Significance of Hole-Magnon interaction on Ferromagnetism in Diluted Magnetic Semiconductors

By

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GOD IS GOOD ALL THE TIME

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Abstract

In this thesis we studied hole-magnon dynamics to understand the contribution of their interaction on the enhancement of ferromagnetism in diluted magnetic semiconductors (DMS). The t-J model is used as the interaction Hamiltonian with a method of perturbation mathematical approach in which canonical transformation is used to obtain convergent values starting with canting the quantum anti-ferromagnetism from its Neel state by some angle θ with respect to the z-axis. Employing a spinless fermion representation for hole operators, Holstein-Primakoff and Bogoliubou transformations are used to change the hole and spin dynamics to the many body problem. Our calculations indicated that motion of a hole in the anti-ferromagnetic background is dependent on the magnetic correlation of the system and the tilted angle. The motion of a hole around the anti-ferromagnetic order is shown to be characterized by high and low energy dispersion fluctuation as the angle changes from 0^0 to 90^0. This fluctuation in energy spectrum is attributed as arising from the pair repair spin alignment which could happen in anti-ferromagnetic(AF) background because of the hole motion effect. This is to mean that the motion of the hole causes a disturbance on the spin cloud of the localized electrons. This also infer that effect of hole motion gives a ferromagnetic (FM) order (maxima) and anti-ferromagnetic (AF) order (minima) fluctuation. Making use of the obtained result, energy dispersion (E_k), spectral function (density function) (A_k) and quasiparticle weight (Z_k) for the $t/J << 1$ and $t/J >> 1$ limit were numerically evaluated and plotted.

Chapter 1

INTRODUCTION

1.1 General introduction

Currently, researchers are getting interested in the newly emerging field of basic physics called spintronics. Spintronics is employed by the spin and charge control activity. One of the issue of this topic can be prominently well explained in the study of diluted magnetic semiconductors (DMS). DMSs are helpful in integrating data processing and magnetic storage facilities in a single chip.

In several DMSs, like $GaMnP$, $GaMnN$, $GaMnSb$ etc, it is unclear whether all reports of Ferromagnetism particularly, at room temperature and above are indeed arising from clustering and segregation effects associated with various Mn complexes or have low solubility and related material problems.

The observed Ferromagnetism of $Ga_{(1-x)}Mn_{(x)}As$ is however well established and is universally believed to be on intrinsic DMS phenomenon. The Mn dopants in $GaMnAs$ serve the dual roles of magnetic impurities providing the local magnetic moments and of acceptors producing in principle one hole per Mn atom. The density, n_h, of holes in $GaMnAs$, however turns out to be by almost an order of magnitude lower than the density, n_i, of the Mn 3d sub-shell localized electrons. The precise role played by relative value of n_i and n_h determine the enhancement of the DMS Ferromagnetism.

There is no agreement even on the low density of charge carriers ($n_h << n_j$) in the system that weather helps or hinders ferromagnetism. An important question in this context is to obtain the functional dependency of the ferromagnetic transition temperature

T_c and the magnetic moment in terms of hole densities n_h and the Mn ion number density n_i. The existence of DMS ferromagnetism seems to be independent of the system being metallic or insulating.

The purpose of this thesis is to analyze the contribution of hole and magnon interaction on ferromagnetism in DMSs like $GaMnAs$. The hamiltonian describing the system is constructed based on standard model, the $t-J$ model Hamiltonian. This model is one of the most frequently used model for the descriptions of hole motion in anti-ferromagnetic (AF) transition metal oxide system. Associated with analytical method, the exact diagonalization employing Bogoliubou transformation and canonical transformation for converging the perturbation theory calculation techniques is used. A number of analytical methods such as spinless fermion approximation for hole operators, mean field approximation for bosons and spin waves and Holstein-primakoff approximation for bosons and so on were used for the investigation of the effective Hamiltonian of the specified model.

The canonical transformation is used for appropriate generalization of the conservation function employed in calculating the average dynamical quantities such as hole spectral density, energy dispersion, etc [1]. This approach is considered in a view that the particles in the system interact with one another in a complex way.

The dispersion and the mean number of magnon and hole in which they interact are calculated for which it leads to determine the effect of their interactions on Ferromagnetism of diluted magnetic semiconductor materials.

The theoretical analysis of transition metal oxide including cuprite, manganite and iron puicitide require faithful description of strongly correlated elections of the localize due to coulomb interaction in partly filled 3D orbital [2]. This interactions lead to the most insulators undoped compounds with spin and orbital degrees of freedom which interact with charge defects arising during under doping [3]. Then magnetic order and transport properties change due to sublattice inter-plane between charge and magnetic orbital degree of freedom. Examples are high temperature super conductivity in cuprates [3, 4, 5] and closed magnetic resistance in manganese [6, 7, 8].

In a system that takes place interaction between charge careers and localized spins is of crucial importance and drives an observed evolution of magnetic order and transform properties captured in the double exchange mechanism [9, 10, 11]. Those changes may also depend on subtle quantum effects in systems with coupled spin orbital charge degrees of freedom [1, 2, 3].

A well known problem in this area is dynamics of one hole added to transition metal oxides which interact with spin $S = \frac{1}{2}$ at the transition metal ion in the oxides planes of high temperature superconductors. The spins from AF order interact with hole due to the super-exchange interactions. The main difficulty in treating the dynamics of the doped holes is the AF quantum fluctuation of the spin background which has to be treated in one appropriate way [3, 4, 5].

Only very few many body problem is exactly solvable. Exact solutions are typically emitted to one dimensional model or to every special choice of interaction parameters. However, an exact solution provides important physical insights in to the nature of quantum states involved, could have to test approximate treatment, and may be used to draw useful conclusions for experimental studies.

This work is organized as follows. In Chapter two a review of literature is presented. The third Chapter deals with the mathematical formulation of a problem using the specified model called $t-J$ model and employed perturbation theory. Chapter four deals with spectral function of hole and magnon distribution function. Under this we have discussed terms like energy dispersion and spectral function for the correlations of hole motion along with, quasi particle weight (quasi survival of a hole in the magnetic polaron) and so on.

Finally, in Chapter five and Chapter six, we discussed and summarized the obtained results.

Chapter 2

REVIEW OF LITERATURE

2.1 Overview of Semiconductors

A semiconductor is a narrow band gap insulator at absolute temperature. It mean that the energy gap between the highest filled band (the valence band) and the lowest unfilled band (or the conduction band) is typically of the order of one electron volt. The electrical conductivity of a semiconductor is typically much less than that of a metal. Purity of a semiconductor is very important for more control while doping is used to vary the electrical properties[1].

Donor impurities are added to increase the number of electrons and acceptor impurities are added to increase the number of holes. Holes act as positive charges, while electrons behave as negative charges. Donor impurities become positively ionized by contributing an electron to the conduction band and acceptors become negatively ionized by accepting electrons from the valence band.

The holes and electrons are thermally activated. Temperature range in which the charge carrier contributed by the impurities dominate the semiconductor is said to be in extrinsic. Otherwise it is said to be intrinsic. Over a certain temperature range, donors can add electrons to the conduction band or acceptors can add holes to the valence band as the 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.

The forbidden band gap for metals is almost all zero but for insulators the forbidden

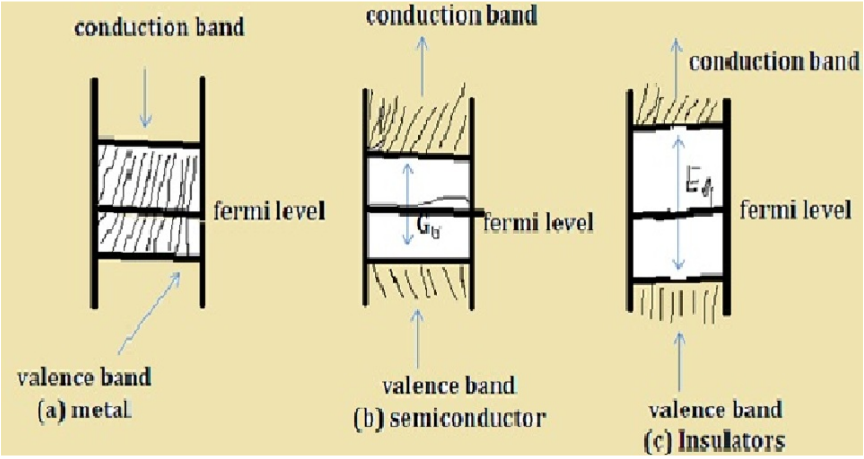

Figure 2.1: Band gap energy for (a) metals,(b) semiconductors and (c) insulators

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band gap is largest of the three. But for semiconductors it is not to small like metals and not to large as insulators[1].

2.2 Electrons and Holes Concentration in Semiconductors

The Fermi function evaluated at the Fermi energy $E_F = \mu$ where μ is assumed near the middle of the band. So the Fermi function $f(E)$ is given by:

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1} \tag{2.2.1}$$

The concentration of electrons in the conduction band and concentration of holes in the valence band can be calculated using the Fermi function.

