STUDY OF CRITICAL TEMPERATURE OF DILUTED MAGNETIC SEMICONDUCTORS (Ga,Mn)As

By

ASNAKE SAHELE

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The undersigned hereby certify that they have read and recommend to the School of Graduate Studies for acceptance a project entitled "**STUDY OF CRITICAL TEMPERATURE OF DILUTED MAGNETIC SEMICONDUCTORS (Ga,Mn)As**" by **ASNAKE SAHELE** in partial fulfillment of the requirements for the degree of **Master of Science in Physics**.

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Advisor: _____
Prof. P. Singh

Examiner: _____
Dr. Chernet Amente

ADDIS ABABA UNIVERSITY

Date: **JUNE 2011**

Author: **ASNAKE SAHELE**

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Abstract

$(Ga, Mn)As$ is a very extensively studied diluted magnetic semiconductor. This type of materials bridge over the incompatibilities in metal-semiconductor in-terfaces in electronics components and which will have an enormous potential for future spintronics applications, where both charge and spin degrees of freedom can be employed simultaneously. In this work an approach based on the green's function to the Ruderman-Kittel-Kasuya-Yosida quantum spin model is used to calculate the magnetic excitation spectrum in the widely studied $(Ga_{1-x}Mn_x)As$ diluted magnetic semiconductors. The resulting magnetic excitation spectrum is then used to estimate The total number of excited magnons, magnetization, and Curie temperature of $(Ga, Mn)As$ diluted magnetic semiconductor. The equation of motion for the magnon Greens function within Tyablikov approximation is solved numerically for systems in which S is larger than $\frac{1}{2}$.

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Chapter 1

Introduction To Semiconductor And Magnetism

1.1 Semiconductor

Starting with the development of the transistor by Bardeen, Brattin, and Shockley in 1947, the technology of semiconductor has exploded. With the creation of integrated circuits and chips, semiconductor devices have penetrated into large parts of our lives. The modern desktop or laptop computer would be unthinkable without microelectronic semiconductor devices.

A semiconductor is a material with electrical conductivity due to electrons flow intermediate in magnitude between that of a conductor and an insulator. One could call a semiconductor a narrow-gap insulator in the sense that its energy gap between the highest filled band (the valance band) and the lowest unfilled band (the conduction band) is typically of the order of one electron volt. The electrical conductivity of a semiconductor is consequently typically much less than that of a metal. This means a conductivity roughly in the range of 10^3 to 10^{-8} $\frac{s}{cm}$. In a metallic conductor, current is carried by the flow of electrons. In semiconductors, current is often schematized as being carried by the flow of electrons or by the flow of positively charged "holes" in the electron structure of the materials. Semiconductor intrinsic electrical properties, in an intrinsic semiconductor the number of electrons in the conduction band is equal to the number of holes in the valence

band, are often permanently modified by introducing impurities by a process known as **Doping** and the materials which added to the semiconductor is called **Dopant**. Usually it is sufficient to approximate that each impurities atom adds one electron or one hole that may flow freely. Upon the addition of a sufficiently large proportion of impurity dopant, semiconductor will conduct electricity nearly as well as metals. Depending on the kind of impurity , a doped region of semiconductor can have more electrons or holes, and is named N-type or P-type semiconducting material, respectively. Junction between N-type and P-type semiconductors creates electric field, which cause electrons and holes to be available to move away from them, and this effect is critical to semiconductor device opration. Over a certain temperature range, donors can add electrons to the conduction band and acceptor can add holes to the valence band as temperature is increased. This can cause the electrical resistivity to decrease with increasing temperature giving a negative coefficient of resistance. This is to be contrasted with the opposite behavior in metals.[1]

1.1.1 Doping process

The pure semiconductor mentioned earlier is basically neutral. It contains no free electrons in its conduction bands. Even with the application of thermal energy, only a few covalent bonds are broken, yielding a relatively small current flow. A much more efficient method of increasing current flow in semiconductors is by adding very small amounts of selected additives to them, generally no more than a few parts per million. These additives are called **Impurities** and the process of adding them to crystals is referred to as **Doping**. The purpose of semiconductor doping is to increase the number of free charges that can be moved by an external applied voltage. Donor impurities are added to increase the number of electrons and acceptor impurities are added to increase the number of holes (which are caused by the absence of electrons in states normally electron occupied and holes act as positive charges). When an impurity increases the number of free electrons, the doped semiconductor is Negative or N-type, and the impurity that is

added is known as **Doner impurity** or an **N-type impurity**. However, an impurity that reduces the number of free electrons, causing more holes, creates a Positive or P-type semiconductor, and the impurity that was added to it is known as **Acceptor impurity** or a **P-type impurity**. Semiconductors which are doped in this manner either with N- or P-type impurities are referred to as **Extrinsic semiconductors**.[2]

1.1.2 N-Type Semiconductor

The N-type impurity loses its extra valence electron easily when added to a semiconductor material, and in so doing, increases the conductivity of the material by contributing a free electron. This type of impurity has 5 valence electrons and is called a **Pentavalent impurity**. Arsenic, antimony, bismuth, and phosphorous are pentavalent impurities. Because these materials give or donate one electron to the doped material, they are also called Doner impurities. When a pentavalent (donor) impurity, like arsenic, is added to germanium, it will form covalent bonds with the germanium atoms. *Fig.*(1.1) illustrates this by showing an arsenic atom (As) in a germanium (Ge) lattice structure. Notice the arsenic atom in the center of the lattice. It has 5 valence electrons in its outer shell but uses only 4 of them to form covalent bonds with the germanium atoms, leaving 1 electron relatively free in the crystal structure. Pure germanium may be converted into an N-type semiconductor by "doping" it with any donor impurity having 5 valence electrons in its outer shell. Since this type of semiconductor (N-type) has a surplus of electrons, the electrons are considered **Majority carriers**, while the holes, being few in number, are the **Minority carriers**.[3]

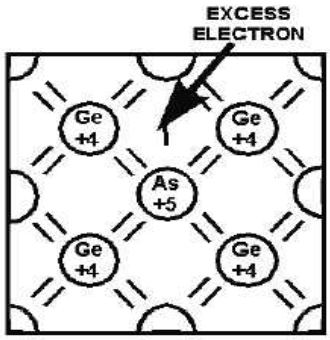


Figure 1.1: Germanium crystal doped with arsenic[3]

1.1.3 P-Type Semiconductor

The second type of impurity, when added to a semiconductor material, tends to compensate for its deficiency of 1 valence electron by acquiring an electron from its neighbor. Impurities of this type have only 3 valence electrons and are called **Trivalent impurities**. Aluminum, Indium, Gallium, and Boron are trivalent impurities. Because these materials accept 1 electron from the doped material, they are also called **Acceptor impurities**. A trivalent (acceptor) impurity element can also be used to dope Germanium. In this case, the impurity is 1 electron short of the required amount of electrons needed to establish covalent bonds with 4 neighboring atoms. Thus, in a single covalent bond, there will be only 1 electron instead of 2. This arrangement leaves a hole in that covalent bond. *Fig.*(1.2) illustrates this theory by showing what happens when germanium is doped with an indium (In) atom.[3]

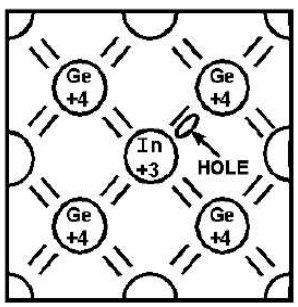


Figure 1.2: Germanium crystal doped with indium.[3]

1.1.4 Intrinsic carrier concentration in semiconductor

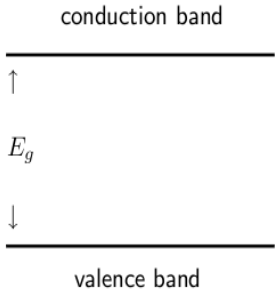
Melissinos gives the formula valid at thermal equilibrium.[4]

$$n_i = N_s exp\left(\frac{-E_g}{2k_\beta T}\right) \tag{1.1.1}$$

where

- n_i is the intrinsic carrier concentration, i.e, the number of electron in the conduction band (and also the number of holes in the valenceband) per unit volume in a semiconductor that is completely free of impurities and defect.
- N_s is the number per unit volume of effectively available states; its precise value depend on the materials, but it is of order $10^{19} cm^{-3}$ at room temperature and increases with temperature.
- E_g is the energy gap (between the bottom of the conduction band and the top of the valence band).
- k_β is Boltzmann's constant, k_β=$1.381 * 10^{-23}\ \frac{J}{K}$.
- T is the absolute temperature in kelvin; it is assumed that $k_\beta T \lesssim \frac{E_g}{5}$

The physical basis of *eq.*(1.1.1) can be understood as follows.



The probability of exciting electron from the top of the valence band to the bottom of the conduction band is proportional to the Boltzmann factor $exp\left(\frac{-E_g}{k_\beta T}\right)$. This process leaves behind a hole in the valence band and is called electron-hole pair creation.

