts of wind across the road can be envisioned to induce collisions, as thermally excited phonons break pairs. With each collision one or two lanes are closed to traffic flow, as a number of single-particle quantum states are eliminated from the macroscopic, many-particle ground state.

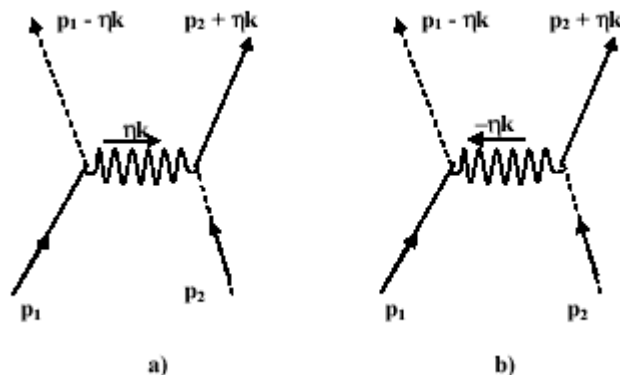


Figure 1.4: *cooper pair*.

1.5 Types of superconductor

There is no difference in the mechanism of superconductivity in type one and type two superconductors. Both types have similar thermal properties at the superconductor-normal transition in zero magnetic field. But the Meissner effect is entirely different. Type one superconductor excludes a magnetic field until superconductivity is destroyed suddenly, and then the field penetrates completely. Type two superconductor excludes the field completely up to a field H_c . Above H_c , the field is partially excluded, but the specimen remains electrically above H_{c2} , the flux penetrates completely and superconductivity vanishes.

To distinguish the important difference between the two types of superconductor first we have to know the meaning of the two characteristic length scale of the superconductor that are the penetration depth (λ) gives the scale over which the magnetic field inside the superconductor is shielded by the supercurrents.

On the other hand the coherence length(ξ) determines the scale over which there exists strong correlations which stabilize the superconducting state, or equivalently, it is a measure of the distance over which the superconducting state, is affected by fluctuations in the external field or other variables. Based on this both(λ)and(ξ) are temperature dependent quantities their ratio, $k = \frac{\lambda}{\xi}$ serves to distinguish type one from type two superconductor[2].

1.5.1 Type one superconductors

The type one superconductors are mainly comprised of metals and metalloids that exhibit some conductivity at room temperature. Superconductors for which $k < (\frac{1}{2})$ are classified as type one, e.g Al, Sn, In, and Pb. Type one superconductors are characterized to be the soft superconductors. They were discovered first and they needed the coldest temperatures to become superconductive. They exhibit a very sharp transition to a superconducting state and they also exhibit a "perfect" diamagnetism fig.1.5. The distinction between the two types of superconductivity in terms of k has to do with the interface energy between the normal and superconducting parts. In type one superconductors the interface energy is positive and the sample tries to minimize it by splitting into macroscopic normal or superconducting domains with the smallest possible interface area.

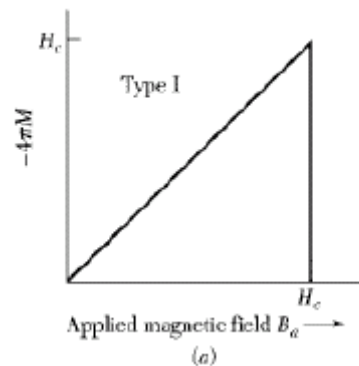


Figure 1.5: *the magnetization versus magnetic field graph to differentiate type one from type two .*

1.5.2 Type two superconductors

The type two category of superconductors is comprised of metallic compounds and alloys, except for the elements Vanadium, Technetium, and niobium. The recently discovered superconducting metal oxide ceramics that normally have ratio of two metal atom to every three oxygen atoms called perovskites belong to the category of type two superconductors. Superconductivity is only partially destroyed in type two superconductors for $H_{C_1} \leq H \leq H_{C_2}$,

Table 1.1: Type one superconductors with the corresponding critical temperature [3]

superconductor	(Tc)	superconductor	Tc(k)
Lead(Pb)	7.196k	Molybdenum(Mo)	0.915k
Lanthanum(La)	4.48k	Zinc(Zn)	0.85k
Tantalum(Ta)	4.47k	Osmium(Os)	0.66k
Mercury(Hg)	4.15k	Zirconium(Zr)	0.61k
Tin(Sn)	3.72k	Americium(Am)	0.60k
Indium(In)	3.41k	Cadmium(Cd)	0.517k
Palladium(Pd)	3.3k	Ruthenium(Ru)	0.49k
Chromium(Cr)	3k	Titanium(Ti)	0.40k
Thallium(Tl)	2.38k	Uranium(U)	0.20K
Rhenium(Re)	1.697k	Hafnium(Hf)	0.128k
Protactinium(Pa)	1.40k	Iridium(Ir)	0.1125k
Thorium(Th)	1.38k	Beryllium(Be)	0.023k
Aluminum(Al)	1.175k	Tungsten(W)	0.0154K
Gallium(Ga)	1.083k	Platinum(Pt)	0.0019k

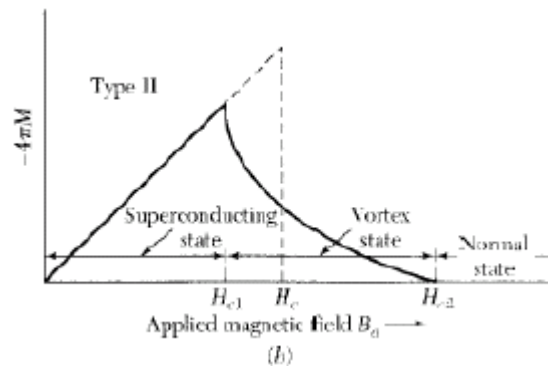


Figure 1.6: the magnetization versus magnetic field graph to differentiate type two from type one.

Table 1.2: Type two superconductors with the corresponding critical temperature [4]

material	Tc(k)	material	Tc(k)
<i>HgBa₂Ca₃Cu₃O₈</i>	133	<i>TmBaSrCu₃O₇</i>	88
<i>Ti₂Ca₂Ba₂Cu₃O₁₀</i>	128	<i>EuBaSrCu₃O₇</i>	88
<i>HgBa₂CaCu₂O₆</i>	127	<i>HoBaSrCu₃O₇</i>	87
<i>HgBa₂Ca₃Cu₄O₁₀</i>	126	<i>GdBaSrCu₃O₇</i>	86
<i>TiCaBa₂Cu₂O₈</i>	119	<i>SmBaSrCu₃O₇</i>	84
<i>TiCa₂Ba₂Cu₃O₈</i>	110	<i>MgB₂</i>	39
<i>BiCa₂Sr₂Cu₃O₁₀</i>	110	<i>Nb₃Ge</i>	23.2
<i>TiCaBa₂Cu₂O₇</i>	103	<i>Nb₃Si</i>	19
<i>HgBa₂CuO₄</i>	94	<i>Nb₃Sn</i>	18.1
<i>YBa₂Cu₃O₇</i>	93	<i>Nb₃Al</i>	18
<i>YBa₄Cu₇O₁₅</i>	93	<i>V₃Si</i>	17.1
<i>Ti₂Ba₂CuO₆</i>	92	<i>Ta₃Pb</i>	17
<i>Bi₂CaSr₂Cu₂O₈</i>	92	<i>V₃Ga</i>	16.8
<i>DyBaSrCu₃O₇</i>	90	<i>Nb₃Ga</i>	14.5
<i>TiSr₂Y_{0.5}Ca_{0.5}Cu₂O₇</i>	90	<i>V₃In</i>	13.9

this region is called the intermediate state since it is really a mixture of normal and superconducting state. In general the intermediate or vortex state is unstable for type one (soft) superconductors but stable for type two (hard) superconductors.

1.6 High-temperature superconductivity

After the fascinating discovery of high temperature superconductivity at 35k in La-Ba-Cu-O by Bednorz and muller [4] in 1986,superconductivity was discovered in Y-Ba-Cu-O system at 90k by Wu et al [5]. With the discovery of two new superconductors Bi-Sr-Ca-Cu-O($T_c \sim 110k$) [6] and Ti-Ba-Ca-Cu-O($T_c \sim 125k$) [7] a new dimension has been added to the field of ever increasing T_c materials. Although many of their properties have been studied extensively during the last few years, the mechanism of superconductivity remains illusive.

In general the magnetic order plays an important role in the physics of these materials, and the presence of strong antiferromagnetic interactions may be intimately related to the mechanism(s) of electron pairing. On the other hand, some variation of the basic theme of electron-phonon interaction, taking also account the strong anisotropy in these systems may be able to capture the reason for electron pairing. All shared feature that is responsible for the occurrence of high T_c superconductivity is the presence of planes containing Cu and O atoms

separated by the planes. Currently high T_c superconductivity is the subject of immense interest because of the following.

1. Its interdisciplinary nature(material scientists,chemists and physicists)
2. Potential application of materials with T_c greater than temperature at which nitrogen liquefies(77)
- 3.Applications in cellular phone systems, superconducting transmission lines, microwave systems,etc.
- 4.The possibility of finding a superconductor at room temperature.

Chapter 2

Review on the study of superconducting Magnesium Diboride (MgB_2)

2.1 Introduction

The intermetallic compound MgB_2 has been sitting in chemical laboratories since the 1950's, but not until January 2001, was discovery of its superconductivity with $T_c \approx 39K$ announced by Nagamatsu and his co-workers [9]. This critical temperature is the highest among superconducting transition temperature of all metallic compounds, but still smaller in comparison with that of some other high T_c superconductors. During past three years there is an intensive research interest in this compound from physics community through out the world. A large number of articles covering both experimental and theoretical areas involving to this compound has been published. So, what makes MgB_2 become a hot topic? As the consequence of large coherence length ($\xi = 50A$), this compound has weak-link free grain boundaries, and there fore, high transport current densities of the order of $10^6 \frac{A}{cm^2}$ and high upper critical magnetic field(39T) in the temperature range from 4.2k to 25k in bulk sample as reported in[10] and [11]. Another important reason to count MgB_2 as a promising candidate for industrial application at temperature lower than 30k is its low cost of material production because this kind of material do not need to use Ag for sheathing as many other high T_c superconducting tapes (or wire).

At this point of time, there is no explicit and firm explanation for mechanism of superconductivity in MgB_2 yet. However, one believes that it can be a conventional BCS phonon-mediated superconductivity. This assumption has been suggested and predicated from boron isotope effect and calculation of energy gap from various experiments.

2.2 Properties of superconducting Magnesium diboride

2.2.1 The crystal structure of MgB_2

Magnesium diboride has very simple graphite-type crystal structure. It consists of hexagonal honey-combed plane of boron atoms separated by hexagonal closed-packed layers of magnesium. At room temperature, lattice parameters $a = b = 3.0851\text{\AA}$, $c = 3.5201\text{\AA}$ has been reported [12]. The lattice vibrations in MgB_2 are much larger due to the strong electron pairs formation.

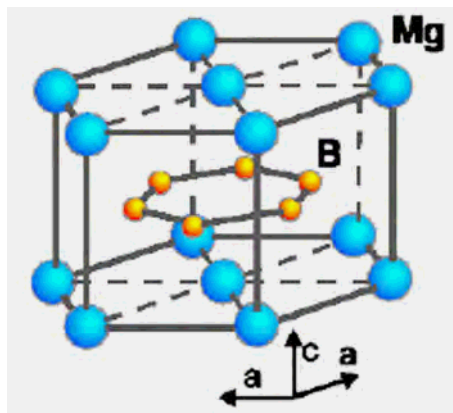


Figure 2.1: *crystal structure of magnesium diboride.*

2.2.2 Physical properties of superconducting Magnesium diboride

The major physical properties that characterize the material magnesium diboride (MgB_2), are listed below .

1. Magnesium diboride (MgB_2) is an isotropic material.
2. Unlike other superconductors it has been verified that MgB_2 has two energy gaps.