Assume the non-degenerate case when E in the conduction band implies $E - \mu >> k_B T$ so:

$$f(E) = e^{-\frac{(E-\mu)}{k_B T}} \tag{2.2.2}$$

The energy versus density of state assumes a parabolic band as shown in Fig. 2.2. It shows with increasing of D(E) direction , f(E) is indicated in the opposite. The parabolic

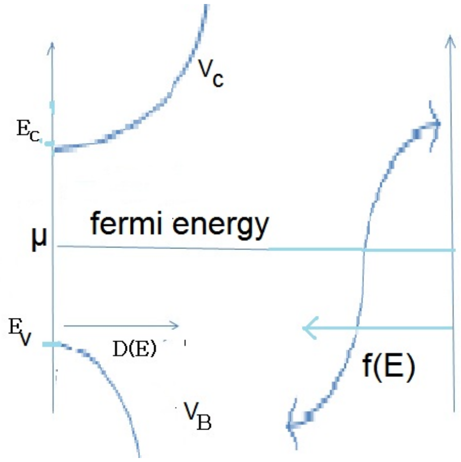

Figure 2.2: Energy gaps, Fermi function and defect level (sketch).

energy function is given by :

$$E = \frac{\hbar^2 k^2}{2m_e^*} + E_c \tag{2.2.3}$$

E_c is the energy of bottom of the conduction band where m_e^* is constant. The density of state is given by:

$$D(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E - E_c} \tag{2.2.4}$$

The number of electrons per unit volume in the conduction band is given by:

$$n = \int_E^\infty D(E)f(E)dE \tag{2.2.5}$$

Evaluating integral of equation (2.2.5) gives:

$$n = 2\left(\frac{m^* K_B T}{2\pi\hbar^2}\right)^{3/2} e^{\frac{(\mu - E_c)}{k_B T}} \tag{2.2.6}$$

For holes, we assume following equation (2.2.3) and(2.2.6):

$$E = E_v - \frac{\hbar^2 k^2}{2m_h^*} \tag{2.2.7}$$

The density of state for holes is given by:

$$D(E)_h = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\sqrt{E_v - E_c} \tag{2.2.8}$$

The number of holes per state is:

$$f_h = 1 - f(E) = \frac{1}{e^{\frac{(\mu - E)}{k_B T}} + 1} \tag{2.2.9}$$

For a non-degeneracy assumption and assume $(\mu - E) >> E$ in the valence, so

$$f(E) = e^{\frac{(E-\mu)}{k_B T}}$$

The number of holes per volume in the valence band is given by

$$p = \int_{-\infty}^{E_v} D_h(E) f_h(E) d(E) \tag{2.2.10}$$

from which we find: $p = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2} e^{\frac{(E_v - \mu)}{k_B T}}$. The density of states in the valence and conduction bands are essentially unmodified by the presence or absence of donors and acceptors hence, are valid with or without donors or acceptors for n and p, respectively. Multiplying n and p, we find $np = n_i^2$.

Where;

$$n_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} \left(m_e^* m_h^*\right)^{3/4} e^{\frac{(-E_g)}{2k_B T}} \tag{2.2.11}$$

$E_g = E_c - E_v$, which is called the band gap and n_i is the intrinsic (without donor or acceptor) electron concentration. $np = n_i^2$ is sometimes called the law of mass action and is generally true since it is independent of μ [7].

2.3 Electron Energies

Each isolated atom has only a certain number of orbital available. These available orbital represent energy level for the electrons. Modern physics tells us that only discrete value of electron energies is possible. An electron cannot have only value of energy usually expressed by eV, but only certain permissible values. No electron can excite at an energy level other than a permissible one. For a single atom a diagram can be drawn for showing the different energy levels available for its electrons. Figure 2.3 is the energy level diagram for the hydrogen atom, as an example the permissible energy levels are numbered $n = 1, 2, \ldots$ in increasing order of energy.

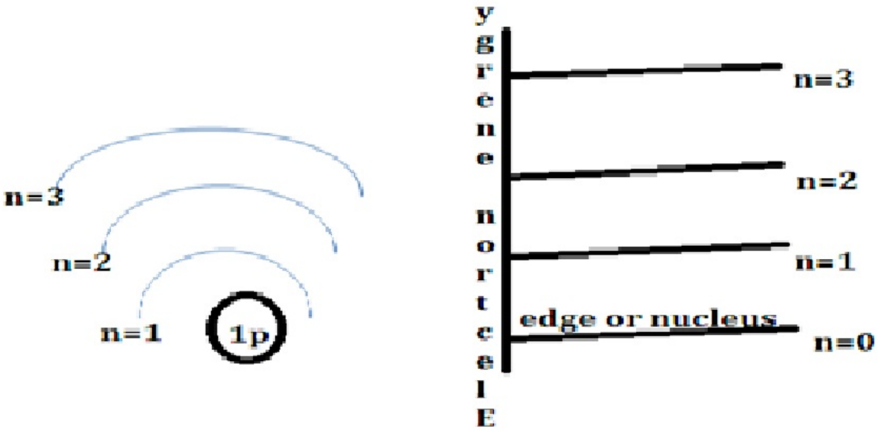

Figure 2.3: Permissible energy level in isolated hydrogen atom.

In any atom, the greater the distance of an electron from the nucleus, the greater is its total energy or the total energy including kinetic and potential energies. An electron orbiting very close to the nucleus to the first shell is tightly bound to the nucleus and posses only a small amount of energy. It would be difficult to knock out this electron. On the other hand an electron orbiting far from the nucleus would have a greater energy and hence easily knocked out of its orbit. This is why it's valence electron entered to the conduction band easily. i.e. the electron in the outer most orbit, having maximum energy that take part in chemical reaction and in bonding the atoms together to form solids.

When energies, like heat, light, or other radiations, are impinged on an atom, the energy of the electrons increase. As a result, lifted to higher energy levels or larger orbit. The atom is then said to be excited. This state doesn't last long and very soon fall back to the original energy level. In this process, the electrons give out energy in the form of heat, light or other radiations.

2.4 Energy Bands In Solids

When atoms bond together to form a solid, the simple diagram of Fig. 2.4 for the electron energies are no longer applicable. In a solid, the orbit of the electron is influenced not only by the charges in its own atom but by nuclei and electrons of energy atom in the solid. Since each electron occupies a different position inside the solid, no two electrons can be seen exactly in the same pattern of surrounding charges. As a result, the orbits of the electron are different.

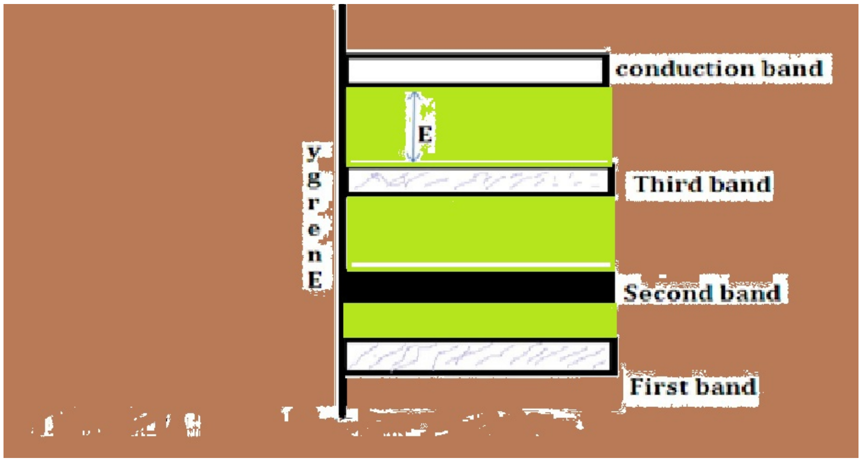

Figure 2.4: Energy band diagram of a solid (S_i)

Now it modifies to that shown in Fig.(2.4). There are millions of electrons, belonging to the first orbit of atoms in the solid. Each of them have different energy. Since there are millions of first orbit electrons the closely spaced energy levels differing very slightly in energy from a cluster or band. Similarly the second orbit and higher orbit electrons also form bands. We now have first energy band, second energy band, third energy band ... etc.

2.5 Magnetism

Magnetism is an interaction of moving charges with other moving charges. The magnetic field is defined in terms of the torque on a magnetic test dipole. It has no sources or sinks; magnetic field patterns never converge on or diverge from a point.

The magnetic and electric fields are intimately related. The principle of induction states that any changing electric field produces a magnetic field in the surrounding space, and vice versa. These induced fields tend to form whirlpool patterns.

The most important consequence of the principle of induction is that there are no purely magnetic or purely electric waves. Disturbances in the electrical and magnetic fields propagate outward as combined magnetic and electric waves, with a well-defined relationship between their magnitudes and directions. These electromagnetic waves are what light is made of. But other forms of electromagnetic waves exist besides visible light, including radio waves, x-rays, and gamma rays.

Fields of force contain energy. The density of energy is proportional to the square of the magnitude of the field. In the case of static fields, we can calculate potential energy either using the previous definition in terms of mechanical work or by calculating the energy stored in the fields. If the fields are not static, the old method gives incorrect results and the new one must be used [12, 13].

2.6 Magnetic Ordering

Among the paramagnetic materials, it is possible especially at low temperatures to distinguish three different sub classes of magnetic materials called Ferromagnetism, Anti-Ferromagnetism, or Ferrimagnetism.

The basis for the distinction is provided by magnetic ordering with spontaneous magnetization. i.e. the alignment of spontaneous atomic or molecular moments with respect to one another and with respect to the crystallographic axes.

The origin of magnetism lies in the orbital and spin motions of electrons and how the electrons interact with one another. The best way to introduce the different types of magnetism is to describe how materials response to magnetic fields. This may be surprising to some, but all matter is magnetic. It is just that some materials are much more magnetic than others are. The main distinction is that in materials there is a very strong interaction between moments.

The magnetic behavior of materials can be classified in to the following five major groups;diamagnetism, Para magnetism, ferromagnetism, ferrimagnetism and anti-ferromagnetism.

Diamagnetism and Para magnetism are those that exhibit no collective magnetic interaction and are not magnetically ordered ferromagnetism, ferromagnetism and Anti ferromagnetism exhibit long-range magnetic order below certain critical temperature. Ferromagnetic and ferri-magnetic materials are usually what we consider as being magnetic (i. e., behaving like iron). Whereas diamagnetic, paramagnetic and anti-ferromagnetic materials are so weekly magnetic that they are usually thought of as nonmagnetic one [13, 14, 15, 16].

2.6.1 Diamagnetism

It is a fundamental property of all matter, although it is usually very weak. It is due to the non-cooperative behavior of orbiting electrons when exposed to an applied magnetics field . Diamagnetic substances are composed of atoms which have no magnetic moments. (i.e. all the orbital shells are filled and there are no up paired electrons). However, when exposed to an external magnetic field, a negative magnetization is produced and thus the susceptibility is negative. When the field is zero, the magnetization is zero. The other characteristic behavior of diamagnetic materials is that the susceptibility is temperature independent. Some well-known substances include quartz (SiO_2), calcite ($CaCo_3$) and water (H_2O)

2.6.2 Paramagnetism

It is the class of materials that have a net magnetic moment due to up paired electrons in a partially filled orbital. One of the most important atoms with un paired electrons in iron. However, the individual magnetic moments do not interact magnetically, and like diamagnetism, its magnetization is zero end with the field is removed.