At thermal equilibrium, the creation of electron-hole pairs is balanced by their recombination. If n is the concentration of conduction-band electrons and p the concentration of valence-band holes, the electron - hole recombination rate is proportional to the product np, according to the general law of mass action of chemical physics. Equating creation to recombination, we conclude that

$$np = Kexp\left(\frac{-E_g}{k_\beta T}\right) \tag{1.1.2}$$

where K is proportionality factor. In an *intrinsic semiconductor*, by definition, $n = p = n_i$. Then $eq.(1.1.1)$ is equivalent to $eq(1.1.2)$. with $K = N_s^2$.

1.1.5 The rigorous calculation of n_i .

The probability of finding an electron in a state of energy E at temperature T, is given by the fermi function

$$f_e = \frac{1}{exp\left(\frac{E - E_f}{k_\beta T}\right) + 1} \tag{1.1.3}$$

where E_f is the fermi energy, the energy at which the probability of occupation by an electron is exactly one-half. At room temperature, the intrinsic fermi level lies very close to the middle of the band gap. For large enough samples, the number of available quantum states in a given energy interval is proportional to the volume of the sample. We denote by $\left(\frac{d\mathbf{n}}{dE}\right) dE$ the number of the available states per unit volume with energy between E and $E + dE$, and we call $\frac{d\mathbf{n}}{dE}$ the density of states. Then the number per unit volume of electron in the conduction band is.

$$n = \int_{E_c}^{\infty} f_e \frac{d\mathbf{n}}{dE} dE \tag{1.1.4}$$

where

$$\mathbf{n} = \frac{1}{3\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{\frac{3}{2}} \epsilon^{\frac{3}{2}} \qquad and \qquad \epsilon = \frac{\hbar^2 k^2}{2m_e^*}$$

The energy of electron in the conduction band is

$$E = E_c + \frac{\hbar^2 k^2}{2m_e^*}$$

E_c is the energy of the bottom of the conduction band. The density of states in a solid is similar to that of free particles near the bottom of a band and is given by

$$D_e(E) = \frac{d\mathbf{n}}{dE} = \frac{(2m_e^*)^{\frac{3}{2}}}{2\pi^2\hbar^3}(E - E_c)^{\frac{1}{2}} \tag{1.1.5}$$

We know evaluate expressions for the electron concentration in the conduction band and the hole concentration in the valence band. we assume the non degenerate case when in the conduction band implies $E - E_f \gg k_\beta T$, so

$$f_e(E) \approx exp\left(\frac{E_f - E}{k_\beta T}\right) \tag{1.1.6}$$

clearly it is convenient to use $E - E_c$ as a variable to deal with states in the conduction band, so we write $Eq.(1.1.6)$ in the form.

$$f_e(E) \simeq exp\left(-\frac{E_c - E_f}{k_\beta T}\right) exp\left(-\frac{E - E_c}{k_\beta T}\right)$$

and substituting back in $Eq(1.1.4)$ we obtain

$$n = exp\left(-\frac{E_c - E_f}{k_\beta T}\right) \frac{(2m_e^*)^{\frac{3}{2}}}{2\pi^2\hbar^3} \int_{E_c}^{\infty} (E - E_c)^{\frac{1}{2}} exp\left(-\frac{E - E_c}{k_\beta T}\right) dE \tag{1.1.7}$$

The integral gives

$$(k_\beta T)^{\frac{3}{2}} \frac{\sqrt{\pi}}{2}$$

and the intrinsic concentration of electrons is become,

$$n_i = 2\left(\frac{m_e^* k_\beta T}{2\pi\hbar^2}\right)^{\frac{3}{2}} exp\left(-\frac{E_c - E_f}{k_\beta T}\right) \tag{1.1.8}$$

Similarly for holes we can obtains:

$$P_i = \int_{-\infty}^{E_v} D_h f_h(E) dE \tag{1.1.9}$$

the energy of hole in the valence band is $E = E_v - \dfrac{\hbar^2 k^2}{2m_h^*}$

and the density of states for holes in the valence band is given by

$$D_h(E) = \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{\frac{3}{2}}(E_v - E)^{\frac{1}{2}} \tag{1.1.10}$$

the fermi-dirac distribution for hole can be written down as

$$f_h(E) = 1 - f_e(E) = 1 - \frac{1}{exp\left(\frac{E-E_f}{k_\beta T}\right)+1} = \frac{1}{1+exp\left(\frac{E_f-E}{k_\beta T}\right)}$$

Again, we make a non degenerate assumption and assume $(E_f - E) \gg k_\beta T$ for E in the valance band, so

$$f_h(E) \approx exp\left(\frac{E-E_f}{k_\beta T}\right) \tag{1.1.11}$$

we can write $Eq.(1.1.11)$ in another form:

$$f_h(E) \approx exp\left(\frac{E-E_v}{k_\beta T}\right) exp\left(\frac{E_v-E_f}{k_\beta T}\right) \tag{1.1.12}$$

now substituting $Eq.(1.1.10)$ and $Eq.(1.1.12)$ into $Eq.(1.1.9)$ we obtain:

$$P_i = \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{\frac{3}{2}} exp\left(\frac{E_v-E_f}{k_\beta T}\right)\int_{-\infty}^{E_v}(E_v-E)^{\frac{1}{2}} exp\left(\frac{E-E_v}{k_\beta T}\right)dE$$

the requirements for the degree of the integral gives

$$(k_\beta T)^{\frac{3}{2}}\frac{\sqrt{\pi}}{2}$$

and the intrinsic concentration of hole is become

$$P_i = 2\left(\frac{m_h^* k_\beta T}{2\pi\hbar^2}\right)^{\frac{3}{2}} exp\left(\frac{E_v-E_f}{k_\beta T}\right) \tag{1.1.13}$$

1.2 Magnetism

1.2.1 The origin of magnetism

In order to understand why semiconductors are traditionally not magnetic and how it is possible to introduce magnetic behavior in these materials, it is first necessary to look at the fundamental origins of magnetic behavior, and then analyze how magnetic behavior can be exploited in the development of dilute magnetic semiconductor compounds.

Magnetism in material is due to electron spin about its axis and orbital motion about the nuclei as shown in $fig.(1.3)$. Bohr suggested a fundamental quantity later called the bohr magento which is the strength of the magnetic field associated with an isolated electron. This magnetic field is a constant and can be calculated as follows.[5]

$$\mu_B = \frac{eh}{4\pi m} = 9.27 \times 10^{-24} Am^2$$

where, e the charge of an electron, h is planks constant and m is the mass of electron.

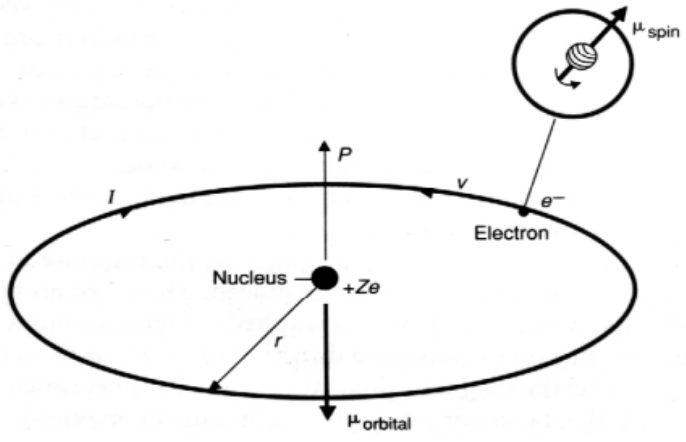


Figure 1.3: Origin of the magnetic moments in atoms due to an electron orbiting the nucleus ($\mu_{orbital}$) and to the electron spin about its axis ($\mu_{spin} = \mu_B$).

1.2.2 Types of magnetism

There are five different types of magnetisms these are.[5]:

- diamagnetism
- paramagnetism
- ferromagnetism
- antiferromagnetism, *and*
- ferrimagnetism

Diamagnetism

Although diamagnetism is in all solid states existent, it can be observed only in atoms or ions with complete filled electron shells. Otherwise the weak diamagnetism is obscured by other types of magnetic ordering. In diamagnets a magnetic moment is induced by an external magnetic field. The electrons precess in direction of the field and act against the inducing field according to the Lenz rule. Therefore, the susceptibility is negative and small ($10^{-9} < |\chi_{dia}| < 10^{-5}$).[5]

Paramagnetism

Paramagnetism exists in atoms or ions with partly filled orbitals possessing unpaired electrons, so that uncompensated magnetic moments can occur. In absence of magnetic fields and long-range interactions, the magnetic moments are distributed statistically. Hence, an average macroscopic magnetic moment vanishes. The magnetic moments can be aligned by an external magnetic field[6]. The susceptibility of paramagnetism is positive and in an order of magnitude of ($10^{-3}<|\chi_{para}|<10^{-2}$).

Three manifestations of the paramagnetism can be distinguished: the Van Vleck paramagnetism, the Langevin paramagnetism and the Pauli paramagnetism.