3. The magnetic penetration depth (length) is about 850Å.
4. No other borides have comparable superconducting transition temperature yet.
5. The superconducting transition temperature of magnesium diboride is approximately 39k.
6. The coherence length of MgB_2 is estimated to be 50Å.
7. It is a very good metal even better than some pure metals with resistivity ratio $\frac{R(300k)}{R(40k)} > 15$ and at 300k, $R = 9\text{ to }10\mu\Omega$ but at 40k : $R = 0.38\mu\Omega$
8. The electronic mean free path at 40k is estimated as 600Å.

2.2.3 Isotopic effect

A large boron isotope effect was firstly reported by Calfield's group [17,18], based on observation of the temperature dependent magnetization, resistance and specific heat on $Mg^{10}B_2$ and $Mg^{11}B_2$ samples .

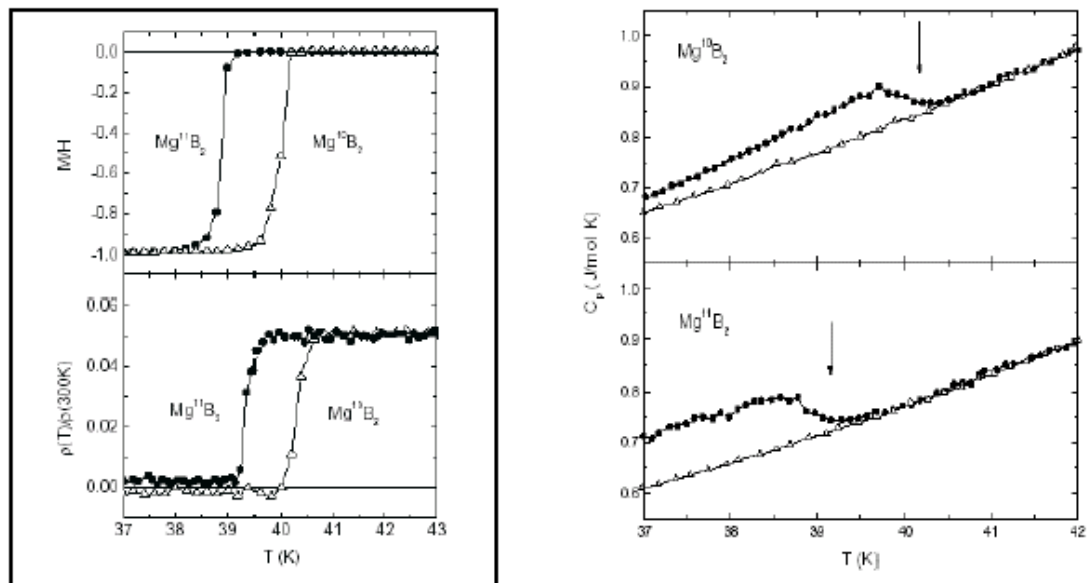


Figure 2.2: (a) magnetization, resistance on $Mg^{10}B_2$ and $Mg^{11}B_2$ vs temperature (b) specific heat on $Mg^{10}B_2$ and $Mg^{11}B_2$ vs temperature.

Obviously, one-kelvin shift of the transition temperature has been observed consistently in all three experiments as shown in fig.2.2. Within the BCS formalism for superconductivity, $T_c \propto$

$$(\hbar\omega_{ph})\exp\left(\frac{-1}{JN_{E_F}}\right),$$

Where $\hbar\omega_{ph}$ is energy of phonon, N_{E_F} is density of state at Fermi level and J is electron-phonon coupling constant. The low mass elements result in higher frequency phonon and therefore, increase transition temperature. Thus, the large boron atoms play very important role in superconductivity of MgB_2 Which is not an exotic mechanism but a phonon mediated BCS one. To check the effect of vibration of Mg atoms to superconductivity of MgB_2 , they also measured magnesium isotope effect. For more convenience one can define isotope exponent for boron $\alpha_B = \frac{\Delta \ln(T_C)}{\Delta \ln(M_B)}$ we can calculate isotope exponent for boron $\alpha_B = 0.26$ also, $\alpha_{Mg} = 0.02$ has been obtained[19]. This value of α_{Mg} prove that vibration modes of Mg atoms have a small contribution on T_c , but boron layers will be the key to find superconducting mechanism in MgB_2 .

2.2.4 Energy gaps in MgB_2

Energy gap plays an important role in BCS theory. Thus studying and calculating energy gaps can help to suggest a mechanism of superconductivity in this compound. Very numerous experiments and calculations have been reported on this issue. However, both number and values of gaps are found to be inconsistent so far. Some experiments, such as specific heat [20],[21],[22], penetration depth,[23], tunneling spectroscopy [24], photo emission spectroscopy [25] point out that there are two energy gaps observed in superconducting state with values between (1.8 – 3)mev for small gap and between (5.8 – 7)mev for the big one[26]. Whereas, some other experiments, found only one gap with values ranging from 2.5 to 5 mev. There is no firm explanation for this inconsistency but it can be improved by the experiments using the high quality large single crystal sample, or by reducing surface effect which is very important for width of the gaps.

2.3 Superconductivity of Magnesium diboride theoretical aspects

Our theoretical understanding of superconductivity in magnesium diboride(MgB_2) has made rapid progress since its discovery by Naganatsu et al[9]. Unlike superconductivity in the high- T_c cuprates we are in a possession of clear picture of its superconducting state now[13]. It seems clear that superconductivity is driven by electron-phonon interaction in MgB_2 . More excitingly, it appears well established both theoretically and experimentally that the rare form

of two gap superconductivity is realized in this compound. Two superconducting gaps of distinctively different size appear to exist on different disconnected parts of its Fermi surface. Since MgB_2 is the clearest example of two gap superconductivity to date, it makes it an interesting object for study and exploration. In the present work we want to review our present understanding of two gap superconductivity in MgB_2 from the theoretical perspective and discuss some of its consequences. The presence of these two different gaps gives rise to a number of anomalous behaviors.

Magnesium diboride possesses a comparatively high critical transition temperature compared with other conventional superconductors of about $T_c = 40k$. Presently only the high T_c cuprates have higher transition temperatures. For that reason the natural question arises whether superconductivity in MgB_2 is of the conventional electron-phonon driven type or if its superconducting state has more similarities with the one in the high T_c cuprates. In the high- T_c cuprates the superconducting state is of an unconventional d-wave type, possessing gap nodes, and electronic pairing mechanisms, like for example exchange of antiferromagnetic spin fluctuations. In contrast to optimally doped high- T_c cuprates MgB_2 shows a strong isotope effect. If the boron-11 isotope is replaced by the lighter boron-10 isotope, T_c increases by about one kelvin indicating an important phonon contribution to the pairing interaction[14]. Low temperature specific heat and penetration depth studies are consistent with an exponential decay, indicating the presence of a full gap without nodes[15,16]. In addition, there are no indications of sizable magnetic interactions in MgB_2 , again in contrast to the high- T_c cuprates. All these observations seem to place MgB_2 among the conventional S-wave electron-phonon driven superconductors. Then the question arises, why it has such a high transition temperature as compared with other conventional superconductors. Here, band structure calculations turned out to be elusive, which we want to review in the following.

The MgB_2 lattice structure consists of alternating layers of Boron and Magnesium atoms forming a honeycomb lattice and the Magnesium atoms a triangular lattice half way between the boron layers. Calculations of the electronic band structure show four bands crossing the Fermi energy leading to four topologically disconnected Fermi surface sheets. Two of these bands are derived from Boron p_z orbitals. They form the so called π bands. The other two bands derive from Boron p_x and p_y orbitals and form the so-called σ bands. Interestingly, all these bands are dominated by Boron p orbitals and contributions from Magnesium orbitals

are very small at the Fermi level. About 58 percent of the total density of states at the Fermi level is residing on the π bands making both σ and π bands about equally important for the electronic properties of MgB_2 . From density-functional calculations of the phonon modes, the highest phonon density of states is found in the energy range around 30mev. However, these phonons only couple weakly to the electrons at the Fermi level and thus do not contribute very much to superconductivity. In fact, the phonons that couple most strongly to the electrons at the Fermi level are found in the energy range around 70mev. These phonon modes evolve from the E_{2g} mode at the Γ point and correspond to a Boron-Boron bond-stretching vibration of the Boron sub lattice. A comparison with the phonon modes in the isostructural but non superconducting compound AlB_2 shows that these E_{2g} phonon modes are strongly softened in MgB_2 consistent with their strong coupling. Correspondingly, the so-called Eliashberg function $\alpha^2F(w)$, which weights the phonon density of states with the coupling strengths and appropriately describes the pairing interaction due to phonons, possesses a strong peak around 70mev and significantly differs from the phonon density of states in contrast to conventional strong-coupling superconductors. The dimension less electron-phonon coupling constant was found to lie between $\lambda \approx 0.7 - 0.9$ from these first-principles calculations from this microscopic information we can obtain a qualitative understanding of why T_c is so high in MgB_2 by looking at the BCS T_c formula $K_B T_c = 1.13 \hbar w_c e^{\frac{-1}{VN(0)}}$ here, w_c is the characteristic phonon frequency, V the interaction strength and $N(0)$ the density of states at the Fermi level, with $\lambda \sim VN(0)$. First of all, the characteristic phonon frequency is comparatively high, because Boron is a light element and the E_{2g} phonon modes in question only involve vibrations of the Boron sub lattice. Secondly, this high frequency phonon at the same time possesses a strong coupling to the electrons at the Fermi level. This means that in MgB_2 we have a favorable coincidence of two effects helping to raise T_c .

2.4 Upper critical field and its an isotropy

The upper critical field is very important magnetic superconductivity parameter. There fore starting from its discovery as a superconducting material a lot of researches were carried out on the analysis of upper critical field(H_{c2}) of magnesium diboride. The upper critical field was investigated by transport, ac susceptibility and dc magnetization measurements in magnetic fields of up to 16T with a temperature range $T = 3K$ and $T_c = 39k$. So far a complete $H_{c2}(T)$

curve was reported for MgB₂ wire showing high residual resistivity ratio of about 25.

The other interesting thing in this section is we want to explore the consequence of the two gap picture presented in the previous section on the temperature dependence of the upper critical field H_{c2} , particularly its anisotropy. Measurements of the upper critical field in MgB₂ single crystals have shown that not only H_{c2} is anisotropic as shown in fig.2.3, but also that this anisotropy is strongly temperature dependent[27,28]. The anisotropy ratio γ is given by $\gamma = \frac{H_{c2}^{ab}}{H_{c2}^c}$, where H_{c2}^{ab} is the upper critical field, when the field is applied along the boron planes, and H_{c2}^c the one for field along c-axis direction perpendicular to the boron planes. At low temperatures γ reaches maximum values around 5. It decreases with increasing temper-

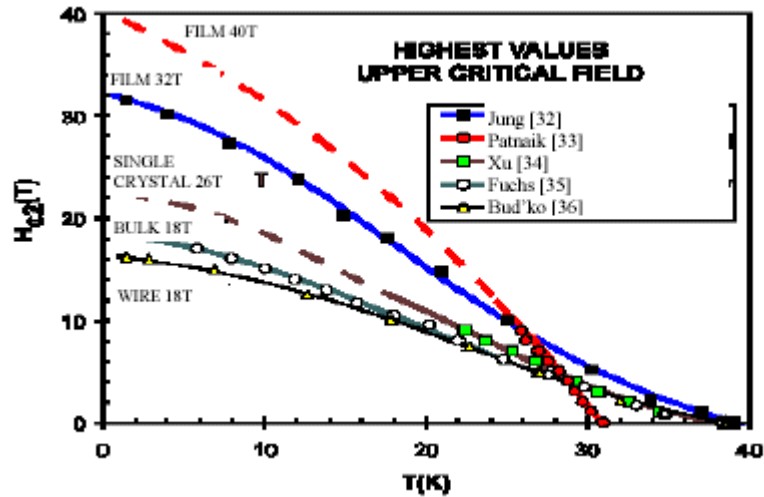


Figure 2.3: the highest values of $H_{c2}(T)$ for MgB₂ in different geometries(bulk,single crystal,wire and films).

ature and reaches values around 2.

The first theoretical work addressing this unusual behavior in MgB₂ was a study with in an anisotropic gap model by Posazhennikova et al[29]. In this work a single anisotropic s-wave gap on an elliptical Fermi surface was considered.