In the presence of a field, there is no a partial alignment of the atomic magnetic moments in the direction and positive susceptibility. In addition, the efficiency of the field in aligning the moments is opposed by the rang dominating effects of temperature. This result in temperature dependent susceptibility is small (but larger than the Diamagnetic contribution) unless the temperature is very low ($<< 100K$) or the field is varying. High paramagnetic susceptibility is independent of the applied field. Under these conditions, paramagnetic susceptibility is proportion to the total iron content.

Many iron-bearing minerals are paramagnetic at room temperature. Some of them, include montcorillonite (clay), Nontronite (Fe- rich clay) Biotitic (silicate) siderite (carbonate) and pyrite (sulfide).

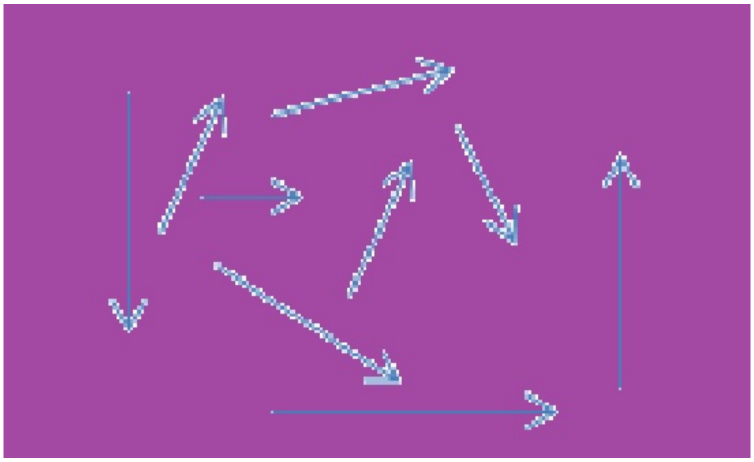

Figure 2.5: Spin alignment in paramagnetic materials.

2.6.3 Ferromagnetism

It is property of substances, which are capable of having magnetization in absence of external magnetic field. Even in absence of external magnetic field, the magnetization in a domain of ferromagnetic material has saturation value (Ms). The electron spins are the sources of permanent magnetic moment. Ferromagnetism is found only in elements that have incomplete energy level such as 3d in Fe Ni and Co; 4f level in Gd.

However, not all elements possessing magnetic moment are ferromagnetic. Ferromagnetism and semiconducting properties coexist in magnetic Semiconductors; such as Europium Chalcogennids and semiconducting spinless materials that have a periodic array of magnetic elements. Magnetic order exists only below certain critical temperature, T_c, called the Curie point $T_c = 774$ K, 1131 K, and 372 K for Fe, Co, and Ni, respectively. Above T_c, all Ferromagnetism show normal paramagnetic behavior. Ferromagnetic susceptibility which is high at the point below T_c can be expressed as curie point. This implies that susceptibility obeys the curie Weiss law. Below the Curie point, a ferromagnetic substance spontaneously magnetize into regions called ferromagnetic domains.

The total magnetic moment of the material is the vector sum of the magnetic moment of the individual domains. It is now known that these assumed domains really exist and are usually between 0.01 and 0.1 cm wide. See fig. 2.6.

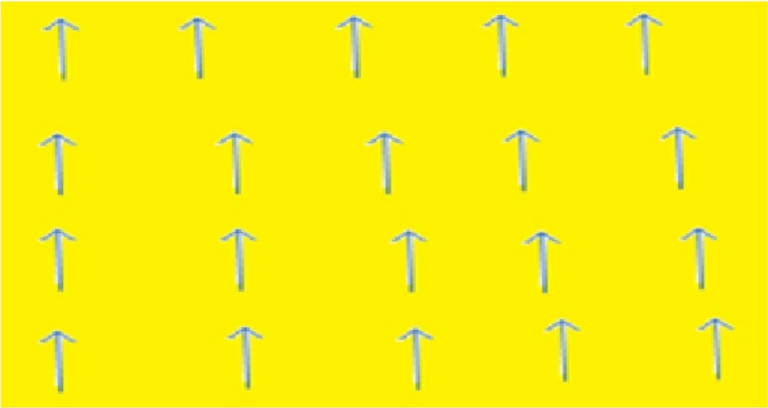

Figure 2.6: Spin alignment in ferromagnetic materials

2.6.4 Ferrimagnetism

In ionic compounds such as oxides, more complex forms of magnetic ordering can occur. As a result of the crystal structure called ferrimagnetism. Ferrimagnetism is only special case of ferromagnetism, for example, magnetite (Fe_3O_4) is a well-known ferromagnetic material. It was considered ferromagnetic until Neel provided the theoretical frame work for understanding ferrimagnetism. The curie temperature of ferromagnetic materials is usually quite higher than the room temperature and saturation magnetization at $0K$ can be the orders of $500G$. Figure 2.7 shows the property.

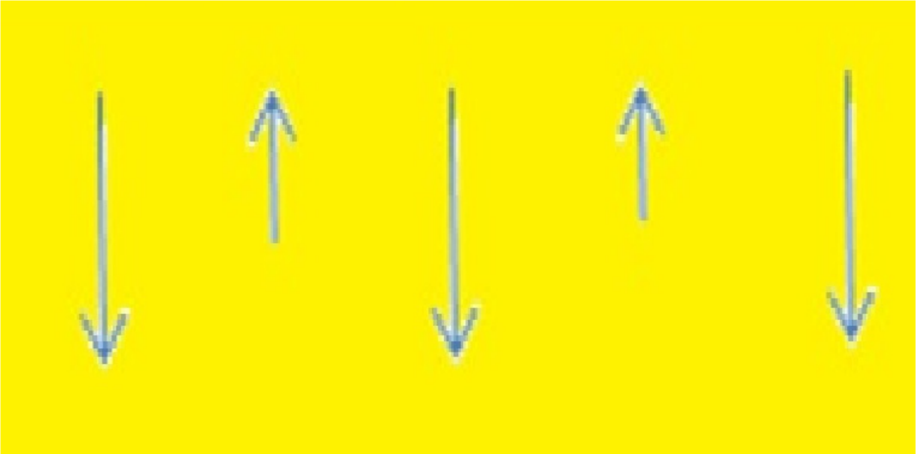

Figure 2.7: Spin alignment in ferri magnetic materials.

2.6.5 Anti-Ferrimagnetism

A more common situation is when the crystal symmetry is such that the localized dipole moment alignment at different lattice sites results in no net macroscopic magnetic field. Then such solid is referred to as anti-ferromagnetism. MnO, FeO, CoC and NiO, are few well-known examples of anti-ferromagnetically ordered solids. The sub lattice moments of anti-ferromagnetic materials are exactly equal but apposite, the net magnetization is zero.

The clue to anti-ferromagnetism is the behavior of susceptibility above a critical temperature (T_c). Above Neel temperature (T_N), the susceptibility obeys the Curie Weiss law for Paramagnets but with a negative intercept indicating negative exchange interactions as shown in figure 2.8.

2.7 Spintronics and it's Application

In course of years spintronics research has spread over all branches of condensed matter physics and materials science. Indeed, because of asymmetry in abundance of electric and magnetic elementary charges, random magnetic fields are weaker than random electric fields. So that electron spin may at the end be better information carrier than the electron

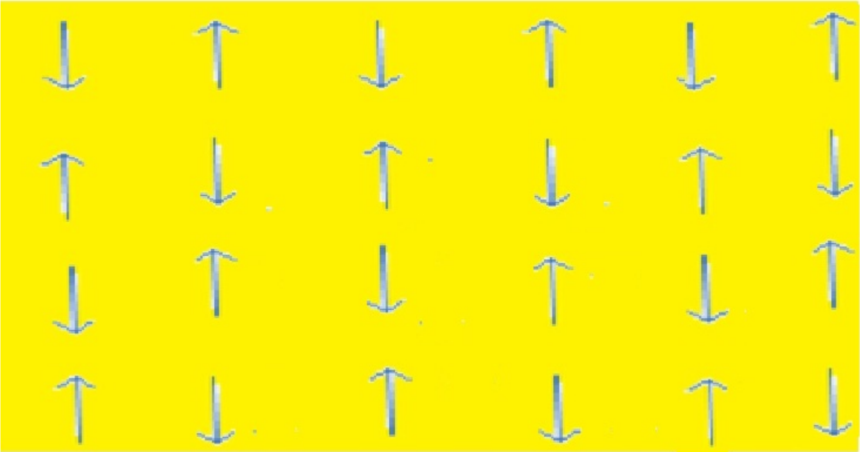

Figure 2.8: Spin alignment in antiferromagnetic materials.

charge in both classical and quantum information technologies [17].

With no doubt, the most advanced are studies on metal magnetic multilayered, in which spin dependent electron scattering and tunneling are employed in reading heads of hard disks and random access magnetic memories (MRAMs) that are now reaching the production stage.

However, particularly interesting appear ferromagnetic semiconductors as they combine resources of magnetic and semiconducting systems.

Now we discuss issues we encounter developing wide-band gap semiconductor systems in which spontaneous magnetization persists to above room temperature. We are interested to describe advances in spintronics research on non-magnetic semiconductors in narrow-band gap semiconductors can serve for spin manipulation. while it is weakness in wide-band gap dielectric constant, and offer a worthwhile opportunity for developing functional quantum gates.

Owing to a short-range character of the direct exchange interaction between tightly localized magnetic orbital, the coupling between d-orbital electron spins proceeds indirectly via $s-p$ bands in tetrahedrally coordinated diluted magnetic semiconductors (DMS). Such a coupling is usually antiferromagnetic, if the $s-p$ bands are either entirely occupied or totally empty (superexchange), but can acquire a ferromagnetic character in the presence of free carriers (zener or RKKY mechanism).