The Langevin paramagnetism appears for magnetic moments of atoms or ions in the ground state. The magnetization is given thermodynamically for N ions in a volume V by:

$$M = -\frac{N}{V}\frac{\partial F}{\partial B} = n\frac{\partial F}{\partial B} \tag{1.2.1}$$

with the number of magnetic moments per unit volume n. The free energy F is defined by

$$exp\left(-\frac{F}{k_\beta T}\right) = \sum exp\left(-\frac{g\mu_B B}{k_\beta T}\right) \tag{1.2.2}$$

for low temperature it is sufficient to provide the $n = 2J + 1$ lowest states. Therefore follows for macroscopic magnetization of free magnets moments $\mu = -g\mu_B J$ without interaction, i.e. the spins be regarded as independent from one another,

$$M = -ng\mu_B J B_J(y) \text{ with } y = \frac{g\mu_B JB}{k_\beta T}$$

In the equation is

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \tag{1.2.3}$$

The Landè g-factor of electrons, μ_B the Bohr magneton and $B_J(y)$ the Brillouin function and described by

$$B_J(y) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}\right) - \frac{1}{2J}\coth\left(\frac{y}{2J}\right) \tag{1.2.4}$$

For high temperatures and weak magnetic fields the Brillouin-function can be simplified, so that the susceptibility can be described by the classical Curie law

$$\chi_{para}^{langevin} = \frac{C}{T} \tag{1.2.5}$$

with the Curie constant C

In contrast the Van Vleck paramagnetism is temperature independent. It arises from magnetic moments of excited states. In case of non-vanishing orbital angular momentum $J = 0$, the Van Vleck paramagnetism is about three orders weaker than the Langevin paramagnetism and, thus, is negligible. The Pauli paramagnetism finally arises from the magnetic moment of delocalized electrons and, therefore, is important for metals.

Ferromagnetism

one group of materials having very different magnetization from the first two group known as ferromagnetic. First magnetic susceptibility χ is positive and very large; about 10^7 times greater than χ in paramagnetic materials. This means that the material under an applied field will create a very large magnetization. Second, large magnetic field can be retained after the applied field is removed. These properties are of great engineering importance.[5]

The most important ferromagnetic element are Fe, Co, and Ni. A large rare earth element; gadolinium (Gd), is also ferromagnetic below 16^0C. Fe, Co and Ni are transition metals and have unpiared inner $3d$ electrons. Fe atome has four unpaired $3d$ electrons, Co has three unpaired $3d$ electrons and Ni has two unpaired $3d$ electrons. The spin of the $3d$ electron of adjacent atoms align in parallel to applied field induces diamagnetic and paramagnetic effect when the field is removed, the effect is disappear by a phenomenon called ***spontaneous magnetization***.

This parallel alignment of atomic magnetic dipoles occurs in microscopic regions called ***magnetic domains***. If the domains are randomly oriented, there will be no net magnetization in a bulk sample. If the domains are aligned in a magnetic field, the magnetic induction of the specimen will be very strong.[5]

The positive susceptibility follows the Curie-Weiss law:

$$\chi^{ferro} = \frac{C}{T - \Theta} \tag{1.2.6}$$

where Θ is the Curie-Weiss temperatures called ordering temperature of the ferromagnetic phase. With rising the temperature decreases the ferromagnetism and passes finally into paramagnetic phase. This second phase transition occur at Θ.

Antiferromagnetism

In the presence of a magnetic field, the magnetic dipoles of atoms in some materials align themselves in opposite direction. Therefore, the atoms do not show a net magnetic moment. Manganese (Mn) and chromium (Cr) exhibit this behavior as they have a negative exchange energy[5]. Exchange interaction which is responsible for parallel alignment of spins is extremely sensitive to inter-atomic spacing and to the atomic positions. This sensitivity causes anti-parallel alignment of spins. When the strength of anti-parallel spin magnetic moments is equal, no net spin moment exists, and resulting susceptibilities are quite small.[28]

The transition temperature below which the spontaneous anti parallel magnetic ordering takes place is called the Néel temperature. Above the Néel temperature, the substance is para-magnetic, and the susceptibility obeys the Curie-Weiss

$$\chi_{afm} = \frac{C}{T + T_{Neel}} \tag{1.2.7}$$

law, Where T_{Neel} is the néel temperature. with a negative paramagnetic Curie temperature, the Néel temperature is similar to the Curie temperature in ferromagnetism.[29]

Ferrimagnetism

In some ceramic compounds, different ions have different magnitude of magnetic moments. When these magnetic moments are aligned in an anti parallel manner, there is a net magnetic moment in one direction. *Fig.*(1.4) is a schematic drawing illustrating the arrangement of dipoles for different magnetism. These ceramic magnetic materials is called ferrites. Their magnetic properties are very much like those of ferromagnet. However , because of their ceramic nature, they have a much lower electrical conductivity than metallic magnets.These properties make them very useful in many electronic application.[5]

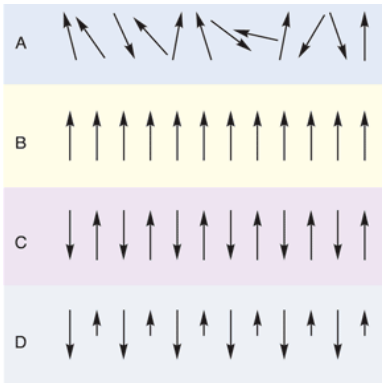


Figure 1.4: Alignment of magnetic dipoles for different type of magnetism: (A) pramagnetic (B) ferromagnetic (C) antiferromagnetic and (D) Ferrimagnetic.

Chapter 2

Overview Of Diluted Magnetic Semiconductors

2.1 Introduction To DMS.

Diluted magnetic semiconductors (DMS) are materials in which a host semiconductors are doped with magnetic impurities, generally atoms of a transition metal such as Manganese (Mn), Iron (Fe), Cobalt (Co), Chromium. There is considerable current interest in these materials because they appear to have great potential for use in spin-polarized electronics (spintronics) or in non-volatile computer memory.[14] The discovery of ferro-magnetism in (Ga,Mn)As with a relatively high temperature has sparked a rapid increase in the number and variety of such materials studied. The aim of much of these work has been to find higher curie temperature or useful transport properties.

Most of the early work in the field focused on II-VI semiconductors, in which a semiconductor composed of a group II and a group VI element, such as CdTe, is doped with Mn. In the II-VI case, Mn and Cd have same valence, hence each Mn ion introduce a spin-$\frac{5}{2}$ moment, but does not introduce any carriers, unless another dopant with a different valence, such as N (a p-type dopant) is introduce.

A major advance in the field occurred with the ability to dope Mn into III-V semiconductors such as InAs and GaAs. These materials differ from the II-VI DMS because

Mn has a different valence to group III elements, and whilst it still introduces a spin-$\frac{5}{2}$ moment, Mn plays the dual role of magnetic ion and acceptor. The low solubility of Mn in III-V semiconductor was the main barrier to fabrication and it has only recently become to grow such materials using low-temperature molecular beam epitaxy.[14]

Following the discovery of a ferromagnetic transition at temperature in excess of 100 K, the diluted III-V magnetic semiconductors, which are realized by doping a semiconducting host materials with low concentration of magnetic impurities (typically manganese), have attracted a great deal of attention from both the experimental and theoretical point of view due to their potential in spintronics application. In DMS, low concentration of magnetic impurities carrying localized magnetic moment (spins) form a diluted spin system. The random spatial Distribution of the magnetic impurities brakes the translational symmetry of the crystal and thus greatly complicates the theoretical description of the materials.[7]

2.2 Types of DMS

The magnetic transition elements for doping purpose have been used to date mainly; Mn,Cr and Fe.

Table 2.1: Magnetic elements used for doping purpose in DMS

Element	Cr^{24}	Mn^{25}	Fe^{26}	Cr^{2+}	Mn^{2+}	Fe^{2+}	Fe^{3+}
Configuration	$3d^5 4S^1$	$3d^5 4S^2$	$3d^6 4S^2$	$3d^4$	$3d^5$	$3d^6$	$3d^5$

The above table gives configuration why Mn^{2+} is more appropriate. In Mn^{2+} doped III-V DMS, there is a valence mismatch between that of $S = 5/2$ Mn and the group III-element. In Cr^{2+} doped III-V the $3d$ electrons is less in number which is 4 pair atom and $S = 4(1/2) = 2$ where less magnetic impurity spins per atom results in weak

ordering in the compound. In Fe^{2+} the $3d$ electrons gives rise to $S = 4(1/2) = 2$ and Fe^{3+} gives the valence match with group III element as in II-VI DMSs case. Therefore, Mn^{2+} with shorter nearest neighbor distance of $2.24\dot{A}$ relatively, is more preferable for doping purpose in which high concentration of 3d spins are required.[8]