Table 2.1: list of superconducting parameters of MgB_2

Parameter	Values
Critical temperature	$T_c = 39\text{to}40\text{k}$
Hexagonal lattice with parameters	$b = a = 0.3086\text{nm}, c = 0.3524\text{nm}$
Theoretical density	$\rho = 2.55 \frac{\text{g}}{\text{cm}^3}$
Carrier density	$N = 1.7\text{to}2.8 \cdot 10^{23} \frac{\text{holes}}{\text{cm}^3}$
Isotope effect	$\alpha_t = \alpha_{Mg} + \alpha_B = 0.3 + 0.02$
Upper critical field	$H_{c2}^{ab}(0) = 14\text{to}39\text{T}, H_{c2}^c(0) = 2\text{to}24\text{T}$
Lower critical field	$H_{c1}(0) = 27\text{to}48\text{mT}$
Irreversibility field	$H_{irr}(0) = 6\text{to}35\text{T}$
Penetration depths	$\lambda(0) = 85\text{to}180\text{nm}$
Coherence lengths	$\xi_{ab}(0) = 3.7\text{to}12\text{nm}, \xi_c(0) = 1.6\text{to}3.6\text{nm}$
Energy gap	$\Delta(0) = 1.8\text{to}7.5\text{mev}$

Chapter 3

Mathematical formalism to find the Upper critical field of Magnesium Diboride (MgB_2)

3.1 Introduction

The multi-band characteristic of the superconducting state in MgB_2 is clearly evident in many measurements. In contrast to conventional superconductors, the upper critical field for a bulk MgB_2 has a positive curvature near T_C [30-32]. Canfield and Crabtree [33] show the anisotropy of the upper critical field of MgB_2 . The anisotropy, quantified as the ratio $\gamma = \frac{H_{c2}^{ab}}{H_{c2}^c}$, is not only large, but it has an unusual temperature dependence.

In this thesis, we study the upper critical magnetic field (H_{c2}) of anisotropic two-band s-wave superconductor (MgB_2) by Ginzburg-Landau theory. We can find the formula of H_{c2} including anisotropy of order parameter and anisotropy of effective mass. When Ginzburg and Landau formulated their phenomenological theory of superconductivity in 1950, almost 50 years had passed since Kamerlingh Onnes discovered the superfluid electron liquid in mercury. The Ginzburg-Landau (GL) theory is based on Landau's theory of second order phase transitions from 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_c is a second-order phase transition. Landau's 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 non

zero in the ordered phase. In the theory of ferromagnetism, for example, the order parameter is the spontaneous magnetisation. In order to describe the transition to a superconducting state, GL took the order parameter to be certain complex wave function $\psi(r)$, which they interpreted as the "effective", wave function of the "superconducting electrons", whose density n_s is given by $|\psi|^2$; today we would say that $\psi(r)$ is the macroscopic wave function of the superconducting condensate. In accordance with Landau's general theory of second-order phase transitions, the free energy of the superconductor depends only on $|\psi|^2$ and may be expanded in a power series close to T_c . Since the purpose of Ginzburg and Landau was to describe the superconductor in the presence of magnetic field H , when the order parameter may vary in space, gradient terms had to be added to the expansion. We also formulate additionally Eilenberger theory to calculate the upper critical field (H_{c2}) of MgB_2 .

3.2 Generalized Ginzburg-Landau equations

In this thesis we use the generalized Ginzburg-Landau equations as a mathematical formalism to solve for the upper critical field of magnesium diboride. The well known phenomenological theory of superconductivity, proposed by Ginzburg and Landau[39] much before the microscopic theory of Bardeen, Cooper and Schrieffer[40] has been quite successful in describing the behavior of conventional superconductors. It is based on the general theory of second-order phase transition[41] assuming the existence of an order parameter which is non zero in the ordered (superconducting) state and zero in the disordered (normal) state.

The conditions for validity of the GL theory were shown to be a restriction to temperatures sufficiently near T_c and to special variations of ψ and A which were not too rapid. In this reevaluation of the GL theory, $\psi(r)$ turned out to be proportional to the gap parameter $\Delta(r)$, both being in general complex quantities. The greatest value of the theory remains interesting the macroscopic behavior of superconductors in which the over all free energy is important instead of the detailed spectrum of excitations.

The basic postulate of GL is that if ψ is small and varies slowly in space, the free-energy density F can be expanded in a series of the form

$$F(s) = F_{no} + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m^*} |(\hbar i\nabla - \frac{e^*A}{c})\psi|^2 + \frac{H^2}{8\pi}. \quad (3.1)$$

Evidently, if $\psi = 0$, this reduces properly to the free energy of the normal state $F_{no} + \frac{H^2}{8\pi}$.

We now consider the remaining three terms describing the superconducting effects. In the absence of fields and gradients, we have $F_s - F_n = \alpha|\psi|^2 + \frac{1}{2}\beta|\psi|^4$ which can be viewed as a series expansion in powers of $|\psi|^2$ or n_s , in which only the first two terms are retained. These two terms should be adequate so long as one stays near the second order phase transition at T_c , where the order parameter $|\psi|^2 \rightarrow 0$. In the above free-energy expansion two cases arise, depending on whether α is positive or negative. If α is positive, the minimum free energy occurs at $|\psi|^2 = 0$, corresponding to the normal state. On the other hand, if $\alpha < 0$, the minimum free energy occurs when $|\psi|^2 = -\frac{\alpha}{\beta}$. When this value of ψ is substituted back in $F_s - F_n = \alpha|\psi|^2 + \frac{1}{2}\beta|\psi|^4$ one finds $F_s - F_n = -\frac{H_c^2}{8\pi} = -\frac{\alpha^2}{2\beta}$.

Recently this theory has been generalized to the superconductors with several superconducting order parameters [42]. In the case of two-band superconductors, the Ginzburg-Landau theory can be generalized by expanding the free energy functional in powers of order parameters ψ_1 , ψ_2 and inter band mixing order parameter ψ_{12} . i.e $F = F_n + F_1 + F_2 + F_{12} + \frac{H^2}{8\pi}$. where F_n is the free energy of the normal state and

F_1 is the free energy of band one,

F_2 is the free energy of band two,

F_{12} is the free energy of the mixed state. But from the generalized Ginzburg- Landau free energy in the general vicinity of the transition temperature

$$F_s(r) = F_n - \alpha|\psi|^2 + \frac{1}{2}\beta|\psi|^4 + \frac{1}{2m}|(-i\hbar\nabla - \frac{qA}{c})\psi|^2 - \int_0^{B_a} M.dB_a. \quad (3.2)$$

By minimizing the total free energy $\int dvF_r$,with respect to variations in the function $\psi(r)$ we have

$$\delta F_s(r) = -\alpha\psi + \beta|\psi|^2 + (\frac{1}{2m})(-i\hbar\nabla - \frac{qA}{c})\psi(i\hbar\nabla - \frac{qA}{c})\delta\psi^* + c.c. \quad (3.3)$$

We integrate by parts to obtain

$$\int dv(\nabla\psi)(\nabla\delta\psi^*) = -\int dv(\nabla^2\psi)\delta\psi^*, \quad (3.4)$$

if $\delta\psi^*$ vanishes on the boundaries, it follows that

$$\delta \int dvF_s = \int dv\delta\psi^*(-\alpha\psi + \beta|\psi|^2\psi + (\frac{1}{2m})(-i\hbar\nabla - \frac{qA}{c})^2\psi) + c.c. \quad (3.5)$$

Now this integral is zero if the term in the brackets is zero. Then

$$\left(\frac{1}{2m}\right)(-i\hbar\nabla - \frac{qA}{c})^2 - \alpha + \beta|\psi|^2)\psi = 0. \quad (3.6)$$

So, this is the Ginzburg-Landau equation.

3.3 Calculation of coherence length

The coherence length(ξ) is a measure of the distance with in which the superconducting electron concentration cannot change drastically-varying magnetic field. It is also a measure of the minimum spatial extent of the transition layer between normal and superconductor . The coherence length is best introduced into the theory through the Ginzburg-Landau equations above. So, the intrinsic coherence length(ξ) may be defined from equation [3.6]. Let $A = 0$ and suppose that $\beta|\psi|^2$ may be neglected in comparison with α . In one dimension the GL equation [3.6] reduces to

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = \alpha\psi. \quad (3.7)$$

Now let's define our wave function is a plane wave of

$$\psi(x) = \exp\left(\frac{ix}{\xi}\right) \quad (3.8)$$

Then,

$$\frac{-\hbar^2}{2m} \left(\frac{i^2}{\xi^2}\right)\psi = \alpha\psi. \quad (3.9)$$

which implies that $\frac{\hbar^2}{2m} \frac{1}{\xi^2} = \alpha$, that is $\xi^2 = \frac{\hbar^2}{2m\alpha}$ then $\xi = \left(\frac{\hbar^2}{2m\alpha}\right)^{\frac{1}{2}}$ since, α is a temperature dependent parameter then we can conclude that coherence length is temperature dependent.

3.4 Flux quantization in a superconducting ring

Flux quantization is a beautiful example of a long-range quantum effect in which coherence of the superconducting state extends over a ring or solenoid. Flux penetration into the superconductor in the intermediate state occurs in definite amounts; i.e the flux is quantized. To demonstrate this we start from the quantum-mechanical expression for the diamagnetic

current density

$$J = \frac{e^*{}^2 |\psi_0|^2}{mc} A_0. \quad (3.10)$$

Where $e^* = 2e$ is the electric charge on an "elementary superconductor" and $|\psi|^2 = n_0$ is the constant electron density in the London expression for the penetration depth, $\psi_0 \rightarrow \psi = \psi_0 \exp(\frac{ie^*}{\hbar c \chi(r)})$, $A_0 \rightarrow A = \nabla \chi$, where χ is an arbitrary gauge function observe that χ is not single-valued. Since a change in χ by an amount

$$\Delta \chi = \frac{2\pi n \hbar c}{e^*} \quad (3.11)$$

(n being an integer) does not change ψ . The flux through the hole is $\Phi = \int \int \nabla \times A \cdot ds$

$$\Phi = \int \int \nabla \times A \cdot ds = \oint A \cdot dl = \oint \nabla \chi \cdot dl = [\chi] = n \phi_0 \quad (3.12)$$

by Stoke's theorem. where from above equation $\phi_0 = \frac{2\pi \hbar c}{e^*}$ is the magnetic flux quantum.