The discovery of carrier-induced ferromagnetism in Zinc blend III-V compounds containing a few percent of Mn in which T_c can exceed $100K$. Followed by the prediction and the observation of ferromagnetism in p-type (II, Mn-VI) materials, opened up new areas for exploration [17]. Spintronics exploits the electron spin along with its charge. In this material, there is a need for manipulating of spin and charge degrees of freedom to yield a desired electronic outcome. All spintronics devices act in order that:

1. Information is stored (written) in to spin as a particular spin orientations (up or down).
2. The spins, being attached to mobile electrons, carry the information along a wire, and
3. The information is read at the terminal.

Spin orientation of conduction electrons survives for a relatively long time (Nano seconds compared to tens of femes seconds during which electron momentum and energy decay). This make spintronics devices particularly attractive for memory, storage and potentially for quantum computing purpose. Here electron spins Would represent a bit (called cubit) of information. What is expected from these materials is to have a large commercial and economic impact in non-volatile memories (the information stays in the memory even if the electronic power is switched off, in contrast to semiconductor memories that we use).

Now we talk about preciously two, the most important successfully technologies today in the world has been the Si integrated circuit (ICs) and the Data storage industry. Both continue to advance at a rapid pace.

On the other hands, the data Storage industry has had a great and significant advance in the elaboration of different devices for this end. For example for magnetic hard disk drive Technology, a typical desktop computer drive today has a 40 GB, whereas in 1995, this capacity was approximately 1GB [11].

All integrated circuits operate and controlling the flow of the carrier charges (electron and hole) through the semiconductor when we applied an electric field. This is the dominant parameter in this type of devices.

For the case of Magnetic data storage, the dominant parameter is the spin of the electron. Where this characteristic intrinsic can be considered as the fundamental origin of the Magnetic moment. This characteristic is more important for ICs that consist in your high speed Signal processing and excellent trustworthy. But the memory elements are volatile (The stored information is lost when the power is switched-off, as data is stored in Capacitors).

A big advantage of magnetic memory technologies is that, there are non-volatile since they employ ferromagnetic materials that by nature have reminisced. A new field of the electronic opens the possibility for the study and understands of the properties a new material that tries combining the two-promise characteristic (charge and spin). This branch of the electronics is now like, semiconductor spin transfer electronics (spintronics).

Spintronics or spin electronics, consist in the study of active control and manipulation of spin degrees of freedom in solid-state system [12]. On this base, several group of investigator in the world are trying looking for material which combining both properties, to create an amazing new generation of electronic devices.

This characteristic open the possibility of developing spintronics devices that could be much smaller, (less than 100 nanometers) which consume less electricity and be more powerful for certain types of computations than is possible with electron-charge based system.

The scientific community hope understand the behavior of electron spin in this kind of material, in order to provide something foundations new about solid state physics that will lead to a new generation of electronic devices based on the orientation of spin in addition to the flow of charges [17, 18].

2.8 Diluted Magnetic Semiconductor

Diluted magnetic semiconductors (DMS) have attracted considerable attention. Because they hold the promise of using electron spin, in addition to its charge flow for creating a new class spintronics(semiconductor devices with unprecedented functionality) [12]. The suggested applications include, spin field effect transistors, which could allow for software reprogramming of the microprocessor hard ware during run times. semiconductor-based spin valves which would result in high-density, non-volatile semiconductor memory chips and even spin quits to be used as the basic building block for quantum computing. The attention was paid primarily to $Mn_xGa_{(1-x)}As$ for several reasons:

1. Significant break through the non-equilibrium growth of $Mn_xGa_{(1-x)}As$, pioneered by H. Ohno and Co-workers, has enabled its practical growth with stoichiometric amount of Mn [13].
2. this material has been experimentally confirmed to be ferromagnetic, with curie temperature as high as 110 K.
3. $Mn_xGa_{(1-x)}As$ alloys are recently compatible with existing $GaAs$ technology, resulting in the practical realization of device structure combining ferromagnetic and non-magnetic layers. Last, but by no means least, injection of spin polarized holes has been observed experimentally and supported theoretically, proving that spintronics devices are feasible.

Data storage media such as hard disks use the spin of electrons in a magnetic study interesting and it is of great technological importance to find DMS system with curie temperature, T_c above room temperature (RT) [13].

It was predicted theoretically, based on a Zener model, that an alloy of $Mn_{(x)}Ga_{(1-x)}As$, with an amount of Mn comparable to that used in $Mn_xGa_{(1-x)}As$, should result in a curie temperature exceeding room temperature. Of course, GaN is a technologically important material in its own right due to its applications in numerous devices, most notably in the blue solid-state laser.

A successful operation of spintronics devices requires more than a ferromagnetic semiconductor. It requires the support of spin-polarized transport so that spin polarized charge carriers may be injected into non-magnetic semiconductor. It was found by Korring-Kohn-Kostoker (KKR) in that Mn [17, 18, 19, 20].

Chapter 3

Formulation of the Problem and Mathematical Techniques

3.1 Description of The Model Hamiltonian

The model presented in the Fig. 3.1, is the same structure as transition metal oxides like MnO. It assumes that spins with general value S occupy transition metal sites. Spins $S(i)$ are coupled by Ferromagnetic (FM) Heisenberg exchange interaction as in the case of the Fig.3.1 for simpler 1D model considered [24]. While holes are located in the valance orbital. The hole at this site change its degrees of freedom which causes to couple with the spins by a local anti-ferromagnetic (AF) exchange as to a hole injected to transition metal oxide [25].

Let J be the strength of exchange interaction constant of localized spins among each other, and t be hole hopping constant as can be referred from Fig. 3.1.

The problem is formulated by the model Hamiltonian of the form

$$\hat{H} = \hat{H}_{hh} + \hat{H}_{mm} + \hat{H}_{m-h} \tag{3.1.1}$$

where

$\hat{H}_{hh}$ refers to freely hopping hole Hamiltonian, $\hat{H}_{mm}$ freely magnons Hamiltonian and $\hat{H}_{m-h}$ magnon-hole interaction Hamiltonian.

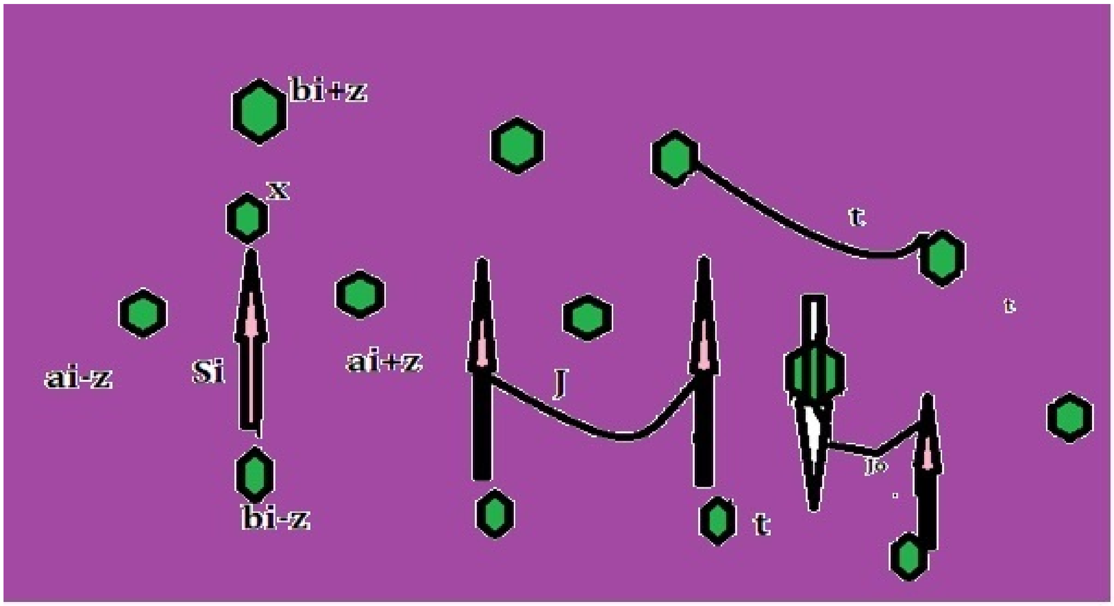

Figure 3.1: A model system that shows interaction of spin wave and hole motion.

3.2 Freely Hopping Hole Hamiltonian

The term H_{hh} in equa. (3.1.1) is free hole hopping energy due to anti-ferromagnetic background of the system considered in fig(3.1). Before we discuss the many body states of creation and annihilation operates we need to formulate the dynamics of a single hole motion.

Assume the hole is located at site r in the orbit, then the system with N sites have a state $\mid r\rangle$. $\mid r\rangle$ is orthogonal and is $\langle r \mid r'\rangle = \delta_{rr'}$.

The general hopping hamiltonian of the hole with translational invariance is

$$\hat{H}_{hop} = \sum_{rr'} t(r-r') \mid r'\rangle\langle r \mid = \sum_{\langle i,j\rangle} t_{ij} \mid r'\rangle\langle r \mid \tag{3.2.1}$$

In particular case of a one dimensional chain with nearest neighbor hopping, it is given by;

$$\hat{H}_{hop} \mid r\rangle = -t(\mid r+a\rangle + \mid r-a\rangle) \tag{3.2.2}$$

Where $r \pm a$ is due to the periodic boundary condition and is always understood a periodic length L.

The mathematical approach we use for the hopping hamiltonian for the hole is identical to the tight-binding approach to electron bands. The dynamics of hole could be studied easier by considering the motion of the hole as a lattice model. Every independent hopping model will yield similar behavior and due to the discreteness of the position of the hole at a discreet parameter, we need to specify the hopping model. A convenience of this hopping model is lattice hopping model formulation.

The lattice hopping formulation deals with one band. One band of the lattice model does not mean necessary to the lowest band of the continuum model, but it tells us where the action is located. As we know from the usual situation the lowest bands are completely filled bands.