2.2.1 (II,Mn)VI diluted magnetic semiconductor

The II-VI DMS are based on semiconductors AB, where A is a group II elements and B is a group VI element (such as $CdTe$ or $ZnSe$). In the II-VI DMS, some of the divalent sites (Cd/Zn) are substituted by a magnetic element, typically Mn. This fraction is denoted by x, so the DMS we consider is $A_{1-x}Mn_xB$. Mn is also a group II element, but in addition it has a half filed $3d$ shell, with a total spin given by hund's rule:$S = \frac{5}{2}$. In the absence of other types of dopant, the system $A_{1-x}Mn_xB$ is an insulator which exhibits antiferromagnetic (AFM) tendencies at low temperature. This is seen, for instance , from measurements of the susceptibility which is found to depend on temperature as $\chi(T) \sim \frac{1}{T+T_N}$, with a neel temperature of a few kelvin. The origin of this AFM tendency is the expected antiferromagnetic exchange between the Mn spins. However, for low doping concentration x, the average distance between Mn spins is large and this AFM direct exchange is rather small. In $CdTe/Cd_{1-x}Mn_xTe$, the dilution decrease the influence of ion-ion interaction, which favors an anti-parallel alignment of Mn^{2+} spins at low temperature. When a Mn^{2+} ion occupies a substitutional Cd site in cubic $CdTe$ crystal, its free ion terms split due to the cubic crystal field.[9]

2.2.2 (III,Mn)V diluted magnetic semiconductors

Soon after the discovery of (In,Mn)As, similar materials have been prepared by introducing Mn atoms into a III-V compound semiconductor.[10] The Mn^{+2} ions in the most widely studied (III,Mn)V alloys provide localized magnetic moments and at the same time act as a source of valence band holes that mediate the exchange interaction between them. Recent experiments have demonstrated that electrical control of the spin properties in these compounds can be used both for manipulation and detection of magnetic signals. This feature makes them promising candidates for the material background of future spintronics applications which also incorporates the existing semiconductor technologies in a seamless way.[11]

The most important and most widely studied prototype materials of the III-V diluted magnetic semiconductor family are (Ga,Mn)As and (Ga,Mn)N. Both of these materials have rather high Curie temperatures, but the electronic properties, and possibly also the origin of magnetism, are quite different.[10] In this project we focused only on (Ga,Mn)As

2.2.3 $(Ga_{1-x}\ Mn_x)As$ Dilute Magnetic Semiconductor

Diluted magnetic semiconductors (DMS) have been studied for three decades in order to search for thermodynamically stable materials with traditional semiconductor characteristics and robust high-temperature ferro-magnetism for new multi-functional electronics DMS devices. $Ga_{1-x}Mn_xAs$ is one of the most important DMS systems. Recent years have witnessed two breakthroughs in its curie temperature. A curie temperature of 110 K ($x = 0.053$) was achieved in 1998 and 173 K ($x = 0.08$) in 2005. It is reasonably believed that higher curie temperature may be achieved in the future.[12]

2.2.3.1 Mechanisms of ferromagnetism in $(Ga_{1-x}\ Mn_x)As$

It is an important challenge of materials science to understand the ferromagnetism in magnetic semiconductors and to develop functional semiconductor systems with the Curie temperatures T_c exceeding comfortably the room temperature.[18]

The fact that the DMS are ferromagnetic independent of their weakly metallic or strongly insulating nature implies a robust character for the underlying mechanism leading to the long range magnetic order in these systems. Clearly the ferromagnetic mechanism should not depend crucially on the carrier system being free valence band holes since the strongly insulating DMS systems do not have any free holes. The currently accepted picture for DMS ferromagnetism is that it is the local antiferromagnetic coupling between the carriers (i.e., holes in (Ga,Mn)As) and the Mn magnetic moments that leads to long range ferromagnetic ordering of Mn local moments. The carrier system also becomes spin-polarized in the process with the carrier magnetic moment directed against the Mn magnetic ordering by virtue of the antiferromagnetic hole-Mn coupling, but the total magnetic moment of the spin polarized carriers is extremely small since $n_c \ll n_i$ and $|S|$ $> |s|$ where S and s are respectively the Mn and the hole spin and n_c and n_i are carrier and local moment density respectively.[18]

There are two basic approaches to understand the magnetic properties of $(Ga_{1-x}\ Mn_x)As$ diluted magnetic semiconductors. The first one is based on mean field theory which originates in the model of Zener. The theories that fall into this general model implicitly assume that the diluted magnetic semiconductor is a more or less random alloy, in other words, the doping atoms will substitute randomly for the lattice constituents. The second class of approach suggests that the magnetic atoms form small clusters that produce the ferromagnetism.[19]

The Zener Model

The theory proposed by Zener indicates that the direct super-exchange interaction between half filled d-shell electrons of TM cations and completely filled p-orbitals of anion is antiferromagnetic (Fig. 2.1). Since the d-shell electrons from both adjacent TM atoms occupy the same p-level, their spins must be opposite according to Pauli exclusion principle. This leads to an antiferromagnetic coupling of nearest-neighbor TM cations through a shared anion. On the other hand, the indirect super exchange interaction between localized d-shell electrons of TM cations mediated by the delocalized band carriers tends to align the spin of the partially filled d-shells in a ferromagnetic manner . In the Zener model, ferromagnetism is only possible when the indirect exchange interaction dominates over the direct superexchange interaction.[21]

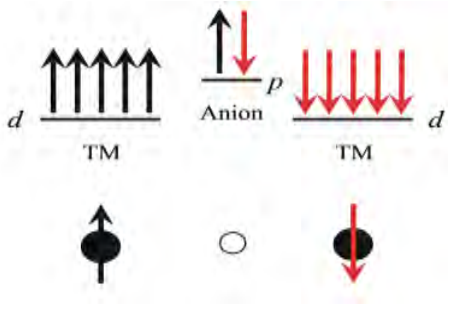


Figure 2.1: Direct superexchange interaction: Antiferromagnetic coupling of adjacent TM cations through shared anion.[21]

The disorder-free p-d Zener model has been successful in explaining a number of experimentally observed properties in ferromagnetic III-V semiconductors, in particular (Ga,Mn)As and (In,Mn)As. The properties are the ferromagnetic transition temperature T_C, magnetization and effective Landé factor, Gilbert constant, spin-polarization of the hole liquid, magnetocrystalline anisotropy with its strain and temperature dependence, magnetic stiffness, stripe domain width, the anomalous Hall effect, magnetic anisotropy of the Coulomb blockade, and optical properties.[23]

The Mean-Field Model

In the mean-field model, the interaction between the localized Mn atoms through free holes in the material leads to a ferromagnetic alignment of Mn atoms (Fig. 2.2). Due to the possibility of direct super exchange Mn-Mn interactions, there is always a competition between the ferromagnetic and antiferromagnetic interactions.[21]

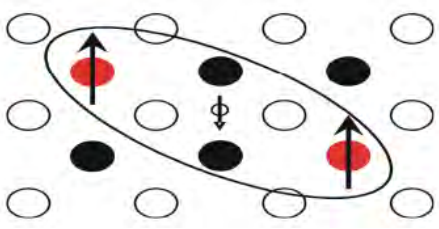


Figure 2.2: The mean-field model: Ferromagnetic coupling of localized Mn spins through the free holes.[21]

The RKKY Model

The RKKY interaction was first proposed by Ruderman and Kittel and later extended by Kasuya and Yoshida. It has originally been developed for nuclear magnetic moments in a metal. It is an indirect interaction of local moments via conduction electrons. If one puts an impurity into the free electron gas, slowly decaying oscillations of the electron charge density centered around the perturbation are found. These so-called Friedel oscillations are a consequence of screening. If the oscillations are different for spin-up and spin-down electrons one expects oscillations of the magnetization density. The mutual interaction of two impurities via the oscillations of their corresponding magnetization densities is then called RKKY interaction.[21] The interaction is characterized by a coupling coefficient, J, given by

$$J(R_i - R_j) = 9\pi \left(\frac{J^2}{\epsilon_f}\right) F(2k_f \mid R_i - R_j \mid) \tag{2.2.1}$$

where k_f is the radius of the conduction electron Fermi surface, R_i is the lattice position of the point moment, ϵ_f is the Fermi energy and

$$F(k) = \frac{xcos(x) - sin(x)}{x^4} \tag{2.2.2}$$

The RKKY exchange coefficient, J, oscillates from positive to negative as the separation of the ions changes and has the damped oscillatory nature. Therefore, depending upon the separation between a pair of ions their magnetic coupling can be ferromagnetic or antiferromagnetic. A magnetic ion induces a spin polarization in the conduction electrons in its neighborhood. This spin polarization in the itinerant electrons is felt by the moments of other magnetic ions within range, leading to an indirect coupling. In rare-earth metals, whose magnetic electrons in the $4f$ shell are shielded by the $5s$ and $5p$ electrons, direct exchange is rather weak and insignificant and indirect exchange via the conduction electrons gives rise to magnetic order in these materials.[22]

2.2.3.2 Transition Temperature of the (Ga,Mn)As DMS

Recent advances in magnetoelectronics and spintronics renewed interest in ferromagnetic semiconductors. Experimental efforts are now focused on the search for semiconductors with ferromagnetism occurring above 300 K.[25]

The recently discovered ferromagnetism in III-V compound semiconductors containing 5% of Mn impurity is relatively high temperatures ($T_c > 100$ K).[24] A similar magnitude of T_c was also reported recently for Ge doped with about 3.5% of Mn atom.[27]

One of the standing issues is related to the fact that the critical temperature, as a function of Mn composition in $Ga_{1-x}Mn_xAs$, are crucially dependent on the details of the growth conditions.[26] In order to incorporate magnetic ion such as Mn into III-V materials beyond solubility limits, low temperature molecular-beam epitaxy (LT-MBE) is usually adopted.