3.5 Ginzburg-Landau free energy and its relation to upper critical field

In the presence of two order parameters ψ_1 and ψ_2 , in a superconductor, the Ginzburg-Landau free energy can be written as [5,6-8]

$$F(\psi_1, \psi_2) = \int d^3 r (F_1(\psi_1) + F_2(\psi_2) + F_{12}(\psi_1, \psi_2) + \frac{H^2}{8\pi}), \quad (3.13)$$

with

$$F_j(\psi_j) = \frac{\hbar^2}{4m_j} |(\nabla - \frac{2\pi i A}{\phi_0}) \psi_j|^2 + \alpha_j(T) \psi_j^2 + \frac{\beta}{2} \psi_j^4, \quad (3.14)$$

i.e $F_1(\psi_1) = \frac{\hbar^2}{4m_1} |(\nabla - \frac{2\pi i A}{\phi_0}) \psi_1|^2 + \alpha_1(T) \psi_1^2 + \frac{\beta_1}{2} \psi_1^4$,

$F_2(\psi_2) = \frac{\hbar^2}{4m_2} |(\nabla - \frac{2\pi i A}{\phi_0}) \psi_2|^2 + \alpha_2(T) \psi_2^2 + \frac{\beta_2}{2} \psi_2^4$, these are free energies of the two separate bands of superconducting MgB2.

$$F_{12}(\psi_1, \psi_2) = \varepsilon(\psi_1 \psi_2^* + c.c) + \varepsilon_1 [(\nabla + \frac{2\pi i A}{\phi_0}) \psi_1^* (\nabla - \frac{2\pi i A}{\phi_0}) \psi_2 + c.c] \quad (3.15)$$

where $F_{12}(\psi_1, \psi_2)$ is free energy of the mixed state and $\varepsilon, \varepsilon_1$ are the interband mixing of two order parameters and their gradients respectively. \vec{H} is the external magnetic field ($\vec{H} = \nabla \times \vec{A}$). α_j, β_j, m_j are the temperature dependent coefficient, temperature - in dependent coefficient and mass of the carriers in band $j(j = 1, 2)$ respectively. Let's assume that there is only magnetic field in the z-direction, $\vec{H} = H\hat{K}$ and vector potential is in y-direction, $\vec{A} = Hx\hat{j}$ that $H = |\vec{H}|$ and x is displacement. Equilibrium or the minimum value of the free energy given in equation(3.13) with respect to the order parameters ψ_1^* and ψ_2^* respectively we get[34,35]

$$\begin{aligned} \frac{\partial F}{\partial \psi_1^*} &= \frac{\hbar^2}{4m_1} \left(\vec{\nabla} + \frac{2\pi i \vec{A}}{\phi_0} \right) \psi_1 \left(\vec{\nabla} - \frac{2\pi i \vec{A}}{\phi_0} \right) + \alpha_1(T) \psi_1 + \\ &\varepsilon \psi_2 + \varepsilon_1 \left(\vec{\nabla} + \frac{2\pi i \vec{A}}{\phi_0} \right) \left(\vec{\nabla} - \frac{2\pi i \vec{A}}{\phi_0} \right) \psi_2 = 0, \end{aligned} \quad (3.16)$$

$$\begin{aligned} \frac{\partial F}{\partial \psi_2^*} &= \frac{\hbar^2}{4m_1} \left(\vec{\nabla} + \frac{2\pi i \vec{A}}{\phi_0} \right) \psi_2 \left(\vec{\nabla} - \frac{2\pi i \vec{A}}{\phi_0} \right) + \alpha_2(T) \psi_2 + \\ &\varepsilon \psi_1 + \varepsilon_1 \left(\vec{\nabla} + \frac{2\pi i \vec{A}}{\phi_0} \right) \left(\vec{\nabla} - \frac{2\pi i \vec{A}}{\phi_0} \right) \psi_1 = 0 \end{aligned} \quad (3.17)$$

where ϕ_0 is the quantum flux. Mathematically it can be represented by $\phi_0 = \frac{2\pi\hbar c}{e}$. For one-dimensional case the above two equations that are equation(3.16) and (3.17) can be reduced to

$$\frac{-\hbar^2}{4m_1} \left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2} \right) \psi_1 + \alpha_1(T) \psi_1 + \varepsilon \psi_2 + \varepsilon_1 \left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2} \right) \psi_2 = 0, \quad (3.18)$$

$$\frac{-\hbar^2}{4m_2} \left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2} \right) \psi_2 + \alpha_2(T) \psi_2 + \varepsilon \psi_1 + \varepsilon_1 \left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2} \right) \psi_1 = 0 \quad (3.19)$$

where $l_s = \frac{\hbar c}{2He}$ and the field is H_{c2} . Let's assume that the wave function (order parameter) is proportional to the exponential function. i.e $\psi \propto \exp\left(\frac{-ax^2}{2}\right)$ which implies that $\psi_1 = \lambda_1 \exp\left(\frac{-ax^2}{2}\right)$ and $\psi_2 = \lambda_2 \exp\left(\frac{-bx^2}{2}\right)$ then by substituting the expression for ψ_1 and ψ_2 in equation[3.18] and [3.19] we get

$$\frac{-\hbar^2}{4m_1} \left(-a(1 - ax^2) - \frac{x^2}{l_s^2} \right) \psi_1 + \alpha_1(T) \psi_1 + \varepsilon \psi_2 - \varepsilon_1 \left(-b(1 - bx^2) - \frac{x^2}{l_s^2} \right) \psi_2 = 0, \quad (3.20)$$

$$\frac{-\hbar^2}{4m_2} \left(-b(1 - bx^2) - \frac{x^2}{l_s^2} \right) \psi_2 + \alpha_2(T) \psi_2 + \varepsilon \psi_1 - \varepsilon_1 \left(-a(1 - ax^2) - \frac{x^2}{l_s^2} \right) \psi_1 = 0. \quad (3.21)$$

Now let's try to write the matrix form of eqs.(3.20) and(3.21)as

$$\begin{pmatrix} -\frac{\hbar^2}{4m_1}(-a(1-ax^2) - \frac{x^2}{l_s^2}) + \alpha_1(T) & \varepsilon - \varepsilon_1(-b(1-bx^2) - \frac{x^2}{l_s^2}) \\ \varepsilon - \varepsilon_1(-a(1-ax^2) - \frac{x^2}{l_s^2}) & -\frac{\hbar^2}{4m_2}(-b(1-bx^2) - \frac{x^2}{l_s^2}) + \alpha_2(T) \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (3.22)$$

Then the determinant of this gives

$$\begin{aligned} & \left(\frac{\hbar^2}{4m_1}a + \alpha_1(T) + x^2 \left(\frac{\hbar^2}{4m_1 l_s^2} - \frac{\hbar^2 a^2}{4m_1} \right) \right) \left(\frac{\hbar^2 b}{4m_2} + \alpha_2(T) + x^2 \left(\frac{\hbar^2}{4m_2 l_s^2} - \frac{\hbar^2 b}{4m_2} \right) \right) \\ & - (\varepsilon + \varepsilon_1 b + x^2 \left(\frac{\varepsilon_1}{l_s} - \varepsilon_1 b^2 \right)) (\varepsilon + \varepsilon_1 a + x^2 \left(\frac{\varepsilon_1}{l_s} - \varepsilon_1 a^2 \right)) = 0. \end{aligned} \quad (3.23)$$

If we assume that $\frac{\hbar^2}{4m_1 l_s^2} - \frac{\hbar^2 a^2}{4m_1} = 0$ where $a^2 = \frac{1}{l_s^2}$ and $\frac{\hbar^2}{4m_2 l_s^2} - \frac{\hbar^2 b^2}{4m_2} = 0$ where $b^2 = \frac{1}{l_s^2}$ then we can get the following simplified equation

$$\left(\alpha_1(T) + \frac{\hbar^2}{4m_1 l_s} \right) \left(\alpha_2(T) + \frac{\hbar^2}{4m_2 l_s} \right) = \left(\varepsilon - \frac{\varepsilon_1}{l_s} \right)^2. \quad (3.24)$$

Now let's assume that $m_1 = m_2 = m$

$$\alpha_1(T)\alpha_2 + \frac{\hbar H e \alpha_1(T)}{2mc} + \frac{\hbar H e \alpha_2(T)}{2mc} + \left(\frac{\hbar H e}{2mc} \right)^2 = \varepsilon^2 - \frac{4H e \varepsilon \varepsilon_1}{\hbar c} + \frac{4H^2 e^2 \varepsilon_1^2}{\hbar^2 c^2} \quad (3.25)$$

$$\left(\frac{\hbar^2 e^2}{4m^2 c^2} - \frac{4\varepsilon_1^2 e^2}{\hbar^2 c^2} \right) H_{C_2}^2 + ((\alpha_1 + \alpha_2) \frac{\hbar e}{2mc} + \frac{4\varepsilon \varepsilon_1 e}{\hbar c}) H_{C_2} + \alpha_1 \alpha_2 - \varepsilon^2 = 0. \quad (3.26)$$

from section 3.3 and 3.4 we have defined the coherence length and quantum flux i.e $\xi = \left(\frac{\hbar^2}{2m\alpha} \right)^{\frac{1}{2}}$ which implies that $\xi_1 = \left(\frac{\hbar^2}{2m\alpha_1} \right)^{\frac{1}{2}}$, $\xi_2 = \left(\frac{\hbar^2}{2m\alpha_2} \right)^{\frac{1}{2}}$, $\xi_{12} = \left(\frac{\hbar^2}{2m\varepsilon} \right)^{\frac{1}{2}}$ that are the 1st band, 2nd band and inter band effective coherence length, respectively. And $\varepsilon_1 = \frac{\hbar^2 k}{4m}$ where k is the gradient of inter band mixing of two order parameters in energy unit. We find that

$$\frac{\pi^2}{\phi_0^2} (1 - k^2) H_{C_2}^2 - \frac{\pi}{\phi_0} \left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right) H_{C_2} + \frac{1}{4} \left(\frac{1}{\xi_1^2 \xi_2^2} - \frac{1}{\xi_{12}^4} \right) = 0. \quad (3.27)$$

so, this equation is a quadratic equation of the form $ax^2 + bx + c = 0$. To find the the solution set of this equation we can use $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$. In our case $x = H_{C_2}$, $b = -\frac{\pi}{\phi_0} \left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right)$,

$a = \frac{\pi^2}{\phi_0}(1 - k^2)$, $c = \frac{1}{4}\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)$. Now let's substitute these values in their right positions i.e

$$H_{c2} = \frac{\frac{\pi}{\phi_0}\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right) \pm \left(\left(\frac{\pi}{\phi_0}\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)\right)^2 - 4(1 - k^2)\frac{\pi^2}{\phi_0^2}\frac{1}{4}\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)\right)^{\frac{1}{2}}}{\frac{2\pi^2}{\phi_0^2}(1 - k^2)} \quad (3.28)$$

which is equal to

$$H_{c2} = \frac{\phi_0}{2\pi(1 - k^2)}\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right) \pm \frac{\phi_0}{2\pi(1 - k^2)}\left(\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)^2 - (1 - k^2)\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)\right)^{\frac{1}{2}}. \quad (3.29)$$

equation(3.28) has two terms in square root that we can make the approximation by considering these two terms. It can be considered in to cases

case I for $\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)^2 \gg (1 - k^2)\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)$. Now let's apply important application of the Taylor and Maclaurin expansions is the derivation of the binomial theorem for negative and/or non integral powers.i.e is let $f(x) = (1 + x)^m$, in which m may be negative and is not limited to integral values. Then,

$$(1 + x)^m = 1 + mx + \frac{m(m-1)}{2!}x^2 + \dots \quad (3.30)$$

By using the approximation in case I we can write equation(3.29) as follows

$$H_{c2} = \frac{\phi_0}{2\pi(1 - k^2)}\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right) \pm \frac{\phi_0}{2\pi(1 - k^2)}\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)\left(1 - \frac{(1 - k^2)\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)}{\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)^2}\right)^{\frac{1}{2}}. \quad (3.31)$$

Now this is a form of equation (3.29) so, we can expand it by using binomial theorem. But in our case $x = -\frac{(1-k^2)\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)}{\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)^2}$, $m = \frac{1}{2}$ then

$$\begin{aligned} (1 - (1 - k^2)\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)\frac{1}{\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)^2})^{\frac{1}{2}} &= 1 - \frac{1}{2}(1 - k^2)\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)\frac{1}{\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)^2} \\ &\quad + \frac{1}{2}\left(\frac{1}{2} - 1\right)\frac{1}{2!}\left((1 - k^2)\left(\frac{1}{\xi_1^2\xi_2^2} - \frac{1}{\xi_{12}^4}\right)\frac{1}{\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2}\right)^2}\right)^2. \end{aligned} \quad (3.32)$$

by substituting eq.(3.29) in eq.(3.31)

$$H_{c2} = \phi_0 \frac{1}{\pi(1-k^2)} \left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right) \pm \frac{\phi_0}{2\pi(1-k^2)} \left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right) \left(1 - \frac{1}{2}(1-k^2) \left(\frac{1}{\xi_1^2 \xi_2^2} - \frac{1}{\xi_{12}^4} \right) \frac{1}{\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right)^2} \right) + \dots \quad (3.33)$$

There fore we have two values of H_{c2} that are $H_{c2}(-)$ and $H_{c2}(+)$. That are

$$H_{c2}(-) = \frac{\phi_0}{\pi(1-k^2)} \left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right) + \left(\frac{1}{2} \right) \frac{\phi_0}{2\pi} \left(\frac{1}{\xi_1^2 \xi_2^2} - \frac{1}{\xi_{12}^4} \right) \frac{1}{\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right)} + \dots, \quad (3.34)$$

and $H_{c2}(+)$ will have

$$H_{c2}(+) = - \frac{\left(\frac{1}{2} \right) \frac{\phi_0}{2\pi} \left(\frac{1}{\xi_1^2 \xi_2^2} - \frac{1}{\xi_{12}^4} \right)}{\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right)} + \dots \quad (3.35)$$