In view of the lattice symmetry, we considered that the eigenstates have a well defined crystal wave vector $|r\rangle$. The transformation of this crystal wavevector to the fourier state is

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{r} e^{ikr} |r\rangle \tag{3.2.3}$$

Substituting equ(3.2.3) in equ(3.2.1),

$$\hat{H}_{hop}|k\rangle = \frac{1}{\sqrt{N}} \sum_{rr'} t(r-r') e^{ikr} |r'\rangle = \frac{1}{\sqrt{N}} \sum_{R} t_{(R)} e^{ikR} \sum_{r}^{\prime} e^{ikr'} |r'\rangle \tag{3.2.4}$$

Where $R = r_i - r_j$ which is the position between sites i and j. And also $E(k)$ is the dispersion energy of free hopping hole given by

$$E_{(k)} = \sum_{R} t_{(R)} e^{ikR} \tag{3.2.5}$$

Now we have seen that $E_{(k)}$ is the fourier transform of the term $t(R)$.

For one dimensional chain equ(3.2.5) the free hole dispersion energy $E(k)$ can be shown to be

$$E_{(k)} = \sum_{R} t_{ij} e^{ikR} = \sum_{<ij>} t_{ij} e^{ik(r_i - r_j)} \tag{3.2.6}$$

t_{ij} is dependent on the distance between site i and site j. i. e., $|R_i - R_j|$. t_{ij}-is the energy (hopping integral) of the hole of nearest neighbor sites i and j. It is calculated from the concept of 1^s hypogenic wave function and given by

$$t_{ij} = 2t\frac{(1 + R_i - R_j)}{a}e^{-\frac{(R_i - R_j)}{a}} \approx 2t \tag{3.2.7}$$

The hole Energy dispersion $E_{(k)}$ can be obtained as

$$E_{(k)} = \sum_n e^{ik(R_i - R_j)}$$

The allowed value of k can be determined using the concept of periodic boundary condition i. e.,

$$e^{ika} \simeq 1$$

This indicates that

$$\cos ka + i \sin ka = 1$$

To satisfied the above equation, the value of $\sin ka$ must be zero and $\cos ka = 1$. As a result of this the value of k should be

$$k = \frac{2\pi}{L}(n) = \frac{2\pi}{L}(n_x, n_y, n_z) \tag{3.2.8}$$

Where n is an integer and is given by

$$n = (n_x, n_y, n_z) = 0 \pm 1 \pm 2 \pm \dots \tag{3.2.9}$$

and $L = aN'$ with $N'^3 = n_x n_y n_z = N$ and a is lattice spacing constant taken as unity.

Taking N as even, $\frac{1}{2}N$ and $-\frac{1}{2}N$ gives identical value of e^{ikr} for all r. So that we take only $\frac{1}{2}N$.

The value of $n = 0$ or $k = 0$ represents a uniform mode for which all $t_{ij} = t_r$ are equal and is independent of r. So that $t_r = t$. $\sigma = R_i - R_j$, $\sigma = 1$, when $R_i = R_j$.

For $i = j$, the sum over k gives Nt. That means,

$$\sum_n e^{ik(R_i - R_j)} = N'^3 = N$$

Then the freely hopping hole energy dispersion E_k for $i = j$, becomes

$$E_k = \frac{1}{N} \sum_{<ij>} t_{ij} e^{ik\sigma} = t \tag{3.2.10}$$

Equation ((3.2.10)) shows the energy of hole for uniform mode is independent of the wavevector k.

On the other hand, for $i \neq j$, E_k is defined as,

$$E_k = \frac{1}{N} \sum_{<ij>} t_{ij} e^{ik\sigma_{ij}}$$

But, $\sigma_{ij} = \sum_{<ij>} (R_i - R_j)$ and

$$\sum_n e^{ik(R_i - R_j)} = \sum_{n_x} e^{ik_x(R_{ix} - R_{jx})} \sum_{n_y} e^{ik_y(R_{iy} - R_{jy})} \sum_{n_z} e^{ik_z(R_{iz} - R_{jz})} \tag{3.2.11}$$

With

$$\sum_n e^{ik\sigma} = \sum_{n_x} e^{ik_x(\sigma_x)} \sum_{n_y} e^{ik_y(\sigma_y)} \sum_{n_z} e^{ik_z(\sigma_z)}.$$

where $k_x = \frac{2\pi}{L}(n_x), k_y = \frac{2\pi}{L}(n_y), k_z = \frac{2\pi}{L}(n_z)$ and $\sum_n e^{ik(R_i - R_j)} = N\sigma_{ij}$

This is the analog for discrete sums of the delta function representation

$$\int e^{ikx} dx = 2\pi\sigma_{ij}$$

Now the energy dispersion of hopping of the hole in the system E_k can be calculated one by one as follows

$$\sum_{n_x} e^{ik_x\sigma_x} = \sum_{n_x} e^{\frac{2i\pi}{L} n_x \sigma(i_x - j_x)}$$

with

$$\frac{-N'}{2} < i_x j_x \leq \frac{N'}{2}$$

$$\sum_{n_x} e^{ik_x\sigma_x} = \sum_{n_x=0}^{\frac{N'}{2}} e^{ik_x\sigma(i_x - j_x)} + \sum_{n_x=1}^{\frac{N'}{2}} e^{ik_x\sigma(i_x - j_x)}$$

The energy dispersion of a free hopping hole for one dimension is now given by

$$E_k = -2tcos(k) \tag{3.2.12}$$

where a is taken as 1.

The difference between the maximum and minimum value of E(k) is called band width. The band width for equa. (3.2.12) is $4t$. The maximum and minimum band width for the hopping hole in one dimension are $2t$ and $-2t$ obtained at $(-\frac{\Pi}{a}, \frac{\Pi}{a})$, respectively.

For small value of wavevector k the hopping hole (hopping operator) is considered as a kinetic energy. To see this, one way is connecting the familiar schrodinger equation to the hopping model. This helps to view the hopping model as a concretization of a free continuum hole. So the wave function chain becomes

$$|\Psi\rangle = \sum_r |r\rangle \tag{3.2.13}$$

Acting ((3.2.2)) on ((3.2.13)) gives

$$\begin{aligned} \hat{H_{hop}}|\Psi\rangle &= -2t|\Psi\rangle - t\sum_r |\Psi\rangle[|r-a\rangle + |r+a\rangle - 2|r\rangle\rangle \\ &= -2t|\Psi\rangle + (-t)\sum_r [|\Psi(r+a)\rangle + |\Psi(r-a)\rangle - 2|\Psi(a)]|r\rangle \end{aligned} \tag{3.2.14}$$

Using Taylor series expansion of $\Psi(r \pm a)$ to second order of the above equation we can see that the second difference of $|\Psi(r)$ in the bracket is approximated to $a^2\frac{d^2}{dr^2}|\Psi(r)$. Then the function $\Psi(r)$ varies slowly compared to a. This shows the equation reduces to the continuum time-independent schrodinger equation

$$\hat{H}_{hop}|\Psi\rangle = \{-2t - \frac{\hbar^2}{2m}\frac{d^2}{dr^2}\}|\Psi\rangle \tag{3.2.15}$$

where $\frac{\hbar^2}{2ma^2} = t$. Therefore the hopping Hamiltonian $\hat{H}_{hop}$ plays exactly the role of kinetic energy operator, which is $-\hbar^2\frac{\nabla^2}{2m}$. This shows for small value of wavevector k, the $\hat{H}_{hop}$ part of the energy grows up in the semiclassical approximation explained in [25]. $\hat{H}_{hop}$ acts on a wave packet with crystal momentum $\hbar k$ propagate it at the group velocity given by,

$$\hbar v_g(k) = \nabla_k E(k)$$

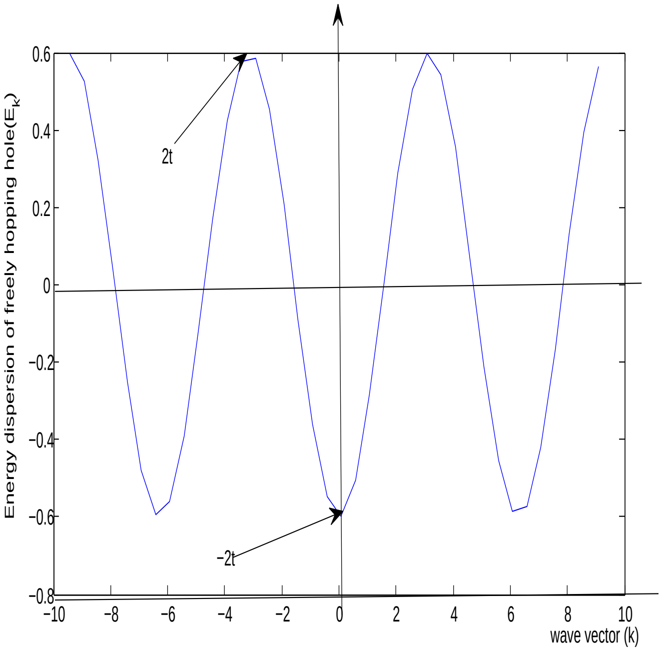

Figure 3.2: Free hole energy dispersion for large k and small k.

As a result of the above statement, we call the kinetic energy term hopping Hamiltonian. Therefore, the free hole dispersion energy is plotted as a function of wavevector k in the Brillioun zone as in the Fig3.2.

The motion of a hole, for example, in a transition metal oxide materials depends on how the system show the magnetic correlation in the system. So based on this idea the motion of a hole could be affected by:

1. Ferromagnetic order of the magnetic component (FM)

Localized electrons spins in a fixed position with the same alignment to have magnetic property. As a result of this a hole can move freely without emission or absorption of magnons in the ferromagnetic order.

2. The anti-ferromagnetic background of spin waves:

Localized electrons spins in opposite position with opposite alignment.