Chapter 3

Mathimatical techenique

3.1 A Green Function Model For Spin Excitation

3.1.1 The double-time temperature dependent Green's function

The method of the double-time temperature dependent Green functions in statistical mechanics are the appropriate generalization of the correlation functions. They are useful in calculating the average of dynamical quantities, and they have great advantages when equations are framed and solved.[8] In this scheme one uses a retarded double-time Green's function which is defined by:

$$\langle\langle \hat{A}(t); \hat{B}(t')\rangle\rangle = -i\theta(t-t')\langle[\hat{A}(t); \hat{B}(t')]_{\pm}\rangle. \tag{3.1.1}$$

Where $\hat{A}(t)$ and $\hat{B}(t)$ are either fermi or Bose operators and, correspondingly, the commutator is

$$[\hat{A}(t), \hat{B}(t)]_{\pm} = \hat{A}(t)\hat{B}(t) \pm \hat{B}(t)\hat{A}(t);$$

and $\theta(t-t')$ is heaviside step function with the value:

$$\theta(t-t') = \begin{cases} 1, \ (t-t') > 0 \\ 0, (t-t') < 0 \end{cases}$$

These operators, $\hat{A}(t)$ and $\hat{B}(t')$ can be expressed as the product of the quantized field operators, i.e.,

$$\hat{A}(t) = e^{iHt} A(0) e^{-iHt} \tag{3.1.2}$$

and

$$\hat{B}(t') = e^{iHt'} B(0) e^{-iHt'} \tag{3.1.3}$$

Single angular brackets, in $Eq.(3.1.1)$, denotes an average with respect to the canonical density matrix of the system at temperature T.

3.1.2 The equation of motion of the Green's Function

We now derive the equation of motion of the Green's function. It is known that $\hat{A}(t)$ and $\hat{B}(t')$ satisfy equation of the form:

$$i\frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t), \hat{H}\right] \tag{3.1.4}$$

Differentiating the green function given by $Eq.(3.1.1)$ with respect to one of the arguments; for example, the first argument, we obtain

$$\begin{aligned} i\frac{d}{dt}\left\langle\left\langle \hat{A}(t); \hat{B}(t')\right\rangle\right\rangle &= i\frac{d}{dt}\left[-i\theta(t-t')\left\langle\left[\hat{A}(t), \hat{B}(t')\right]_{\pm}\right\rangle\right] \\ &= \frac{d}{dt}\theta(t-t')\langle[\hat{A}(t), \hat{B}(t')]_{\pm}\rangle - i\theta(t-t')\left\langle\left[i\frac{d}{dt}\hat{A}(t), \hat{B}(t')\right]\right\rangle \\ &= \frac{d}{dt}\theta(t-t')\langle[\hat{A}(t), \hat{B}(t')]_{\pm}\rangle + \left\langle\left\langle i\frac{d}{dt}\hat{A}(t); \hat{B}(t')\right\rangle\right\rangle \end{aligned} \tag{3.1.5}$$

Since

$$\theta(t-t') = \int_{-\infty}^{t} \delta(t-t')dt \tag{3.1.6}$$

One can verify that

$$\frac{d}{dt}\theta(t-t') = \delta(t-t') \tag{3.1.7}$$

Substitute $Eq.(3.1.7)$ into $Eq.(3.1.5)$ and we can rewrite $Eq.(3.1.5)$ as:

$$i\frac{d}{dt}\left\langle\left\langle \hat{A}(t);\hat{B}(t')\right\rangle\right\rangle = \delta(t-t')\langle[\hat{A}(t),\hat{B}(t')]_{\pm}\rangle + \left\langle\left\langle [\hat{A}(t),\hat{H}];\hat{B}(t')\right\rangle\right\rangle \tag{3.1.8}$$

To solve the differential equation of motion, we should consider the Fourier time transform of the Greens function and the delta function.

$$G_{AB}(t-t') = \left\langle\left\langle \hat{A}(t);\hat{B}(t')\right\rangle\right\rangle = \int_{-\infty}^{\infty} d\omega G_{AB}(\omega) exp[-i\omega(t-t')] \tag{3.1.9}$$

$$\delta(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} exp(-i\omega(t-t')) \tag{3.1.10}$$

By inserting $Eq.(3.1.9)$ and $Eq.(3.1.10)$ into $Eq.(3.1.8)$ we obtain

$$\begin{aligned} i\frac{d}{dt}\int_{-\infty}^{\infty} d\omega G_{AB}(\omega) exp[-i\omega(t-t')] \quad &= \frac{1}{2\pi}\int_{-\infty}^{\infty} exp(-i\omega(t-t'))\langle[\hat{A}(t),\hat{B}(t')]_{\pm}\rangle \\ &+ \left\langle\left\langle [\hat{A}(t),\hat{H}];\hat{B}(t')\right\rangle\right\rangle \end{aligned}$$

$$\begin{aligned} \omega\int_{-\infty}^{\infty} d\omega G_{AB}(\omega) exp[-i\omega(t-t')] \quad &= \frac{1}{2\pi}\int_{-\infty}^{\infty} exp(-i\omega(t-t'))\langle[\hat{A}(t),\hat{B}(t')]_{\pm}\rangle \\ &+ \left\langle\left\langle [\hat{A}(t),\hat{H}];\hat{B}(t')\right\rangle\right\rangle \end{aligned} \tag{3.1.11}$$

The Fourier transform of $Eq.3.1.11$ can be obtained by multiplying its both sides by

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dt e^{i\epsilon(t-t')} \tag{3.1.12}$$

thus,

$$\begin{aligned} \omega\int_{-\infty}^{\infty} d\omega G_{AB}(\omega)\frac{1}{2\pi}\int_{-\infty}^{\infty} dt e^{i(\epsilon-\omega)(t-t')} \quad &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(\epsilon-\omega)(t-t')} dt\langle[\hat{A},\hat{B}]_{\pm}\rangle \\ &+ F.T.of\left\langle\left\langle [\hat{A}(t),\hat{H}];\hat{B}(t')\right\rangle\right\rangle \end{aligned} \tag{3.1.13}$$

The above equation can be rewritten as:

$$\omega\int_{-\infty}^{\infty} G_{AB}(\omega)\delta(\epsilon-\omega)d\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty}\delta(\epsilon-\omega)d\omega\langle[\hat{A},\hat{B}]_{\pm}\rangle + \left\langle\left\langle [\hat{A},\hat{H}];\hat{B}\right\rangle\right\rangle \tag{3.1.14}$$

where

$$\delta(\epsilon-\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dte^{i(\epsilon-\omega)(t-t')} \tag{3.1.15}$$

and

$$\int_{-\infty}^{\infty}\delta(\epsilon-\omega)d\omega=1 \qquad at \qquad \omega=\epsilon \tag{3.1.16}$$

Now put equation $Eq.(3.1.16)$ into $Eq.(3.1.14)$ we obtain:

$$\omega G_{AB}(\omega)=\frac{1}{2\pi}\langle[\hat{A},\hat{B}]_{\pm}\rangle+\left\langle\left\langle[\hat{A},\hat{H}];\hat{B}\right\rangle\right\rangle \tag{3.1.17}$$

The above equation, Eq.(3.1.17), is the Fourier form of equation Eq.(3.1.11),.

3.1.3 Green's function approach to the RKKY model

The Hamiltonian which describes N_{imp} interacting quantum (or classical) spins randomly distributed on a given lattice of N sites is the standard spin RKKY Hamiltonian.

$$\hat{H}=-\frac{1}{2}\sum_{i\neq j}^{'}J_{ij}\hat{\mathbf{s}}_i\cdot\hat{\mathbf{s}}_j \tag{3.1.18}$$

Where J_{ij} is the RKKY effective spin exchange interaction[13] between local spin $\hat{S}_i$ and $\hat{S}_j$ ($\hat{S}_i$ and $\hat{S}_j$ are both quantum spin operators) and $\hat{\mathbf{s}}_i\cdot\hat{\mathbf{s}}_j=\frac{1}{2}\left(S_i^+S_j^-+S_i^-S_j^+\right)+S_i^zS_j^z$. Here, the magnetic atoms are distributed randomly in the full lattice of the undoped semiconductor. The prime of the summation in Eq.(3.1.18) means that the summation is done only over the sites occupied by magnetic impurities. Hence, we use Green's function approach to treat the model Eq.(3.1.18).