Case II for $\left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right)^2 \ll (1-k^2) \left(\frac{1}{\xi_1^2 \xi_2^2} - \frac{1}{\xi_{12}^2} \right)$ when we use this case the term in the square root becomes complex . There fore we can conclude that the second case is in valid because we don't have complex field rather it is real

$$H_{c2}(-) = \frac{\phi_0}{2\pi(1-k^2)} \left(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2} + \frac{k}{\xi_{12}^2} \right) - \frac{\phi_0}{2\pi} \left(\frac{1}{\xi_{12}^4} - \frac{1}{\xi_1^2 \xi_2^2} \frac{1}{(1-k^2)} \right)^{\frac{1}{2}} + \dots \quad (3.36)$$

Now, from case I and case II we have obtained two equations for the upper critical field (H_{c2}) that are equations(3.34) and(3.35). Next step, we will check the conditions to get physical solution of (H_{c2}). We have the critical field of one band model as $H_{c2} = \frac{\phi_0}{2\pi\xi^2}$. Just to obtain $H_{c2} = \frac{\phi_0}{2\pi\xi^2}$ from two-band model we have used $\alpha_2 = \varepsilon = \varepsilon_1 = 0$ so, from the above mentioned equations only equation(3.34) is reduced to $H_{c2} = \frac{\phi_0}{2\pi\xi^2}$ that means this equation can be the solution of two band model. Finally, the analytical equation of upper critical field is

equation(3.34) and we can rewrite to be

$$H_{c2} = \frac{\phi_0}{2\pi\xi_{12}^2} \left(\frac{\xi_{12}^2}{\xi_1^2} + \frac{\xi_{12}^2}{\xi_2^2} + 2k \right) \left(\frac{1}{(1-k^2)} - \frac{(\frac{\xi_{12}^4}{\xi_1^2\xi_2^2} - 1)}{(\frac{\xi_{12}^2}{\xi_1^2} + \frac{\xi_{12}^2}{\xi_2^2} + 2k)^2} + \dots \right) \quad (3.37)$$

3.6 Anisotropic mass tensor model

Since magnesium diboride is a two-band S-wave superconductor that shows the layered property. In the layered superconductors, since the overlap of electron wave function is larger with in the layers than between layers , it can be assumed that the electrons have a high effective mass for motion normal to the layers and a low effective mass for motion with in a layer . From the definition of group velocity we know that

$$v_g = \frac{dw}{dk} \quad (3.38)$$

where the frequency(w) associated with a wave function of energy(E) is $w = \frac{E}{\hbar}$, and so

$$v_g = \frac{1}{\hbar} \frac{dE}{dk} \text{ or } v = \frac{1}{\hbar} \nabla_k E(k). \quad (3.39)$$

Now, we consider a change of the component of the group-velocity with time

$$\frac{dv_g}{dt} = \frac{1}{\hbar} \frac{d}{dt} \frac{\partial E(k)}{\partial k} = \frac{1}{\hbar} \left(\frac{\partial^2 E}{\partial k^2} \frac{\partial k}{\partial t} \right) \text{ but } \frac{\partial k}{\partial t} = \frac{F}{\hbar} \quad (3.40)$$

whence

$$\frac{dv_g}{dt} = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right) F; \text{ or } F = \frac{\hbar^2}{d^2 E}{dk^2} \frac{dv_g}{dt}. \quad (3.41)$$

If we identify $\frac{\hbar^2}{\left(\frac{d^2 E}{dk^2}\right)}$ as a mass, then equation(3.40) assumes the form of Newton's second law.

We define the effective m^* by

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2}. \quad (3.42)$$

It is easy to generalize this to take account of an anisotropic energy surface as for electrons in MgB2. We introduce the components of the reciprocal effective mass tensor,

$$\left(\frac{1}{m^*}\right)_{\mu\nu} = \frac{1}{\hbar^2} \frac{d^2 E_K}{dk_\mu dk_\nu}; \frac{dv_\mu}{dt} = \left(\frac{1}{m^*}\right)_{\mu\nu} F_\nu \quad (3.43)$$

where μ, ν are cartesian coordinates. Now, let the mass tensor $\{m\}$ has the form

$$\{m\}^{-1} = \begin{pmatrix} m^{-1} & 0 & 0 \\ 0 & m^{-1} & 0 \\ 0 & 0 & M^{-1} \end{pmatrix} \quad (3.44)$$

where M greater than m . As we know from above calculation the coherence length(ξ) depends on the effective mass as $\xi \propto \frac{1}{m^{\frac{1}{2}}}$, the coherence length also becomes a tensor and given by

$$\{\xi\} = \begin{pmatrix} \xi & 0 & 0 \\ 0 & \xi & 0 \\ 0 & 0 & \delta\xi \end{pmatrix} \quad (3.45)$$

where $\delta = \left(\frac{m}{M}\right)^{\frac{1}{2}}$. The effect of anisotropy mass tensor on the upper critical field is included by replacing ξ in equation(3.36) with coherence length tensor $\{\xi\}$. the calculation procedure is as same as above. Then we get

$$H_{c2} = \frac{\phi_0}{2\pi\xi_{12}^2(\sin^2\Theta + \delta^2\cos^2\Theta)} \left(\frac{\xi_{12}^2}{\xi_1^2} + \frac{\xi_{12}^2}{\xi_2^2} + 2k \right) \left(\frac{1}{1-k^2} - \frac{\left(\frac{\xi_{12}^2}{\xi_1^2\xi_2^2} - 1\right)}{\left(\frac{\xi_{12}^2}{\xi_1^2} + \frac{\xi_{12}^2}{\xi_2^2} + 2k\right)^2} \right) + \dots \quad (3.46)$$

where θ is the angle between magnetic field and the layer of superconductor. Since we consider the MgB2 superconductor it has a hexagonal crystal structure and the anisotropy is most likely to occur along the c-direction similar to other hexagonal crystal such as Upt_3 [43] and Upd_2Al_3 [44]. We can conclude that MgB2 is a layered superconductor with anisotropy by the nature of the crystal structure. It is seem that H_{c2} of MgB2 can be described by eq.[3.46]. On a recent paper of Koshelev and Golvbov[45], they propose that MgB2 can not be described by the anisotropy mass Ginzburg-Landau theory. The recently discovered superconductor MgB2 [46] gives an example of a superconductor which is not described by the anisotropic

GL theory. This very unusual feature is a consequence of a specific band structure of this compound. It is well established that the superconductivity in MgB2 resides in the quasi-two dimensional band (σ - band) and three- dimensional band (π - band). We demonstrate that, due to such band structure, the anisotropic Ginzburg-Landau theory practically does not have region of applicability, because gradient expansion in the c-direction breaks down. Although this model cannot describe the H_{c2} of MgB2 superconductor, we think that this model should be suitable for the other two - band S-wave superconductors.

3.7 Anisotropic order parameters

Let's assume that order parameters are proportional to the energy gaps, i.e $\psi \propto \Delta$. Now, we there fore propose a BCS model for MgB2 with a superconducting order parameter given by

$$\Delta(k) = \Delta \left(\frac{1 + az^2}{1 + a} \right) \quad (3.47)$$

Where the parameter (a) determines the anisotropy, $z = \cos \theta$ and θ is the polar angel. Since the energy gap is a product of the amplitude Δ and anisotropic function, we can write the order parameters in the form

$$\psi = \psi_0(T) f(\vec{k}) \quad (3.48)$$

where $f(\vec{k}) = \frac{1+az^2}{1+a}$ is the anisotropy function. \vec{k} is the wave vector. substitution of eq.(3.47) in to eq.(3.36), we can get the formula of H_{c2} as

$$H_{c2} = \frac{\phi_0}{2\pi\xi_{12}^2} \left(\frac{\xi'_{12}{}^2}{\xi_1^2} + \frac{\xi'_{12}{}^2}{\xi_2^2} + 2\Omega^{\frac{1}{2}}k \right) \left(\frac{1}{1 - \Omega k^2} - \frac{\left(\frac{\xi'_{12}{}^2}{\xi_1^2 \xi_2^2} - 1 \right)}{\left(\frac{\xi'_{12}{}^2}{\xi_1^2} + \frac{\xi'_{12}{}^2}{\xi_2^2} + 2\Omega^{\frac{1}{2}}k \right)^2} \right) + \dots \quad (3.49)$$

where $\Omega = \frac{\langle f_1(\hat{k})f_2(\hat{k}) \rangle^2}{\langle f_1^2(\hat{k}) \rangle \langle f_2^2(\hat{k}) \rangle}$ and $\xi'_{12} = \left(\frac{\hbar^2}{2m\xi_1\Omega^{\frac{1}{2}}} \right)^{\frac{1}{2}} = \frac{\xi}{\Omega^{\frac{1}{4}}}$ and $\langle \dots \rangle$ is the averaged over Fermi surface. $f_1(k)$ and $f_2(k)$ are the anisotropy function of first and second band.

3.8 Additional method by Eilenberger theory

Eilenberger theory is a generalization of BCS theory to in homogenous superconducting states and contains Ginzburg-Landau theory as a limiting case for $T \rightarrow T_c$ [49,50]. It holds in the limit $K_F \xi \ll 1$, where ξ is the coherence length and K_F the Fermi momentum. Since Ginzburg-Landau theory is limited to the vicinity of T_c ; Eilenberger theory is the method of choice, if one wants to calculate properties of type-II superconductors in the vortex state at lower temperatures from microscopic grounds . Near the upper critical field the gap function becomes small and there fore one can use the linearized Eilenberger equations to determine H_{c2} .

On the basis of this one can now calculate the upper critical field by using the linearized two band Eilenberger equations. For $w_n > 0$ they read,

$$(w_n + \vec{v}_{F,\alpha}(\frac{\hbar}{2}\vec{\nabla} - i\frac{e}{c}\vec{A}(\vec{r})))f_\alpha(\vec{r}, \hat{k}; w_n) = -\Delta_\alpha(\vec{r}) \quad (3.50)$$

along with the gap equation

$$\Delta_\alpha(\vec{r}) = -\pi T \sum_{\alpha'} \sum_{|w_n| < w_c} \lambda^{\alpha\alpha'} \langle f'_\alpha(\vec{r}, \hat{k}'; w'_n) \rangle_{\alpha'} \quad (3.51)$$

Here, f_α is the anomalous Eilenberger propagator and $\Delta_\alpha(\vec{r})$ the (spatially dependent) gap function for the two bands $\alpha \in \{\pi, \delta\}$. The pairing interaction $\lambda^{\alpha\alpha'}$ becomes a two-by-two matrix in the band indices.