The motion of a hole could be affected strongly by the degree of magnetic correlation

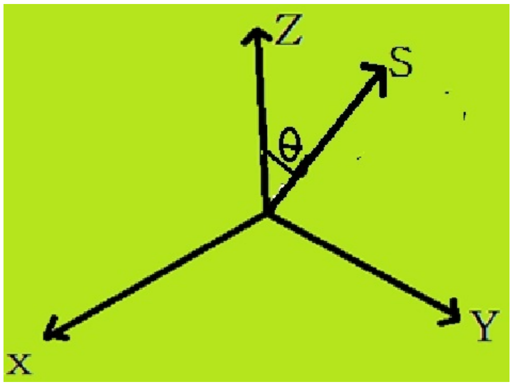

Figure 3.3: Deviation of spin from $x - y$ plane to the z-plane by canting at an angle θ

of the magnetic order. These two mechanisms (factors) mentioned above have their own effect on hole motion and it causes the hole to make interference with its surrounding spin cloud. To study this interference, we can start from the pure AF state to the pure FM state. This can be obtained by canting the AF order from Neel state (ground state), let say from $x - y$ plane to z-plane, at an angle θ using an external magnetic field $\mathbf{H}$. This field causes the magnetic order to cant by an angle θ as shown in the Fig 3.3.

3.2.1 Quantization of energy

In quantum mechanics, it is a general law that a symmetry implies a conservation law.our system is considered as a discrete symmetry and it has a discrete symmetry of translation by lattice vectors. Corresponding to the conservation of crystal momentum.

In simplify our model, we need to introduce a non-generic symmetry for its qualitative behavior. This introduction is a transformation of a single hole problem to a many body problem in a second quantization using a model builder of a system using creation and annihilation operators for the occupation number representation.

We setup a discrete Hilbert spaces for spinless Fermions on a Bravais lattice in a d-dimensions with periodic boundary condition having one orbital on each of the $N = L^d$ sites by the pauli exclusive principle. The occupation number $n(r)$ at site r is either 0 or 1 which gives $M = 2^N$ distinct states. i. e., orthogonal by definition which forming the finite basis for the Hilbert space.

The more elementary representation of the N_f fermion wave function is given by

$$\Psi(r_1, r_2, r_3...r_{N_f}) \tag{3.2.16}$$

A given configuration occupation appears as $N_f!$ amplitude differing only by permutations of the $\{r_i\}$ with the constraints to be equal modulo, the sing of the permutation is ±.

The creation operator $C^+(r)$ is defined to act on the basis states such that it's site r is vacuum in $|\Psi(r)\rangle$. Then $C^+(r)|\Psi(r)\rangle$ has the same occupations as $|\Psi(r)\rangle$, except that site r is occupied too. Where as if site r is occupied in state $|\Psi\rangle$, then $C^+(r)|\Psi\rangle = 0$.

Now the real space occupation (or density) operator $\hat{n}(r)$ at r is

$$\hat{n}(r) = C^+(r)C(r) \tag{3.2.17}$$

A state with zero occupation is called vacuum state which is denoted by $|0\rangle$. All the basis states in terms of the vacuum state is given by

$$|n_1 n_2 n_3 ...\rangle = \prod_{i=1}^{N} C^+(r))^{(ni)}|0\rangle \tag{3.2.18}$$

Each factor makes just one fermion and the product runs over N sites. Every basis state $|\alpha\rangle$ is an eigenstates of $n\hat{(r)}$. i.e

$$\hat{n}(r)|\alpha\rangle = n_i|\alpha\rangle$$

.

Fermion operators have a standard anti-commutation relations [25],

$$[C(r), C^+(r')] = C(r)C^+(r') + C^+(r')C(r) = \delta rr'$$

for any site r

$$C(r)|0\rangle = 0 \tag{3.2.19}$$

A string of $C^+(r)$ acting on $|0\rangle$ causes to move annihilation operators towards the right and creation operators towards the left until an annihilation operator reaches $|0\rangle$ as shown in equa (3.2.18), the commutation relation implies that,

$$C_i^+ C_j^+ |0\rangle = -C_j^+ C_i^+ |0\rangle$$

.

The wave function of our system is just a vector of M complex numbers $\Psi_{n_1 n_2 n_3 \ldots n_N}$ where M is the number of basis states.

For spinless fermion in one orbital per site is $M = 2^N$, since each site may be empty or full. For the string of occupations that α serves as a level for each basis state, the wave function is given by Ψ_α. The system state is now written as $\sum \Psi_\alpha |\alpha\rangle$. Then the schrodinger equation is just the matrix equation:

$$-\frac{\hbar}{i}\frac{d}{dt}\Psi_\alpha = \sum_\beta H_{\alpha\beta}\Psi_\beta \tag{3.2.20}$$

Using the second quantized form the hopping hamiltonian (kinetic energy part) can be written as

$$\hat{H}_{hop} = -\sum_{<ij>} t_{<ij>}(C^+_{i\sigma}C_{j\sigma} + h.c) \tag{3.2.21}$$

here $\langle ij\rangle$ means we sum one over each nearest neighbor pair (ij) and h.c denotes hermitian conjugate, it mean for the reverse hopping $C^+_j C_i$. One action of $\hat{H_{hop}}$ moves just one fermion which hops from one site to another nearest neighbor. The number of fermion operators is always even [31] this means the numbers of real hole operators is conserved. So every term should have equal number of creation and annihilation operators.

3.2.2 Spinless Fermion Representation for Hole Operator

The fermion operators of the hole could be considered as a configuration of spins and can be mapped to a one dimensional (1D) lattice gas of particles. Every ↑ spin becomes an occupied site and every ↓ spin becomes a vacant one. The total possible number of 'up'steps (fermions) is denoted by $C^+(r)$ and its corresponding is $C(r)$

Using the spinless fermion approximation, the "up" and "down" steps of the hole operators defined for both sub space[A, B] as

$$\hat{C}^+ i = Ci \uparrow = gi$$

$$\hat{C}i = g^{+}ia_i$$

$$\hat{C}_j^{+} = C_j \uparrow = f_j b_j^{+}$$

$$\hat{C}_j = f_j^{+}$$

By using fourier transformation, the creation and annihilation hole operators in momentum space can be expressed in terms of creation and annihilation boson operators

$$C_i^{+} = \sqrt{\frac{2}{N}} \sum_{i\epsilon A} g_k^{+} a_k e^{-ir_i(k-\theta)} \tag{3.2.22}$$

$$C_i^{+} = \frac{1}{2}(1 + e^{ir_i(k-\theta)}) g_i^{+} + \frac{1}{2}(1 - e^{ir_i(k-\theta)}) g_i^{+} a_i \tag{3.2.23}$$

Solving equ(3.2.22) and equ(3.2.23) gives,

$$\hat{C}_i \uparrow = cos\left(\frac{\theta}{2}\right) g_i + sin\left(\frac{\theta}{2}\right) g_i^{+} a_i \tag{3.2.24}$$

In the same manner, for the other hole operators in the two sub spaces

$$C_i \downarrow = cos\left(\frac{\theta}{2}\right) g_i^{+} a_i - cos\left(\frac{\theta}{2}\right) g_i$$

$$\hat{C}_j \uparrow = sin\left(\frac{\theta}{2}\right) f_j + cos\left(\frac{\theta}{2}\right) f_j^{+} b_j$$

$$C_j \downarrow = sin\left(\frac{\theta}{2}\right) f_j^{+} b_j - cos\left(\frac{\theta}{2}\right) f_j$$

where f_j and g_i are the fermion operators and a_i and b_j are the Holstein-Primakoff bosons. Now using the above information, the Hamiltonian for the kinetic part can be shown by substituting the above values which after few steps gives

$$\begin{aligned} H_t =& - tsin\theta \sum_k \gamma'_k (g_k f_k^+ + g_k^+ f_k) \\ & - t\frac{\sqrt{2}}{N} cos\theta \sum_{kk'} \mid \gamma_k g_k f'_k b_{k'-k} - \gamma'_k g_k f_k^+ a_{k-k'} + h.c \mid \end{aligned} \qquad (3.2.25)$$

Now it is convenient to define the new fermion bonding and anti-bonding operators:

$$g_k = \frac{(l_k + m_k)}{\sqrt{2}}$$

$$f_k = \frac{(l_k - m_k)}{\sqrt{2}}$$

respectively. When fermions g and f are expressed as a function of the bonding and anti-bonding fermions and the boson a and b in terms of the Bogoliubou operators υ and ν. Bogoliubou approximation is helpful for avoiding the divergent terms(scattered terms). The process can be done using diagonalizing the higher perturbation terms. Now the above can be shown as:

$$\begin{aligned} H_t =& \sum_{kk'} E_k (m_k^+ m_k^+ - l_k l_{k'}) + t\sqrt{\frac{2}{N}} \sum_{kk'} [\mid M_{kk'}^+ \upsilon_{k-k'}^+ (m_k l_{k'}^+ - l_k m_{k'}^+ + h.c) \mid \\ & + \mid M_{qk}^- \nu_{k-k'} (l_k l_{k'}^+ - m_k m_{k'}^+ + h.c) \mid] \end{aligned} \qquad (3.2.26)$$

Where $\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y)$

$M_{kk'}^{\pm} = -\frac{i}{2}\cos\theta(U_{k-k'}^{\pm}\gamma'_k - V_k'^{\pm}\gamma_k)$ and $E_k = -4t\sin\theta\gamma_k$ is free hopping band of a bare hole dispersion

3.3 Free Magnon Hamiltonian

The Hamiltonian of freely interacting magnons is due to Ferromagnetic order of localized electrons in 3d sub shell in the transition metal site. It is described by the Heisenberg model. It is treated in the spin wave approximation (SWA). Primely, we assumed the semi classical uncanted AF order which lies in the $x - y$ plane. However, the external magnetic field pointing in the z-direction causes the AF order to tilt the spins to angle θ out of the $x - y$ plane.