Usually, one needs more than one Green's function when spin S is larger than $\frac{1}{2}$. For our random spin system we construct double-time spin Green's functions between spin operators at two magnetic sites $\mathbf{R}_i$ and $\mathbf{R}_j$,

$$G_{ij}^n(t,t')=\langle\langle\hat{S}_i^+(t);(\hat{S}_j^-(t'))^n(\hat{S}_j^+(t'))^{n-1}\rangle\rangle \tag{3.1.19}$$

where n takes $1, 2, 3, ..., 2S$. As a rule, we needs $2S$ independent Green's function for spin S.[12]

Now, we can write the equation of motion in-terms of the spin operators.

$$\omega\langle\langle S_i^+; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle = \frac{1}{2\pi}\langle[S_i^+; (S_j^-)^n (S_j^+)^{n-1}]\rangle + \langle\langle[S_i^+, \hat{H}]_-; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle \quad (3.1.20)$$

We use the following commutator relation:

$$[S_i^+, (S_j^-)^n (S_j^+)^{n-1}] = [2n\hbar S_j^z + \hbar^2(n^2 - n)](S_j^-)^{n-1}(S_j^+)^{n-1}\delta_{ij} \quad (3.1.21)$$

Now lets evaluate the second term in the right side of Eq.(3.1.20)

we start from evaluating the commutation relation:

$$\begin{aligned}
[S_i^+, \hat{H}]_- &= -\left\{[S_i^+, \frac{1}{2}{\sum}' J_{il} S_i^+ S_l^-]_- + [S_i^+, \frac{1}{2}{\sum}' J_{il} S_i^- S_l^+]_- + [S_i^+, \frac{1}{2}{\sum}' J_{il} S_i^z S_l^z]\right\} \\
&= -\left\{\frac{1}{2}{\sum}' J_{il}[S_i^+, S_i^+ S_l^-]_- + \frac{1}{2}{\sum}' J_{il}[S_i^+, S_i^- S_l^+]_- + \frac{1}{2}{\sum}' J_{il}[S_i^+, S_i^z S_l^z]\right\}
\end{aligned}$$

from the property of commutator:

$$[A, BC] = [A, B]C + B[A, C] \quad (3.1.22)$$

we have

$$\begin{aligned}
[S_i^+, S_i^+ S_l^-]_- &= (2\hbar S_l^z \delta_{il}) S_i^+ \\
[S_i^+, S_i^- S_l^+]_- &= (2\hbar S_i^z) S_l^+ \\
[S_i^+, S_i^z S_l^z]_- &= -\hbar S_i^+ S_l^z - S_i^z \hbar S_l^+ \delta_{il}
\end{aligned}$$

Thus for $i \neq l$,

$$[S_i^+, \hat{H}]_- = -\hbar {\sum}' J_{il} S_i^z S_l^+ + \hbar {\sum}' J_{il} S_i^+ S_l^z \quad (3.1.23)$$

Now we have

$$\langle\langle[S_i^+, \hat{H}]_-; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle = \langle\langle -\hbar {\sum}' J_{il} S_i^z S_l^+ + \hbar {\sum}' J_{il} S_i^+ S_l^z; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle \quad (3.1.24)$$

Use the decoupling which is used by Tyablikov:

$$\langle\langle S_i^z S_l^+; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle = \langle S_i^z\rangle \langle\langle S_l^+; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle \tag{3.1.25}$$

assumed that each spin has same average z-component

$$\begin{aligned}\langle\langle [S_i^+, \hat{H}]_-; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle &= -\hbar \sum{}' J_{il} \langle S^z\rangle \langle\langle S_l^+; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle \\ &+\hbar \sum{}' J_{il} \langle S^z\rangle \langle\langle S_i^+; (S_j^-)^n (S_j^+)^{n-1}\rangle\rangle \\ &= -\hbar \langle S^z\rangle \sum_{l\neq i}{}' J_{il} G_{lj}^n + \hbar \langle S^z\rangle \sum_{l\neq i}{}' J_{li} G_{ij}^n\end{aligned}$$

The equation of motion is become:

$$\omega G_{ij}^n = \frac{\delta_{ij}}{2\pi} C_n + \hbar \langle S^z\rangle \sum_{l\neq i}{}' J_{li} G_{ij}^n - \hbar \langle S^z\rangle \sum_{l\neq i}{}' J_{il} G_{lj}^n \tag{3.1.26}$$

where $C_n = [2n\hbar S_j^z + \hbar^2(n^2 - n)](S_j^-)^{n-1}(S_j^+)^{n-1}$

When we rearrange the above equation we get:

$$(\omega - \langle S^z\rangle \sum_{l\neq i}{}' J_{il}) G_{ij}^n = \frac{\delta_{ij}}{2\pi} C_n - \langle S^z\rangle \sum_{l\neq i}{}' J_{il} G_{lj}^n \tag{3.1.27}$$

Note: that the Hamiltonian of our system is given by

$$\hat{H} = -\sum_{l\neq i}{}' J_{li} \hat{S}_i \cdot \hat{S}_l \tag{3.1.28}$$

Generally speaking, the full lattice is always regular and has translational symmetry. As long as all its sites are occupied by local spins, (see Fig.(3.1)(a)), Fourier transformation can be done directly between real space and k space for Green's function because the identities

$$\frac{1}{N} \sum_{k\in Bz} e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} = \delta_{ij} \tag{3.1.29}$$

and

$$\frac{1}{N} \sum_{j=1}^{N} e^{i\vec{R}_j\cdot(\vec{k} - \vec{k'})} = \delta_{kk'} \tag{3.1.30}$$

can be used, where BZ denotes the first Brillouin zone of the full lattice and N is the total number of the lattice sites. When local spins are distributed randomly in the lattice (see

Fig.(3.1)(b)), the k vector can still be used. In fact it can be accessible experimentally although dopants are distributed randomly.[12]

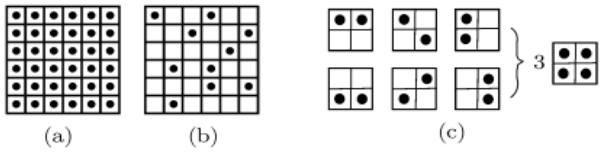


Figure 3.1: (a) The lattice formed by the cations of the un- doped semiconductor. The total number of the sites is N. The full configuration is defined by occupying each site with a local spin. (b) A given spin configuration. There are N' randomly distributed spins, where $N' < N$. (c) A demonstration of the configuration average of a summation over a single index with $N = 4$ and $N' = 2$. In this case we have six spin configurations, $\Omega = 6$, and they correspond to $\Omega N'/N$ full configurations when the prime summation is changed into the regular summation over the full configuration.[12]

The Fourier transformation of the Green's function in k space is given by

$$\langle\langle \hat{S}_i^+(t); (\hat{S}_j^-(t'))^n (\hat{S}_j^+(t'))^{n-1} \rangle\rangle = \frac{1}{N} \sum_k g_{kk'}^n(E) e^{ik\cdot(R_i - R_j)}$$

$$g_{kk'}^n(E) = \frac{1}{N} \sum_{ij} \langle\langle \hat{S}_i^+(t); (\hat{S}_j^-(t'))^n (\hat{S}_j^+(t'))^{n-1} \rangle\rangle e^{ik\cdot(R_i - R_j)}$$

where N is the total number of spins in the lattice.

Eq.(3.1.27) becomes:

$$\frac{1}{N} \sum_k e^{ik(R_i - R_j)} \left(\omega - \langle S^z \rangle \sum_{i \neq l}{}' J_{il} \right) g_{kk'}^n = \frac{\delta_{ij}}{2\pi} C_n - \langle S^z \rangle \sum_{i \neq l}{}' J_{il} \frac{1}{N} \sum_k g_{kk'}^n e^{ik.(R_l - r_j)} \tag{3.1.31}$$

For $i = j$ we have:

$$\left(\omega - \langle S^z \rangle \sum_{i \neq l}{}' J_{il} \right) g_{kk'}^n = \frac{1}{2\pi} C_n - \langle S^z \rangle \sum_{i \neq l}{}' J_{il} \frac{1}{N} \sum_k g_{kk'}^n e^{ik.(R_l - r_i)} \tag{3.1.32}$$

$$\left[\omega - \langle S^z \rangle \sum_{i \neq l}{}' J_{il} \left(1 - \frac{1}{N} \sum_k e^{ik.(R_l - r_i)} \right) \right] g_{kk'}^n = \frac{1}{2\pi} C_n \tag{3.1.33}$$

We have a given spin configuration for specific sample. It appears that we have to calculate the prime summation over the given spin configuration in order to calculate the

green's functions. Actually, we do not need to do it because the k vector is still usable and experimentally accessible for doped systems. Accordingly, what we need is the average of the prime summation over all the possible spin configuration. More details about this configuration average are given below.[12]

For an independent prime summation f, we can define its configuration average over all the spin configuration as

$$\langle f \rangle_c = \frac{1}{\Omega} \sum_{c_i \in C} f(c_i) \tag{3.1.34}$$

Where C is the set of all the Ω different spin configuration of the same number of magnetic moments. For a configuration average on a prime summation over a single index. Such as $\left\langle \sum_{i=1}^{'N'} A_i \right\rangle_c$, we have

$$\begin{aligned} \left\langle \sum_{i=1}^{N'} A_i \right\rangle_c &= \frac{1}{\Omega} \left[\sum_{c_j \in C} \left(\sum_{i=1}^{'N'} A_i \right) \right] \\ &= \frac{1}{\Omega} \left[\frac{\Omega N'}{N} \sum_{i=1}^{N} A_i \right] \\ &= \frac{N'}{N} \sum_{i=1}^{N} A_i \end{aligned}$$