The variational method for the calculation of the upper critical field from equation(3.50) and (3.51) shall be described. This method was used in refs.(51,52). Now by defining the operator

$$L_\alpha = 2|w_n| + \text{sgn}w_n \vec{V}_{F,\alpha}(\vec{K})[\hbar\vec{\nabla} - i\frac{2e}{c}\vec{A}(\vec{r})] \quad (3.52)$$

where $\vec{V}_{F,\alpha}$ is the Fermi velocity of band α , \vec{A} the vector potential due to the internal magnetic field within the system, and $w_n = (2n + 1)\pi T$ the Matsubara frequencies, Eq.(3.50) can be inverted using the identity

$$L_\alpha^{-1} = \int_0^\infty ds \exp(-sL_\alpha) \quad (3.53)$$

which leads to

$$f_\alpha(\vec{r}, \hat{k}; w_n) = -2 \int_0^\infty ds \exp(-sL_\alpha) \Delta_\alpha(\vec{r}). \quad (3.54)$$

Introducing this into the gap equation Eq.(3.51) we can eliminate f_α :

$$\Delta_\alpha(\vec{r}) = 2\pi T \sum_\alpha \sum_{w_n < w_c} \lambda^{\alpha\alpha'} \langle \int_0^\infty ds \exp(-sL'_\alpha) \Delta_{\alpha'}(\vec{r}) \rangle_{\alpha'}. \quad (3.55)$$

This equation is a linear equation for $\Delta_\alpha(\vec{r})$ as is usual in weak - coupling theory we can eliminate the cut off frequency w_c in favor of the critical temperature T_c . For this purpose we consider Eq.(3.55) in the absence of a magnetic field at T_c . Then the gap function $\Delta_\alpha(\vec{r})$ becomes homogeneous and we find

$$\Delta_\alpha = 2\pi T_c \sum_{|w_n(T_c)| < w_c} \int_0^\infty ds \exp(-2s|w_n(T_c)|) \sum_{\alpha'} \lambda^{\alpha\alpha'} \Delta'_{\alpha'}, \quad (3.56)$$

$$= 2\pi T_c \sum_{w_n(T_c) > 0}^{w_c} \frac{1}{w_n(T_c)} \sum_{\alpha'} \lambda^{\alpha\alpha'} \Delta'_{\alpha'}. \quad (3.57)$$

This is an eigen value equation for Δ_α and the largest eigen value λ_+ of the matrix $\lambda^{\alpha\alpha'}$ determines T_c . Thus we find $\frac{1}{\lambda_+} = 2\pi T_c \sum_{w_n(T_c) > 0}^{w_c} \frac{1}{w_n(T_c)}$ for $w_c \gg T_c$ the following relation holds:

$$2\pi T_c \sum_{w_n(T_c) > 0}^{w_c} \frac{1}{w_n(T_c)} - 2\pi T \sum_{w_n(T) > 0}^{w_c} \frac{1}{w_n(T)} \approx \ln \frac{T}{T_c} \quad (3.58)$$

and thus we can write Eq.(3.57) in the form

$$\frac{1}{\lambda_+} - \ln \frac{T}{T_c} = 2\pi T \sum_{w_n(T) > 0}^{w_c} \frac{1}{w_n(T)} = 2\pi T \sum_{|w_n(T)| < w_c} \int_0^\infty ds \exp(-2s|w_n(T)|). \quad (3.59)$$

Multiplying this equation by $\sum_{\alpha'} \lambda^{\alpha\alpha'} \Delta'_{\alpha'}(\vec{r})$ it can be subtracted from Eq.(3.55) and we can get

$$\begin{aligned} \Delta_\alpha(\vec{r}) + \sum_{\alpha'} \lambda^{\alpha\alpha'} \Delta_{\alpha'}(\vec{r}) \left(\frac{-1}{\lambda_+} + \ln \frac{T}{T_c} \right) &= \sum_{\alpha'} \lambda^{\alpha\alpha'} 2\pi T \sum_{|w_n| < w_c} \langle \int_0^\infty ds [\exp(-sL_{\alpha'}) \\ &\quad - \exp(-2s|w_n|)] \Delta_{\alpha'}(\vec{r}) \rangle_{\alpha'}, \end{aligned} \quad (3.60)$$

$$= \sum_{\alpha'} \lambda^{\alpha\alpha'} 4\pi T \sum_{w_n > 0}^{w_c} \int_0^\infty ds \exp(-2sw_n) \langle [\exp(-is\vec{V}_{F,\alpha'} \cdot \vec{\Pi}) - 1] \Delta_{\alpha'}(\vec{r}) \rangle_{\alpha'}. \quad (3.61)$$

Here, we have eliminated the $sgnw_n$ factor assuming inversion symmetry of the Fermi velocity

$\vec{V}_{F,\alpha}(\hat{k}) = -\vec{V}_{F,\alpha}(-\hat{k})$ and introduced the operator

$$\vec{\Pi} = \frac{\hbar}{i} \vec{\nabla} - \frac{2e}{c} \vec{A}(\vec{r}). \quad (3.62)$$

In Eq.(3.60) we may now extend the w_n summation to infinity and sum it up :

$$\begin{aligned} \sum_{w_n > 0} \exp(-2sw_n) &= \sum_{n=0}^{\infty} \exp(-2s(2n+1)\pi T) \\ &= \exp(-2s\pi T) \sum_{n=0}^{\infty} (\exp(-4s\pi T))^n = \exp(-2s\pi T) \left(\frac{1}{1 - \exp(-4s\pi T)} \right) \\ &= \frac{1}{2\sinh(2s\pi T)}. \end{aligned} \quad (3.63)$$

Note that integration and summation in Eq.(3.61) may only be interchanged because the divergence for $s \rightarrow 0$ has been eliminated. So we find from Eq.(3.61)

$$\begin{aligned} I &= \Delta_{\alpha}(\vec{r}) + \sum_{\alpha'} \lambda^{\alpha\alpha'} \Delta_{\alpha'}(\vec{r}) \left(-\frac{1}{\lambda_+} + \ln \frac{T}{T_c} \right) \\ &= \sum_{\alpha'} \lambda^{\alpha\alpha'} \int_0^{\infty} \frac{du}{\sinh u} \langle [\exp(-iu \vec{V}_{F,\alpha'} \cdot \frac{\vec{\Pi}}{(2\pi T)}) - 1] \Delta_{\alpha'}(\vec{r}) \rangle_{\alpha'}. \end{aligned} \quad (3.64)$$

In the presence of an external magnetic field $\vec{H} = \vec{\nabla} \times \vec{A}$, it is convenient to choose the field direction as the z-axis of the coordinate system . In these coordinates $\Delta_{\alpha}(\vec{r})$ does not depend on z. Choosing the gauge $\vec{A} = Hx\hat{y}$ the operator $\vec{\Pi}$ simplifies to

$$\vec{\Pi} = \frac{\hbar}{i} \vec{\nabla} - \frac{2e}{c} \vec{A}(\vec{r}) = \begin{pmatrix} -i\hbar \frac{\partial}{\partial x} & & \\ -i\hbar \frac{\partial}{\partial y} - \frac{2e}{c} Hx & & \\ & & 0 \end{pmatrix} = \sqrt{\frac{eH}{c}} \begin{pmatrix} a + a^+ & & \\ i(a - a^+) & & \\ & & 0 \end{pmatrix} \quad (3.65)$$

where we have introduced raising and lowering operators $2\sqrt{\frac{eH}{c}}a = -i\hbar \frac{\partial}{\partial x} - \hbar \frac{\partial}{\partial y} + 2i\frac{eH}{c}x$ and $2\sqrt{\frac{eH}{c}}a^+ = -i\hbar \frac{\partial}{\partial x} + \hbar \frac{\partial}{\partial y} - 2i\frac{eH}{c}x$. From Eq.(3.64) one can conclude that only the components of the Fermi velocity perpendicular to the magnetic field direction has contribution. There fore,

$$\vec{V}_{F,\alpha} \cdot \vec{\Pi} = \sqrt{\frac{eH}{c}} [(v_{x,\alpha} + iv_{y,\alpha})a + (v_{x,\alpha} - iv_{y,\alpha})a^+] \quad (3.66)$$

where $v_{x,\alpha}$ and $v_{y,\alpha}$ are the components of the Fermi velocity perpendicular to the magnetic

field. \vec{H} now if we introduce a scaling of the x- and y-coordinates of in the form

$$x = e^\tau \bar{x}, y = e^{-\tau} \bar{y}. \quad (3.67)$$

The above equation (3.66) becomes as follows. Where e^τ is a scaling factor that can scale the coordinates x and y in such a way as to preserve the area. i.e

$$\vec{\Pi} = \begin{pmatrix} -i\hbar e^{-\tau} \frac{\partial}{\partial x} \\ -i\hbar e^\tau \frac{\partial}{\partial y} - \frac{2e}{c} e^\tau H \bar{x} \\ 0 \end{pmatrix} = \sqrt{\frac{eH}{c}} \begin{pmatrix} e^{-\tau}(\bar{a} + \bar{a}^+) \\ ie^\tau(\bar{a} - \bar{a}^+) \\ 0 \end{pmatrix} \quad (3.68)$$

In this case the raising and lowering operators are also expressed in terms of these new coordinates. Now, if we introduce this new expressions of the function $\vec{\Pi}$ to equation(3.66) it becomes

$$\vec{V}_{F,\alpha} \cdot \vec{\Pi} = \sqrt{\frac{eH}{c}} [(e^{-\tau} v_{x,\alpha} + ie^\tau v_{y,\alpha})\bar{a} + (e^{-\tau} v_{x,\alpha} - ie^\tau v_{y,\alpha})\bar{a}^+]. \quad (3.69)$$

By using the expression in Eq.(3.69), one can write the exponential operator in Eq.(3.64) as follows

$$e^{-iu \vec{V}_{F,\alpha} \cdot \frac{\vec{\Pi}}{(2\pi T)}} = e^{F+E} \quad (3.70)$$

where

$$F = -\frac{iu}{2\pi T} \sqrt{\frac{eH}{c}} (e^{-\tau} v_{x,\alpha} - ie^\tau v_{y,\alpha})\bar{a}^+, \text{ and } E = -\frac{iu}{2\pi T} \sqrt{\frac{eH}{c}} (e^{-\tau} v_{x,\alpha} + ie^\tau v_{y,\alpha})\bar{a}. \quad (3.71)$$

But we know that there is a mathematical identity which is

$$e^{F+E} = e^{-\frac{[F,E]}{2}} e^F e^E. \quad (3.72)$$

That is the commutator of $[F, E]$ gives

$$[F, E] = \frac{U^2 eH}{c(2\pi T)^2} (e^{-2\tau} v_{x,\alpha}^2 + e^{2\tau} v_{y,\alpha}^2). \quad (3.73)$$

There fore up on substitution of Eq.(3.71),(3.72), and Eq.(3.73) in equation(3.70) we can get.

$$e^{-u \vec{V}_{F,\alpha} \cdot \frac{\vec{\Pi}}{(2\pi T)}} = e^{-u^2 \frac{eH}{2c(2\pi T)^2} (e^{-2\tau} v_{x,\alpha}^2 + e^{2\tau} v_{y,\alpha}^2)} e^{\frac{-iu}{2\pi T} \sqrt{\frac{eH}{c}} (e^{-\tau} v_{x,\alpha} - ie^\tau v_{y,\alpha})\bar{a}^+} e^{-i \frac{u}{2\pi T} \sqrt{\frac{eH}{c}} (e^{-\tau} v_{x,\alpha} + ie^\tau v_{y,\alpha})\bar{a}}. \quad (3.74)$$

Now, having in mind this, one can consider equation(3.65)as an eigen value problem. Then from that consideration the highest eigenvalue and its corresponding eigenfunction of the right hand side operator will determine the upper critical field ($H_{c2}(T)$). But what we know from Abrikosov's solution of Ginzburg-Landau theory is that the solution for an isotropic s-wave superconductor will be Abrikosov's vortex state wave function $\psi_{\Lambda}(\vec{r})$. And this wave function has the property that it is destroyed by the operator 'a' which is

$$a\psi_{\Lambda}(\vec{r}) = 0. \quad (3.75)$$

Then since in our case the superconductor is an isotropic superconductor we should expect a distortion of the vortex lattice. There fore here we will start from a variational ansatz Eq.(3.64) by choosing a different wave function, which obeys that

$$\bar{a}\Delta_{\alpha}(\vec{r}) = 0. \quad (3.76)$$

This implies the choice $\Delta_{\alpha}(\vec{r}) = \Delta_{\alpha}\psi_{\Lambda}(e^{-\tau}x, e^{\tau}y)$. From this equation the scaling parameter τ can be used as a varational parameter. Now let's introduce this variational wave function in to the Eq.(3.64) just to avoid the e^E and e^F operators and we are left with the equation

$$\Delta_{\alpha} = \sum_{\alpha'} \lambda^{\alpha\alpha'} \left[\frac{1}{\lambda_+} - \ln \frac{T}{T_c} - \nu_{\alpha'}\left(\tau, \frac{H_{c2}}{T^2}\right) \right] \Delta_{\alpha'}. \quad (3.77)$$

That is the expression for ν is

$$\nu\left(\tau, \frac{H_{c2}}{T^2}\right) = \int_0^{\infty} \frac{du}{\sinh u} \langle 1 - e^{u^2 \frac{eH_{c2}}{8c\pi^2 T^2} (e^{-2\tau} v_{x,\alpha}^2(\hat{k}) + e^{2\tau} v_{y,\alpha}^2(\hat{k}))} \rangle. \quad (3.78)$$

since $\lambda^{\alpha\alpha'}$ is 2×2 matrix then Eq.(3.77) as a whole it is a 2×2 matrix there fore to determine the upper critical field we should set a criterion that the largest eigenvalue of the right hand side becomes 1. So, the criterion leads to the following characterstic equation

$$(1 - \eta)\nu_{\sigma} + \eta\nu_{\pi} + \ln t = -\Lambda_{\pm}(\nu_{\sigma} + \ln t)(\nu_{\pi} + \ln t). \quad (3.79)$$

From this equation $t = \frac{T}{T_c}$ and the parameres η and Λ_{\pm} are given by $\eta = \frac{\lambda_+ \pi - \lambda_-}{\lambda_+ - \lambda_-}$ and $\Lambda_{\pm} = \frac{\lambda_+ \lambda_-}{\lambda_+ - \lambda_-}$ where λ_+ and λ_- are the larger and smaller eigenvalues of the matrix $\lambda^{\alpha\alpha'}$, respectively.