The free magnon hamiltonian mentioned in our model hamiltonian of equa. (3.1.1) is magnetic part of the Hamiltonian which takes the spin dynamics (magnon effect). This spin dynamics is described better by the linear spin wave theory (LSWT) for the satisfactory approximation of the Hamiltonian. This theory of approximation could be transformed into many body problem in second quantization. It uses the spin operators via the Holstein-Primakoff transformation. For the AF Heisenberg model, the spin systems consisting of two interpenetrating sub-lattices A and B, [A, B] and simplify the notation by performing rotation of spin on the B sub lattice.

For the AF Heisenberg model, the spin systems consisting of the two sublattice is described by the Hamiltonian

$$H_J = -\sum_{<ij>} J_{ij} S_{A_i}.S_{B_j} - g\mu_B H \sum_{i\varepsilon A} S^z_{Ai} + g\mu_B H \sum_{j\varepsilon B} S^z_{Bj} \tag{3.3.1}$$

For $J < 0$ (where J is exchange interaction constant) the spins coupled to the nearest neighbors on the lattices. The quantity H represents an external magnetic field which is used to polarized the spins to the z-axis, as shown in Tig. 3.3, to an angle θ from the z-axis.

H_J stands for Heisenberg magnons interaction Hamiltonian with Zeeman term: The term J_{ij} is the anti-ferromagnetic (AF) exchange interaction due to localized electrons at site i and j. J_{ij} is defined mathematically as:

$$J_{ij} = J|\psi_{ij}|^2 = Je^{-2}(\frac{Ri - Rj}{a_0}) = \frac{J}{2N}$$

The product $S_{A_i}.S_{B_j}$ in the equa(3.3.1) is stated as

$$S_{A_i}.S_{B_j} = [\hat{s_{ix}} + \hat{s_{iy}} + \hat{s_{iz}}][\hat{s_{jx}} + \hat{s_{jy}} + \hat{s_{jz}}] \tag{3.3.2}$$

We know that, spin angular momentum is defined as

$$\overrightarrow{s} = \overrightarrow{r} \times \overrightarrow{p}$$

where $\overrightarrow{r}$ is the position of all magnons and $\overrightarrow{p}$ is the momentum of the magnons. Their values are given as

$$\overrightarrow{r} = \hat{x}_i + \hat{y}_j + \hat{z}_k$$

$$\overrightarrow{p} = -i\hbar\frac{\partial}{\partial r}$$

Then the spin operators interims of the coordinates are defined bellow

$$\hat{s}_{(i)} = \hat{s}_{(ix)}\hat{i} + \hat{s}_{(iy)}\hat{j} + \hat{s}_{(iz)}\hat{k}$$

$$\hat{s}_{(j)} = \hat{s}_{(jx)}\hat{i} + \hat{s}_{(jy)}\hat{j} + \hat{s}_{(jz)}\hat{k}$$

but

$$\hat{s}_{ix} = \hat{y}_i\hat{p}_z - \hat{z}_i\hat{p}_y = -i\hbar(\hat{y}_i\frac{\partial}{\partial z} - \hat{z}_i\frac{\partial}{\partial y})$$

$$\hat{s}_{iy} = \hat{z}_i\hat{p}_x - \hat{x}_i\hat{p}_z = -i\hbar(\hat{z}_i\frac{\partial}{\partial x} - \hat{x}_i\frac{\partial}{\partial z})$$

$$\hat{s}_{iz} = \hat{x}_i\hat{p}_y - \hat{y}_i\hat{p}_x = -i\hbar(\hat{x}_i\frac{\partial}{\partial y} - \hat{y}_i\frac{\partial}{\partial x})$$

$$\hat{s}_{jx} = \hat{y}_j\hat{p}_z - \hat{z}_j\hat{p}_y = -i\hbar(\hat{y}_j\frac{\partial}{\partial z} - \hat{z}_j\frac{\partial}{\partial y})$$

$$\hat{s}_{iy} = \hat{z}_j\hat{p}_x - \hat{x}_j\hat{p}_z = -i\hbar(\hat{z}_j\frac{\partial}{\partial x} - \hat{x}_j\frac{\partial}{\partial z})$$

$$\hat{s}_{iz} = \hat{x}_j\hat{p}_y - \hat{y}_j\hat{p}_x = -i\hbar(\hat{x}_j\frac{\partial}{\partial y} - \hat{y}_j\frac{\partial}{\partial x})$$

also we know that the total spin S is given by

$$S^2 = S_x^2 + S_y^2 + S_z^2$$

But$S$ depends on the canted angle θ and angular harmonic ϕ.that is

$$S = s(sin\theta cos\phi, sin\theta sin\phi, cos\phi) = s(S_i^z, \phi)$$

as a result of the spherical harmonics, the spin operators depend on each coordinates. The coordinates are defined as

$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\cos\phi$$

$$z = \cos\theta$$

therefore

$$S^2 = -\hbar^2(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial x} + \frac{1}{\sin\theta^2}\frac{\partial}{\partial\phi})$$

The raising and lowering spin operators are defined

$$S_i^+ = s_{ix} + is_{iy} = \hbar e^{i\emptyset}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\emptyset})$$

$$S_i^- = s_{ix} - is_{iy} = \hbar e^{i\emptyset}(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\emptyset})$$

This leads to

$$S^+S^- = S^2 - S_z^2 + \hbar S_z$$

$$S^-S^+ = S^2 - S_z^2 - \hbar S_z$$

Applying the above equations for the general case as,

$$S^2 = \frac{1}{2}(S^+S^- + S^-S^+) \tag{3.3.3}$$

The action of H_J on a function $\mid \Psi\rangle$ produce magnon dispersion energy (ω). It can be calculated as;

$$H_j|\Psi\rangle = \omega_q|\Psi\rangle \tag{3.3.4}$$

We know that;

$$H_J = \sum_{<ij>} J_{i,j}S_{A_i}.S_{B_j} - g\mu_B H\sum_{i\varepsilon A} S_{Ai}^z + g\mu_B H\sum_{j\varepsilon B} S_{Bj}^z$$

For initial condition $\mid \Psi\rangle$ is $\mid \Psi^0\rangle$ and $\omega_{(q_n)}$ is ω. The exact Eigenvalue ω and Eigenstate $\mid \psi^0\rangle$ can be calculated as follows.

As we have mentioned in equa(3.3.1), it need to apply a technical problem that encounters for the H_J of the Heisenberg model. Heisenberg model encounters for the H_J as follows:

$$\hat{S}_i\hat{S}_j = (S_i^x + S_i^y + S_i^z)(S_j^x + S_j^y + S_j^z) = S_i^xS_j^x + S_i^yS_j^y + S_i^zS_j^z$$

where

$$S_i^x = \frac{1}{2}(S_i^+ + S_i^-)$$

$$S_i^y = \frac{(S_i^+ + S_i^-)}{2i}$$

and one can similarly do for the j site. Note that i stands for the site in sub-lattice A and j stands for the site in sub-lattice B.

The Heisenberg model Hamiltonian (H_J) becomes:

$$H_J = -\frac{1}{2}\sum_{ij} J_{ij}[\frac{S_i^+S_j^- + S_i^-S_j^+}{2} + S_i^zS_j^z] \tag{3.3.5}$$

Using commutation relation S_i^+,S_j^+,S_i^-,S_j^- and H_J for equa. (3.3.5) do not commute with H_J due to the presence of S_i^+ in the state. But $S_i^zS_j^z$ term commute with H_J and is obviously diagonal in the usual matrix basis. In analogy $[S^x, H] = [S^y, H_J] = 0$.

Now we can find simultaneously Eigen states of H_J, and S^2 for all spins aligned in the Z-direction, we consider the state:

$$\mid \psi\rangle =\mid S.S\rangle_{1(Spin1)}, \mid S.S\rangle_{2(spin2)} \cdots \mid S.S\rangle N_{(spinN)} \tag{3.3.6}$$

Now we have;

$$H \mid \psi\rangle = -\sum J_{ij}\frac{1}{2}(S_i^+S_j^-) \mid \psi\rangle + S_i^-S_j^+ \mid \psi\rangle + S_i^zS_J^z \mid \psi\rangle$$

The first two terms $S_i^+ \mid \Psi\rangle = 0$, the quantum number m_i cannot be increased further. Thus

$$H \mid \psi\rangle = \omega \mid \phi\rangle = -\frac{1}{2N}JS^2 \mid \psi_0\rangle \tag{3.3.7}$$

where $\omega = -\frac{1}{2N}JS^2$ is the ground state magnon energy dispersion.

3.3.1 Holestein-Primakoff transformation

This transformation is a systematic approach for transforming the spin dynamics to second quantization in the form of bosons operators. According to this transformation, the spin vector operators are related with boson creation (a_i^+, b_j^+) and annihilation (a_i, b_j) operators. a_i^+ and a_i are creation and annihilation boson operators in sub-space A and b_j^+ and b_j are creation and annihilation boson operators in sub-space B. Based on these concept the spin components in both sub-space are shortly defined as follows,

$$s_{xi} = \cos\theta(S - a_i^+a_i) - i\sqrt{\frac{s}{2}}\sin\theta(a_i - a_i^+)$$

$$s_{yi} = \sqrt{\frac{s}{2}}(a_i + a_i^+)$$

$$s_{zi} = -\sin\theta(S - a_i^+ a_i) - i\sqrt{\frac{s}{2}}\cos\theta(a_i - a_i^+)$$

$$s_{xj} = -\cos\theta(S - b_j^+ b_j) - i\sqrt{\frac{s}{2}}\sin\theta(b_j - b_j^+)$$

$$s_{yj} = \sqrt{\frac{s}{2}}(b_j + b_j^+)$$

$$s_{zj} = \sin\theta(S - b_j^+ b_j) - i\sqrt{\frac{s}{2}}\cos\theta(b_j - b_j^+)$$

The lowering and raising operators now become;

$$s_i^+ = s_{xi} + is_{yi} = \sin 2\theta\sqrt{2s}\sqrt{(1 - \frac{a_i^+ a_i}{2s})}a_i$$

$$s_i^- = s_{xi} - is_{yi} = \sin 2\theta\sqrt{2s}a_i^+\sqrt{(1 - \frac{a_i^+ a_i}{2s})}$$

$$s_j^+ = s_{xj} - is_{yj} = -\sin 2\theta\sqrt{2s}(1 - \frac{b_j^+ b_j}{2s})^{\frac{1}{2}}b_j$$

$$s_j^- = s_{xj} - is_{yj} = -\sin 2\theta\sqrt{2s}b_j^+(1 - \frac{b_j^+ b_j}{2s})^{\frac{1}{2}}$$

Here the origin $R_0 = 0$ belongs to sublattice A (spin up).