Where $\sum_{c_j}$ means that the summation is done over spin configuration $C_j (c_j \in C)$, as demonstrated in Fig.(3.1). As a result, we derive

$$\begin{aligned} \left\langle \sum_{j=1}^{'N'} e^{i(k-k')\cdot R_j} \right\rangle &= \frac{N'}{N} \sum_{j=1}^{N} e^{i(k-k')\cdot R_j} \\ &= N' \delta_{kk'} \end{aligned} \tag{3.1.35}$$

As for a configuration average on a prime summation over double indexes such as $\langle \sum_{i\neq j}^{N'} B_{ij} \rangle_c$, the configuration average can be performed as follows

$$\begin{aligned} \left\langle \sum_{i\neq j}^{'N'} B_{ij} \right\rangle_c &= \frac{1}{\Omega}\left[\sum_{c_k\in C}\left(\sum_{i\neq j}^{'N'} B_{ij}\right)\right] \\ &= \frac{1}{\Omega}\left[\Omega\frac{N'(N'-1)}{N(N-1)}\sum_{i\neq j} B_{ij}\right] \\ &= \frac{N'(N'-1)}{N(N-1)}\sum_{i\neq j}^{N} B_{ij} \end{aligned} \tag{3.1.36}$$

After using the configuration average, the Fourier transformation in Eq.(3.1.33) can be completed and the Green's functions are obtained as

$$G_{ij}^n = \sum_k g_{ik}^n e^{k\cdot R_j}, \qquad g_{ik} = \sum_{k'} g_{kk'} e^{ik'\cdot R_i} \tag{3.1.37}$$

Here $g_{kk'}^n$ is expressed as

$$g_{kk'}^n = \frac{1}{N}\frac{C_n}{\omega - \langle S^z\rangle N'(J_0 - J_k)} \tag{3.1.38}$$

Where

$$J_k = \frac{1}{N'^2}\left\langle \sum_{i,l=1}^{N'} J_{il} e^{-ik\cdot(R_i - R_l)} \right\rangle_c \tag{3.1.39}$$

According to Eq.(3.1.38) and Eq.(3.1.39), the spin excitation energy spectrum is given by

$$E(k) = \langle S^z\rangle \frac{1}{N'}\left\langle \sum_{i\neq l}^{'N'} J_{il}\left[1 - e^{ik\cdot(R_l - R_i)}\right]\right\rangle_c \tag{3.1.40}$$

$$= \langle S^z\rangle \frac{1}{N'}\frac{N'(N'-1)}{N(N-1)}\sum_{i\neq l}^{N} J_{il}\left[1 - e^{ik\cdot(R_l - R_i)}\right] \tag{3.1.41}$$

$$= \langle S^z\rangle \frac{N'-1}{N(N-1)}\sum_{i=1}^{N}\sum_{\delta} J_{i,i+\delta}\left(1 - e^{ik\cdot\delta}\right) \tag{3.1.42}$$

Where the equality in Eq.(3.1.41) comes from Eq.(3.1.36) and the equality in Eq.(3.1.42) is obtained through making a cutoff approximation for the rang of the RkkY exchange interaction of the lattice site.[12]

Now simplify $E(k)$, the resulting spin excitation spectra are given by

$$E(k) = \langle S^z \rangle \frac{N'-1}{N(N-1)} NJ \sum_{\delta} \left(1 - e^{ik\cdot\delta}\right) \tag{3.1.43}$$

$$= \langle S^z \rangle \frac{N'(1-\frac{1}{N'})}{N(1-\frac{1}{N})} J \sum_{\delta} \left(1 - e^{ik\cdot\delta}\right) \tag{3.1.44}$$

$$= \langle S^z \rangle \frac{N'}{N} J \sum_{\delta} \left(1 - e^{ik\cdot\delta}\right) \tag{3.1.45}$$

$$= x_m \langle S^z \rangle J \sum_{\delta} \left(1 - e^{ik\cdot\delta}\right) \tag{3.1.46}$$

Here the equality Eq.(3.1.43) is obtained because the δ summation is independent of the specific lattice site. The equality in Eq.(3.1.45) is becomes because $\frac{1}{N} \approx 0$ and $\frac{1}{N'} \approx 0$. x_m in Eq.(3.1.46) , defined as $\frac{N'}{N}$, is the dimensionless effective concentration of magnetic impurities. Consider the case of a simple cubic lattice. In this case the nearest neighbors are along the $\pm x$, $\pm y$, and $\pm z$ axes at a distance a and we have.

$$\sum_{\delta} 1 - e^{ik\cdot\delta} = 2 - e^{ik\cdot\delta} - e^{-ik\cdot\delta}$$

$$= 2 - (e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} + e^{ik_z a} + e^{-ik_z a})$$

$$= 2 - 2(cosk_x a + cosk_y a + cosk_z a) \tag{3.1.47}$$

The energy spectrum relations becomes finally

$$E(k) = 2x_m \langle S^z \rangle J[1 - (cosk_x a + cosk_y a + cosk_z a)]$$

$$= 2x_m \langle S^z \rangle J(1 - coska) \tag{3.1.48}$$

For small k , $1 - coska \approx \frac{a^2 k^2}{2}$, Eq.(3.1.48) is reduces to approximately

$$E(k) = x_m \langle S^z \rangle J a^2 k^2 \tag{3.1.49}$$

Chapter 4

Calculation of Magnetization and critical temperature of $(Ga, Mn)As$ DMS

4.1 The total number of excited magnons

The total number of excited magnons in all modes at temperature T, can be estimated. Therefore,

$$\sum_k \langle n_k \rangle = \sum_k \frac{1}{e^{\frac{\epsilon_k}{k_\beta T}} - 1} \tag{4.1.1}$$

where, $\epsilon_k = Dk^2$ and $D = x_m \langle S^z \rangle Ja^2$

we can replace the summation by integration over a k space, hence

$$2\pi^2 \sum_k \langle n_k \rangle = \int_0^\infty \frac{k^2}{e^{\frac{Dk^2}{k_\beta T}} - 1} dk \tag{4.1.2}$$

Now, let $x = \frac{Dk^2}{k_\beta T} \implies k = \sqrt{\frac{k_\beta T x}{D}}$ and $kdk = \frac{k_\beta T x}{D}$

Substitute the above equation we obtain

$$2\pi^2 \sum_k \langle n_k \rangle = \int_0^\infty \frac{\sqrt{\frac{k_\beta T x}{D}} \frac{k_\beta T}{2D}}{e^x - 1} dx \tag{4.1.3}$$

For low temperature $x \to \infty$ and we have $e^x - 1 \approx e^x$

$$\begin{aligned} 2\pi^2 \sum_k \langle n_k \rangle &= \frac{1}{2} \left(\frac{k_\beta T}{D} \right)^{\frac{3}{2}} \int_0^\infty \frac{\sqrt{x}}{e^x} dx \\ &= \frac{1}{2} \left(\frac{k_\beta T}{D} \right)^{\frac{3}{2}} \int_0^\infty \sqrt{x} e^{-x} dx \end{aligned} \tag{4.1.4}$$

To solve the integral we have to introduce the gamma function

$$\Gamma(t) = \int_0^\infty x^{1-t} e^{-x} dx \tag{4.1.5}$$

and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$

in our case $t = \frac{1}{2}$ so, the integral becomes,

$$\int_0^\infty \sqrt{x} e^{-x} dx = \sqrt{\pi}$$

finally we have

$$\sum_k \langle n_k \rangle = \frac{1}{4} \left(\frac{k_\beta}{\pi D} \right)^{\frac{3}{2}} T^{\frac{3}{2}} \tag{4.1.6}$$

4.2 Magnetization

The temperature dependent magnetization, M(T), can be written as:

$$M(T) = M(0) - 2\mu_B \sum_k \langle n_k \rangle \tag{4.2.1}$$

where $M(0) = 2\mu_B nS$ is ground state magnetization or magnetization at absolute zero where all spins align parallel.[8]

Now substitute the value of M(0) into the above equation we obtain

$$M(T) = 2\mu_B nS - 2\mu_B \sum_k \langle n_k \rangle \tag{4.2.2}$$

take $2\mu_B nS$ as a common factor we have:

$$M(T) = 2\mu_B nS \left(1 - \frac{1}{nS} \sum_k \langle n_k \rangle\right) \tag{4.2.3}$$

Substituting Eq(4.1.6) into Eq(4.2.3),

$$M(T) = 2\mu_B nS \left[1 - \frac{1}{4nS} \left(\frac{k_\beta}{\pi D}\right)^{\frac{3}{2}} T^{\frac{3}{2}}\right] \tag{4.2.4}$$

where n is number of atoms per unit volume equal to $\frac{Q}{a^3}$ and $Q = 1, 2, 4$ for sc,bcc,fcc lattice constant respectively. $(Ga, Mn)As$ has fcc lattice structure with $n = \frac{4}{a^3}$ with lattice constant of about $a = 5.65\mathring{A}$.[8]

Now substituting the value of D and n into Eq.(4.2.4) we got

$$\begin{aligned} M(T) &= M(0)\left[1 - \frac{1}{4\frac{4}{a^3}\langle S^z\rangle}\left(\frac{k_\beta}{\pi x_m J\langle S^z\rangle a^2}\right)^{\frac{3}{2}} T^{\frac{3}{2}}\right] \\ &= M(0)\left[1 - \frac{1}{16\langle S^z\rangle}\left(\frac{k_\beta}{\pi x_m J\langle S^z\rangle}\right)^{\frac{3}{2}} T^{\frac{3}{2}}\right] \end{aligned} \tag{4.2.5}$$

where $M(0) = 2\mu_B nS$ and x_m is the concentration of magnetic impurity

We can also write Eq.(4.2.5) as a ratio of temperature dependent magnetization,M(T) and ground state magnetization,M(0) and we have,

$$\frac{M(T)}{M(0)} = 1 - \frac{1}{16\langle S^z\rangle}\left(\frac{k_\beta}{\pi x_m J\langle S^z\rangle}\right)^{\frac{3}{2}} T^{\frac{3}{2}} \tag{4.2.6}$$

From Eq.(4.2.6),we can plot reduced magnetization vs. temperature.