Now let's try to write Eq.(3.78) in the following way i.e

$$I(y) = \int_0^{\infty} \frac{du}{\sinh u} (1 - e^{-yu^2}) \quad (3.80)$$

where $y = \frac{eH_{c2}}{8c\pi^2 T^2} (e^{-2\tau} v_{x,\alpha}^2(\hat{k}) + e^{2\tau} v_{y,\alpha}^2(\hat{k}))$. Consider Eq.(3.80), this integral equation is difficult to solve analytically, so, to solve this equation we should use some limiting expressions for small and large arguments of y . That means large y implies that the temperature approaches to zero and small y implies that the temperature approaches to critical temperature (T_c). That is when $T \rightarrow T_c$, H_{c2} also approaches to zero. Then by using Riemann zeta function we can reduce Eq.(3.81) to

$$I(y) = \frac{7}{2}\zeta(3)y - \frac{93}{4}\zeta(5)y^2 \text{ for } y \ll 1 \text{ and} \quad (3.81)$$

$$I(y) = \frac{1}{2} \ln(4\gamma y) \text{ for } y \gg 1$$

. where, $\zeta(n)$ is the Riemann zeta function and $\ln \gamma = 0.577215$ Euler's constant. by using the integral $I(y)$, Eq.(3.78) can be written as

$$\iota(\tau, \frac{H_{c2}}{T^2}) = \langle I[\frac{eH_{c2}}{8c\pi^2 T^2} (e^{-2\tau} v_{x,\alpha}^2(\hat{k}) + e^{2\tau} v_{y,\alpha}^2(\hat{k}))] \rangle_{\alpha}. \quad (3.82)$$

Then by using the limiting expressions in eq. (3.81) as follows i.e when $T \rightarrow T_c$ we have linear order in H_{c2}

$$\iota_{\alpha} = \frac{7}{2}\zeta(3) \frac{eH_{c2}}{8c\pi^2 T_c^2} (e^{-2\tau} \langle v_{x,\alpha}^2 \rangle_{\alpha} + e^{2\tau} \langle v_{y,\alpha}^2 \rangle_{\alpha}). \quad (3.83)$$

Since H_{c2} goes to zero for $T \rightarrow T_c$, both ι_{α} and $\ln t$ decrease linearly and the right hand side of Eq.(3.80) can be neglected, because it becomes quadratic in $\ln t$. Thus in linear order we have

$$-\ln \frac{T}{T_c} = (1-\eta)\iota_{\sigma} + \eta\iota_{\pi} = \frac{7\zeta(3)eH_{c2}}{16c\pi^2 T_c^2} \{e^{-2\tau} [(1-\eta)\langle v_{x,\sigma}^2 \rangle_{\sigma} + \eta\langle v_{x,\pi}^2 \rangle_{\pi}] + e^{2\tau} [(1-\eta)\langle v_{y,\sigma}^2 \rangle_{\sigma} + \eta\langle v_{y,\pi}^2 \rangle_{\pi}]\}, \quad (3.84)$$

$$-\ln \frac{T}{T_c} = \frac{7\zeta(3)eH_{c2}}{16c\pi^2 T_c^2} \{e^{-2\tau} [(1-\eta)\langle v_{x,\sigma}^2 \rangle_{\sigma} + \eta\langle v_{x,\pi}^2 \rangle_{\pi}] + e^{2\tau} [(1-\eta)\langle v_{y,\sigma}^2 \rangle_{\sigma} + \eta\langle v_{y,\pi}^2 \rangle_{\pi}]\}. \quad (3.85)$$

From this expression by rearranging the terms we can get H_{c2} as follows

$$H_{c2} = -\frac{16c\pi^2 T_c^2 \ln \frac{T}{T_c}}{7\zeta(3)e \{e^{-2\tau} [(1-\eta)\langle v_{x,\sigma}^2 \rangle_{\sigma} + \eta\langle v_{x,\pi}^2 \rangle_{\pi}] + e^{2\tau} [(1-\eta)\langle v_{y,\sigma}^2 \rangle_{\sigma} + \eta\langle v_{y,\pi}^2 \rangle_{\pi}]\}}. \quad (3.86)$$

Minimizing this expression with respect to τ one can find

$$e^{2\tau} = \sqrt{\frac{(1-\eta)\langle v_{x,\sigma}^2 \rangle_\sigma + \eta\langle v_{x,\pi}^2 \rangle_\pi}{(1-\eta)\langle v_{y,\sigma}^2 \rangle_\sigma + \eta\langle v_{y,\pi}^2 \rangle_\pi}}. \quad (3.87)$$

Chapter 4

Results and Discussion

4.1 Determination of H_{c2} by GL Approach

We have used the Ginzburg-Landau theory as a mathematical formalism for a two band superconducting state in MgB₂. So, we do have two order parameters, ψ_1 and ψ_2 , then it can be written as follows

$$F(\psi_1, \psi_2) = \int d^3r (F_1(\psi_1) + F_2(\psi_2) + F_{12}(\psi_1, \psi_2) + \frac{H^2}{8\pi}). \quad (4.1)$$

Using this famous phenomenological theory we obtained the expression for upper critical field of superconducting magnesium diboride as

$$H_{c2} = \frac{\phi_0}{2\pi\xi_{12}^2} \left(\frac{\xi_{12}^2}{\xi_1^2} + \frac{\xi_{12}^2}{\xi_2^2} + 2k \right) \left[\frac{1}{1-k^2} - \frac{(\frac{\xi_{12}^2}{\xi_1^2\xi_2^2} - 1)}{(\frac{\xi_{12}^2}{\xi_1^2} + \frac{\xi_{12}^2}{\xi_2^2} + 2k)^2} + \dots \right]. \quad (4.2)$$

where the parameters have their usual meaning such as the coherence length (ξ), quantum flux (ϕ_0) and others. Which reduces to $H_{c2} = \frac{\phi_0}{2\pi\xi^2}$ for single band case as expected by using $\alpha_2 = \varepsilon = \varepsilon_1 = 0$

Since MgB₂ is considered as a two-band s-wave superconductor, it shows the layered property. In the layered superconductors, since the overlap of electron wave function is larger

with in the layers than between layers, it can be assumed that the electrons have a high effective mass formation normal to the layers and a low effective mass formation with a layer. In other words to show this anisotropic property we have used a mass tensor $\{m\}$. Obviously, the coherence length becomes a tensor because it depends on the effective mass as $\xi \propto \frac{1}{\sqrt{m}}$. The effect of anisotropic mass tensor on the upper critical field is included by replacing ξ in our equation for H_{c2} with coherence length tensor $\{\xi\}$. We obtained

$$H_{c2} = \frac{\phi_0}{2\pi\xi_{12}^2(\sin^2\theta + \delta^2\cos^2\theta)} \left(\frac{\xi_{12}^2}{\xi_1^2} + \frac{\xi_{12}^2}{\xi_2^2} + 2k \right) \left(\frac{1}{1-k^2} - \frac{\left(\frac{\xi_{12}^2}{\xi_1^2\xi_2^2} - 1 \right)}{\left(\frac{\xi_{12}^2}{\xi_1^2} + \frac{\xi_{12}^2}{\xi_2^2} + 2k \right)^2} + \dots \right) \quad (4.3)$$

Recently Koshelev and Golubov, suggested that MgB2 cannot be described by the anisotropic mass Ginzberg-Landau theory. The anisotropic mass Ginzberg-Landau theory has a temperature-limited to describe H_{c2} of MgB2 less than 2 percent away from T_c . Such a small temperature region is difficult to accurately probe experimentally. So, this angular dependence of the upper critical field shows strong deviations from the results expected from anisotropic Ginzburg-Landau theory. The reason for this is that the c-axis coherence length in the two bands strongly differ. As a result the validity of Ginzburg-Landau theory is reduced to a very narrow region near the critical temperature T_c .

On the other hand by using anisotropic order parameters we have got expression for upper critical field of superconducting magnesium diboride. In this case we assumed that order parameters are proportioned to the energy gaps, i.e $\psi \propto \Delta$. And we write the order parameters in the form $\psi = \psi_0(T)f(\vec{k})$ by substituting this expression of order parameter in our Ginzburg-Landau free energy formalism eq.(3.13) we obtained

$$H_{c2} = \frac{\phi_0}{2\pi\xi_{12}^{\prime 2}} \left(\frac{\xi_{12}^{\prime 2}}{\xi_1^{\prime 2}} + \frac{\xi_{12}^{\prime 2}}{\xi_2^{\prime 2}} + 2\sqrt{\Omega}k \right) \left(\frac{1}{1-\Omega k^2} - \frac{\left(\frac{\xi_{12}^{\prime 2}}{\xi_1^{\prime 2}\xi_2^{\prime 2}} - 1 \right)}{\left(\frac{\xi_{12}^{\prime 2}}{\xi_1^{\prime 2}} + \frac{\xi_{12}^{\prime 2}}{\xi_2^{\prime 2}} + 2\sqrt{\Omega}k \right)^2} + \dots \right) \quad (4.4)$$

for symmetry $f_1(k) = f_2(k) = 1$ which implies that $\Omega = 1$ then the above equation(3.48) will be reduced to equation (3.36). Following the anisotropy model of Haas and Maki [48], the function $f(\theta) = \frac{1+a'\cos^2\theta}{1+a'}$ where θ is the polar angel and a' is anisotropy parameter. Let's

consider that both band have the same anisotropy function, but they have the difference in anisotropy parameter. That is $f_1(\theta) = \frac{1+a'\cos^2\theta}{1+a'}$ and $f_2(\theta) = \frac{1+b'\cos^2\theta}{1+b'}$. In this model, the average over fermi surface is

$$\langle f(\theta) \rangle = \frac{1}{2} \int_0^\pi d\theta \sin\theta f(\theta). \quad (4.5)$$

That means for $\langle f_1(\theta) \rangle = \frac{1}{2} \int_0^\pi d\theta \sin\theta f_1(\theta) = \frac{1}{2} \int_0^\pi d\theta \sin\theta \left(\frac{1+a'\cos^2\theta}{1+a'} \right)$ and for $\langle f_2(\theta) \rangle = \frac{1}{2} \int_0^\pi d\theta \sin\theta \left(\frac{1+b'\cos^2\theta}{1+b'} \right)$ in the same way as $\langle f_1^2(\theta) \rangle = \frac{1}{2} \int_0^\pi d\theta \sin\theta \left(\frac{1+a'\cos^2\theta}{1+a'} \right)^2 = \frac{15+10a'+3a'^2}{15(1+a')^2}$.

By using the same procedure $\langle f_2^2(\theta) \rangle = \frac{15+10b'+3b'^2}{15(1+b')^2}$, $\langle f_1(\theta)f_2(\theta) \rangle = \frac{5(3+b')+a'(5+3b')}{15(1+a')(1+b')}$ we get $\Omega = \frac{(5(3+b')+a'(5+3b'))^2}{(15+a'(10+3a'))(15+b'(10+3b'))}$. If $a' = b'$, we get $\Omega = 1$ this means that if each band has the same anisotropy function and anisotropy parameter, the anisotropy will show no effect on H_{c2} . Ω is dependent on anisotropy parameters. If we know the values of anisotropy parameters, we can get the value of Ω to simplify, we will consider Ω as a constant parameter. We consider the experimental data of MgB2 and make the assumption that the upper critical field in ab-plane (H_{c2}^{ab}) and c-axis (H_{c2}^c) can be found by set of the suitable parameters. We can write Eq.(3.48) in the form that $H_{c2} = H_{c2}(a_1, a_2, \Omega, k)$, where $a_1 = \frac{\hbar^2}{2m\lambda_1}$, $a_2 = \frac{\hbar^2}{2m\lambda_2}$. After fitting Eq.(3.48) to the experimental data of upper critical field of

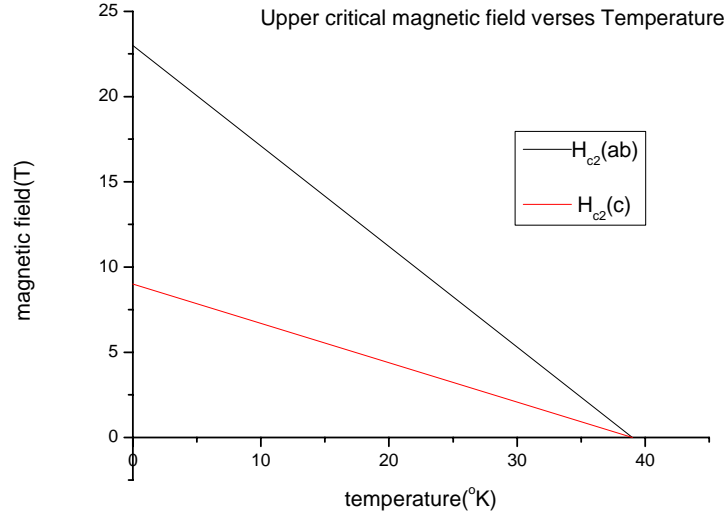


Figure 4.1: *magnetic field vs temperature.*

single crystal MgB2, the upper critical field in ab-plane (H_{c2}^{ab}) is $H_{c2}^{ab} = H_{c2}(6.5, 6.5, 0.7, 0.5)$, and in c-axis (H_{c2}^c) is $H_{c2}^c = H_{c2}(13, 13, 0.7, 0.5)$, as shown in fig.(4.1). In fig.(4.2) the ratio of

upper critical field ($\gamma = \frac{H^{ab}}{H_c^c} = \frac{H_{c2}(6.5,6.5,0.7,0.5)}{H_{c2}(13,13,0.7,0.5)}$) versus temperature is shown. The maximum γ at $T = 0K$ is equal to 2.4. Our result is in the range of 1 to 13 and when temperature is increased, γ is decreased. (although, it is almost constant in low temperature region). This behavior agrees with the result of Miranovic, Machida and Kogan[53] and Canfield and Crabtree[54]. Upper critical field decreases with increasing temperature and the same is true for

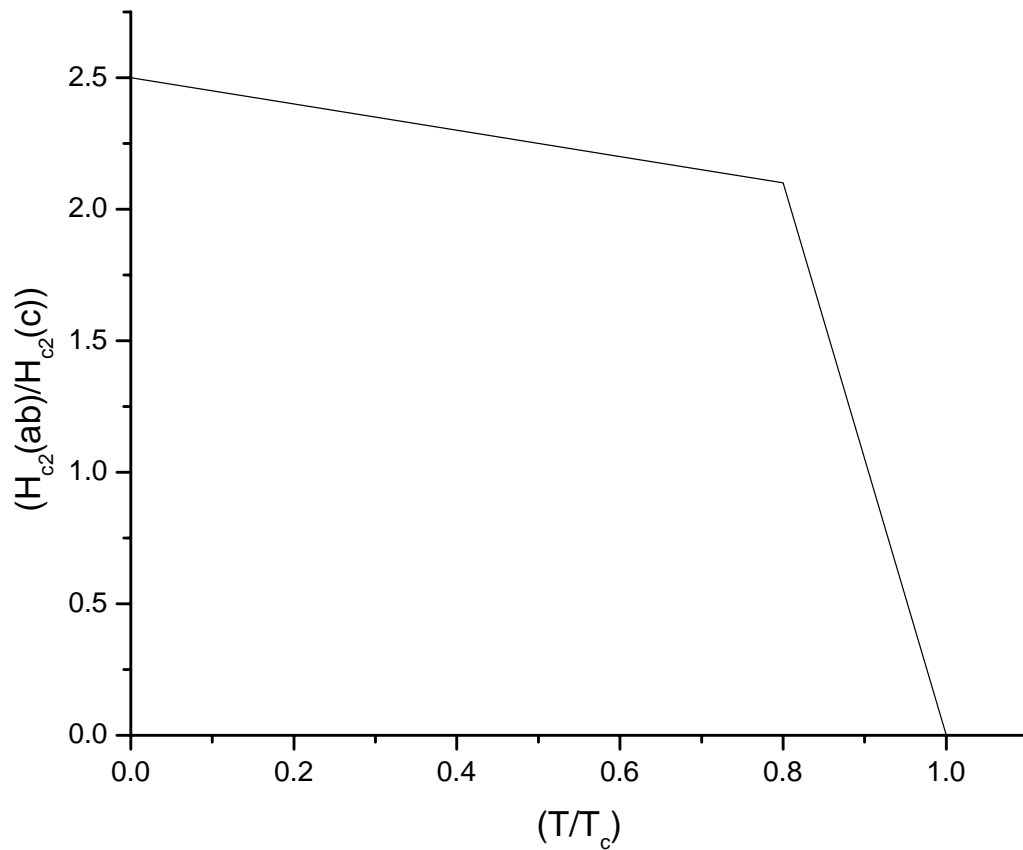


Figure 4.2: *anisotropic property of magnetic field vs temperature.*

upper critical field anisotropy, which is in agreement with experiment .

4.2 Determination of upper critical field of the superconductor by Eilenberger theory

As mentioned above in chapter three the recently discovered superconductor MgB2 gives an example of a superconductor which is not described by the anisotropic GL theory. This unusual feature is a consequence of a specific band structure of this compound. So, to resolve this we have used the Eilenberger theory also to calculate the upper critical field of superconducting magnesium diboride in the vicinity of T_c as shown in fig.4.3. The result is

$$H_{c2} = -\frac{16c\pi^2 T_c^2 \ln \frac{T}{T_c}}{7\zeta(3)e\{e^{-2\tau}[(1-\eta)\langle v_{x,\sigma}^2 \rangle_\sigma + \eta\langle v_{x,\pi}^2 \rangle_\pi] + e^{2\tau}[(1-\eta)\langle v_{y,\sigma}^2 \rangle_\sigma + \eta\langle v_{y,\pi}^2 \rangle_\pi]\}}. \quad (4.6)$$

Which is in terms of the average Fermi velocities of the two bands and the interband pairing strength η . For the single band case with $\eta = 0$ $v_{x,\sigma} = v_{y,\sigma}$ and $\ln \frac{T}{T_c} \approx \frac{T}{T_c} - 1$ $\hbar \sim 1$ $\Delta \sim T_c$. We can obtain the usual expression of single band superconductor which is $H_{c2} = \frac{\phi_0}{2\pi\xi^2}$.

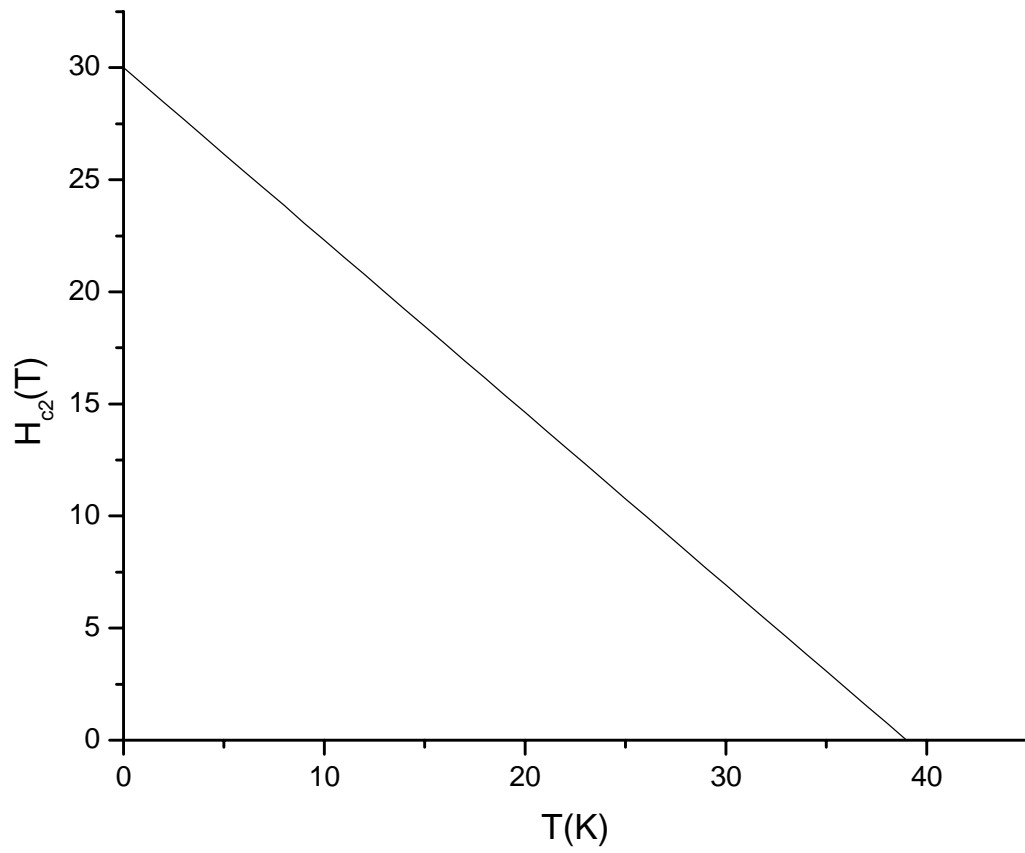


Figure 4.3: *Magnetic field verses temperature by Eilenberger theory.*

Chapter 5

Conclusion and Summary

5.1 Introduction

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

5.2 Conclusion

The aim of this thesis is to determine the upper critical field of superconducting magnesium diboride by using two-band Ginzburg-Landau approach. From the calculation, the effect of an anisotropy in mass tensor and anisotropy of order parameters on upper critical field are considered in our model. We use model of an anisotropic order parameters on upper critical field in our numerical calculation to compare to experimental data of MgB₂. The parameters of the upper critical field in ab-plane (H_{c2}^{ab}) and c-axis (H_{c2}^c) can be found by fitting to experimental data. Finally, we can find the ratio of critical field that depend on temperature in the range of experimental result. So, we can conclude that this temperature dependency and anisotropic nature of the upper critical field comes from two-gap superconductivity or anisotropic s-wave superconductivity nature of this compound. That is since the coherence length depends on the energy gap it will have different value in σ - band and π - band. As we know the coherence length is strongly temperature dependent quantity as a result it can cause temperature dependency and anisotropy nature on the upper critical field of MgB₂. In

addition to this we plotted the graph of upper critical field versus temperature and anisotropy of upper critical field versus temperature in chapter four. So, the the graphs we obtained are fit the experimentally plotted graphs. In the same way the graph that we plotted by using Eilenberger theory has the same nature. Finally, further work is there fore needed to elucidate the nature of superconductivity and the interesting physical properties observed in MgB₂ at both the microscopic level and the macroscopic level.

5.3 summary

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

In chapter one we have seen the historical back ground of superconductivity, the development of superconductivity up to present day, the theories of superconductivity employed by various researchers and types of superconductivity.

Chapter two of this thesis dealt about the mechanism of superconducting state in MgB₂ and the relation ship between upper critical field anisotropy and two-band nature of the superconductor .

We presented the mathematical formalism to find the upper critical field of MgB₂ in chapter three . In this chapter we have seen also anisotropic nature of upper critical field .

In chapter four we have discussed the results what we have got in chapter three .

Finally we concluded all what we have done in this thesis and summarized the main points of this work in chapter five .

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Declaration

This thesis is my original work and has not been presented for a degree in this University or any other University and all sources of material used for the thesis have been duly acknowledged.

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June 2006