For better estimation the exchange integral of local magnetic moments, at different sites separated by distance of GaAs lattice constant($a = 5.56\mathring{A}$), J=31.1951 $\times 10^{-23}$joule; spin of the Mn $3d$ sub-shell of an atom $S = \frac{5}{2}$; the g-factor $g = 2$; and the Boltzmann constant $k_\beta = 1.38 \times 10^{-23}$ are used.[8]

Graph of reduced magnetization vs. temperature, for three value of magnetic impurity concentration, x_m, is shown below.

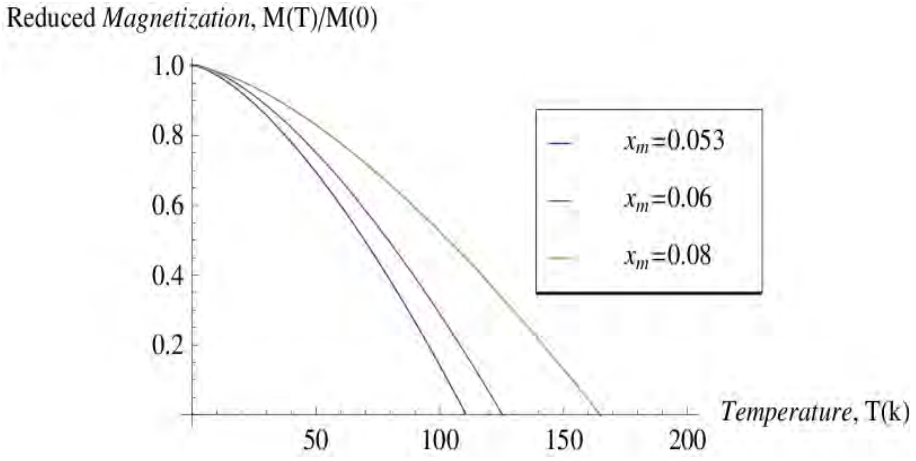


Figure 4.1: graph of reduced magnetization vs. temperature

4.3 Critical Temperature

We can determined the critical temperature T_c by taking the limiting case of Eq.(4.2.6) where $\frac{M(T)}{M(0)}$ approaches 0, i.e., for $\frac{M(T)}{M(0)} \to 0$ when $T \to T_c$.
recall Eq.(4.2.6) and Put $T = T_c$ into the equation we have

$$0 = 1 - \frac{1}{16S}\left(\frac{k_\beta}{2\pi x_m J_{nm} S}\right)^{\frac{3}{2}} T_c^{\frac{3}{2}}$$

$$\left[T_c^{\frac{3}{2}} = \frac{(2SJ_{nm}x_m)^{\frac{3}{2}}16\pi^2}{k_\beta^{\frac{3}{2}}}\right]^{\frac{2}{3}}$$

$$T_c = 2\pi \times (16)^{\frac{2}{3}} \frac{SJ_{nm}}{k_\beta} x_m \tag{4.3.1}$$

Following Eq.(4.3.1) the critical temperature,T_c, vs. impurity concentration, x_m, is plotted. And therefore,

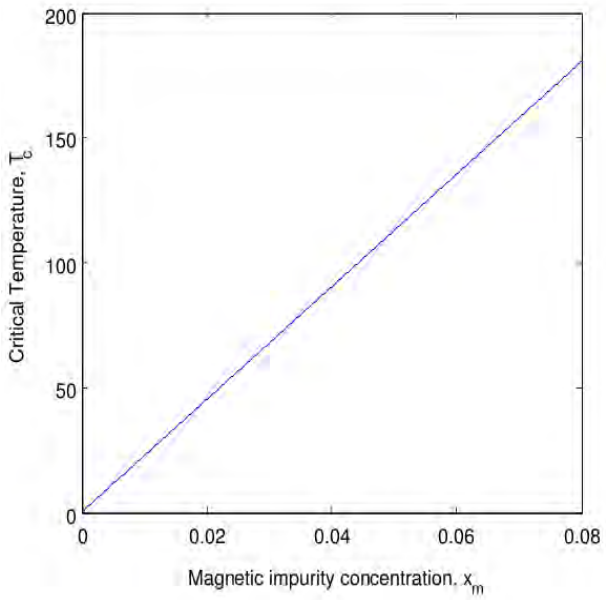


Figure 4.2: graph of critical temperature vs. impurity concentration

Chapter 5

Summary

A semiconductor is a material with electrical conductivity due to electrons flow intermediate in magnitude between that of a conductor and an insulator. Semiconductor intrinsic electrical properties are often permanently modified by introducing impurities by a process known as Doping and the materials which added to the semiconductor is called Dopant. Semiconductors which are doped with either with N-or P-type impurities are referred to as Extrinsic semiconductors

There are two types of impurities these are:

- N-type impurities which add free electron to the semiconductor and semiconductors with this impurities is called N-type semiconductors
- P-type impurities which contributes hole and semiconductors with this impurities is called P-type semiconductors.

the intrinsic concentration of electron is given by

$$n_i = 2\left(\frac{m_e^* k_\beta T}{2\pi\hbar^2}\right)^{\frac{3}{2}} exp\left(-\frac{E_c - E_f}{k_\beta T}\right)$$

and that of hole is

$$P_i = 2\left(\frac{m_h^* k_\beta T}{2\pi\hbar^2}\right)^{\frac{3}{2}} exp\left(\frac{E_v - Ef}{k_\beta T}\right)$$

- Diluted magnetic semiconductors (DMS) are materials in which a host semiconductors is doped with magnetic impurities, generally atoms of a transition metal such as manganese(Mn), iron (Fe), cobalt (Co), chromium.

- Diluted magnetic semiconductors are promising candidates for spintronics materials, as they naturally overcome the material incompatibilities in metal-semiconductor interfaces.

- Of particular interest are the III-V based semiconductor materials made magnetic by inclusion of Mn (or some other suitable transition metal) that can easily be integrated in the existing III-V semiconductor technologies.

- In order to exploit the possibilities of this new family of materials it is crucial to understand the fundamental mechanisms behind ferromagnetism in semiconductor based materials.

- (Ga,Mn)As and (Ga,Mn)N are considered as important prototype materials because of their relatively high Curie temperatures T_C , and further these materials provide us with a good testing ground in the quest for new, similar materials with optimized properties.

- In the present work we have obtained energy spectrum of magnetic spin excitation in (Ga,Mn)As, starting with Hamiltonian Eq.(3.1.18) and Green's function approach, as

$$E(k) = 2x_m\langle S^z\rangle J(1 - coska)$$

Approximately we have for long wave length magnons

$$E(k) = x_m\langle S^z\rangle Ja^2k^2$$

- The total number of excited magnons is given by

$$\sum_k \langle n_k \rangle = \frac{1}{4}\left(\frac{k_\beta}{\pi D}\right)^{\frac{3}{2}} T^{\frac{3}{2}}$$

where $D = x_m\langle S^z\rangle Ja^2$ and x_m is the concentration of magnetic impurity.

- From the total number of excited magnons the Magnetization can be calculated and we have

$$M(T) = 2\mu_B nS\left[1 - \frac{1}{4nS}\left(\frac{k_\beta}{\pi D}\right)^{\frac{3}{2}} T^{\frac{3}{2}}\right]$$

- The reduced magnetization is become

$$\frac{M(T)}{M(0)} = 1 - \frac{1}{16\langle S^z\rangle}\left(\frac{k_\beta}{\pi x_m J\langle S^z\rangle}\right)^{\frac{3}{2}} T^{\frac{3}{2}}$$

- from the limiting case, $\dfrac{M(T)}{M(0)} \to 0$ when $T \to T_c$, we can determine the critical temperature and we have

$$T_c = 2\pi \times (16)^{\frac{2}{3}} \frac{SJ_{nm}}{k_\beta} x_m$$

- Magnetization vs. T and T_c vs. x_m have been plotted as shown in Figs.(4.1 and 4.3)

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Declaration

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

Name: Asnake Sahele

Signature:– – – – – – – – – – –

Place and time of submission: Addis Ababa University, June 2011

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

Name: Prof. P. singh

Signature:– – – – – – – – – ––