Next we need to introduced the sub-lattice spin wave variables $a_q^+(a_q)$ spin wave variables for sub-lattice A and $b_q^+(b_q)$ spin wave variables for sub-lattice B. This spin wave variables are related with creation and annihilation boson operators $a_i^+(a_i)$ and $b_j^+(b_j)$ using the fourier transform of the bosonic operators $a's$ and $b's$

$$a_q = \frac{2}{\sqrt{N}}\sum_i e^{(iqR_i)}a_i$$

and

$$a_q^+ = \frac{2}{\sqrt{N}}\sum_i e^{(iqR_i)}a_i^+$$

$$b_q = \frac{2}{\sqrt{N}}\sum_j e(iqR_i)b_j$$

and

$$b_q^+ = \frac{2}{\surd N}\sum_j e^{(iqR_i)} b_j^+$$

the revers fourier transform of the Bosonic operators $a's$ and $b's$ are defined as:

$$a_i^+ = \sqrt{\frac{2}{N}}\sum_k e^{ikRi} a_k^+$$

$$b_j^+ = \sqrt{\frac{2}{N}}\sum_k e^{ikRj} b_k^+$$

The summation runs over all N atoms of the sub-lattices A and B, respectively. Applying the series expansion of the above s^+ and s^- equations up to the quadratic order, gives:

i. For Sub-lattice A:

$$\hat{S^+_{Ai}} = \sin 2\theta(\frac{4s}{N})^{\frac{1}{2}}[\sum_{q1} e^{(iq1R_i)} - \frac{1}{8SN}\sum_{q1q2q3} e^{(i(q_1-q_2-q_3)R_i)} a_{q1}^+ a_{q2} a_{q3} + ...]$$

$$\hat{S^-_{Ai}} = \sin 2\theta(\frac{4s}{N})^{\frac{1}{2}}[\sum_{q1} e^{(iq1R_i)} - \frac{1}{8SN}\sum_{q1q2q3} e^{(i(q_1+q_2+q_3)R_i)} a_{q_1}^+ a_{q_2}^+ a_{q_3} + ...]$$

$$\hat{S^z_{A_i}} = \cos\theta[S - \frac{s}{N}\sum_{q_1} e^{i(q_1-q_2)R_i} {a^+}_{q_1} a_{q_2}]$$

ii. For Sub-lattice B:

$$\hat{S^+_{Bj}} = -\sin 2\theta(\frac{4s}{N})^{\frac{1}{2}}[\sum_{q1} e^{(iq_1R_j)} - \frac{1}{8SN}\sum_{q_1q_2q_3} e^{(i(q_1-q_2-q_3)R_j)} b_{q_1}^+ b_{q_2} b_{q_3} + ...]$$

$$\hat{S^-_B}j = -\sin 2\theta(\frac{4s}{N})^{\frac{1}{2}}[\sum_{q_1} e^{(iq_1R_j)} - \frac{1}{8SN}\sum_{q_1q_2q_3} e^{(i(q_1+q_2+q_3)R_j)} d_{q_1}^+ b_{q_2}^+ b_{q_3} + ...]$$

$$\hat{S^z_B}j = -\sin\theta[S + \frac{s}{N}\sum_{q_1} e^{i(q_1-q_2)R_j} b_{q_1}^+ b_{q_2}]$$

where N is the number of latices sites and k runs along the magnetic Brillioun zone.

Taking the expansion up to quadratic order, the magnetic part of $t-J$ Hamiltonian takes the form:

$$H_J = E_c + \sum_k \mid A(a_k^+ a_k + b_k^+ b_k) + D\gamma_k(a_k^+ b_k + a_k b_k^+) + C\gamma_k(a_k b\_k + a_k^+ b\_k^+) \mid \quad (3.3.8)$$

where the constants: $A = 4JS\cos 2\theta + B\sin\theta, D = JS\sin^2\theta, C = JS\cos^2\theta$ and

$$E_c = -2JS^2N\cos^2\theta - BN\sin\theta$$

minimization of E_c with respect to θ gives for the constant B: i.e. $B = 8JS\sin\theta$ substituting the value of B for the constant A gives:

$$A = 4JS\cos 2\theta + 8JS^2\sin\theta$$

we know,

$$\cos 2\theta = 1 - 2\sin^2\theta$$

Substituting $1 - 2\sin^2\theta$ for $\cos 2\theta$, the value of the constant A becomes $A = 4JS$.

Substituting the values of the constants for the H_J Hamiltonian it's value cancels the linear terms of the magnetic part and justify the use of the quadratic form.
i.e.,

$$H_J = E_c + JS\sum_k \mid 4(a_k^+a_k + b_k^+b_k) + \sin^2\theta\gamma_k(a_k^+b_k + a_kb_k^+) + \cos^2 k\gamma_k((a_kb\_k) + a_k^+b\_k^+)\cdots \mid$$

H_J has a $4x4$ matrix. For this case we need digitalization of H_J. H_J can be diagonalizing using two steps. These steps are:

1. First taking a transformation as: $\alpha_k^+ = a_k^+ + b_k^+$ and $\beta_k^+ = a_k^+ - b_k^+$

2. Secondly taking Bogoliubou transformation of α and β to the new Bosonic operators η and ν as:

$$\alpha_k = \upsilon_k^+\eta_k^+ + \nu_k\eta_k^+$$

$$\beta_k = \upsilon_k^-\eta_k + \nu_k^+\eta_{-k}$$

where:

$$U_k^\pm = \sqrt{\frac{A + D\gamma_k}{2\omega_k^\pm} + \frac{1}{2}}$$

$$V_k^{\pm} = \mp \frac{\gamma_k}{\mid \gamma_k \mid} \sqrt{\frac{A + D\gamma_k}{2\omega_k^{\pm}} + \frac{1}{2}}$$

Once the transformations are taken into account the harmonic magnetic part becomes:

$$H_J = E_c - 2JSN + \sum_k [(\omega_k^+ + \omega_k^-)\eta_k^+ \nu_k + \omega_k^+ \eta_k^+ \eta_K + \omega_k^- \nu_k^+ \nu_k]$$

where the two magnon dispersion branches:

$$\omega_k^{\pm} = 2JS\sqrt{(1 \pm \gamma_k)(1 \mp \cos\theta\gamma_k)}$$

which is defined in the magnetic Brillion zone, and

$$\gamma_k = \frac{(\cos k_x + \cos k_y)}{2}$$

To identify the magnon dispersion energy as a ferromagnetic order or anti ferromagnetic order we use numerical method, as shown below: for $k = (0,0), \gamma_k = 1$ then $\omega_k^- \approx 0$ which is approaching to zero linearly. Then, the situation shows anti ferromagnetic order. $\omega_k^+ \approx 4JS\sin^2\theta$ this shows the magnon dispersion approaches quadratically. So that the system is in a FM order.

3.4 Hole-Magnon Interaction Hamiltonian

The third term H_{h-m} mentioned in equa (3.1.1) stands for the Hole-magnon interaction Hamiltonian. The detail of this one is our attention to do further.

The equations of motion of the system given in equa (3.1.1) for the hoping of a hole in an anti-Ferromagnetic background and free spin wave due to ferromagnetic order is explained based on the $t-J$ model. The $t-J$ model is best for the description of charge motion interacting with spin particles in anti-ferromagnetic order. This $t-J$ model Hamiltonian is stated as follows:

$$H = H_t + H_J = -\sum_{<j,i>} t_{ij}(C_{i\sigma}^+ C_{i\sigma} + h.c) + \sum_{<j,i>} J_{ij} S_i.S_j + g\mu_B H \sum_{<j,i>} S_i^z S_j^z \qquad (3.4.1)$$

where $H_t = \sum_{<j,i>} t_{ij}(C_{i\sigma^+} C_{i\delta} + h.c)$, is the Hamiltonian for the hopping of hole (kinetic energy part), and $H_J = \sum_{<j,i>} J_{ij} S_i.S_j + g_s\mu_B H \sum S_i^z$ is the Heisenberg spin waves hamiltonian (magnon-magnon exchange interaction).

The Hamiltonian (H) in equa (3.4.1))has two parts. These are:

•The kinetic energy due to hopping of a hole (H_t) and

•The magnetic energy (H_0) due to spin of localized electrons in 3d sub shell).

The main features of hole motion reveals strong re-normalization of the tight-bonding results for the band energies due to hole motion by the cloud of spin excitations. The degree of interaction between hole motion and cloud of spins in transition metal oxides affects by the strength of J and t measured in the magnetic Brillouin zone (MBZ). For $t > J$ (ferromagnetic order(FM)), the hole can hope and couples strongly with magnons, and for $t < J$ (antiferromagnetism (AF)) background, the hole moves freely and its energy is higher.

Using the pure $t - J$ model given in equa (3.4.1), we can find the interactional Hamiltonian (H) by a mathematical method called perturbation theory as clearly presented in the following section.

3.4.1 Effective Hamiltonian Through Perturbation Theory

The Hamiltonian given in equa (3.4.1) can be calculated for obtaining the effective Hamiltonian by means of perturbation theory. For this method to do, we need the Hamiltonian of equa(3.4.1) by classified or decompose in to unperturbed system(H_0), and perturbed system (H_p).

So the Hamiltonian due to hopping of hole takes as a perturbation (H_t) and the Hamiltonian due to spin wave exchange interaction (H_J) considered as (unperturbed). That is,

$$\hat{H} = \hat{H}_0 + \hat{H}_p \tag{3.4.2}$$

where $\hat{H}_0 = \hat{H}_J$ and $\hat{H}_p = \lambda \hat{H}_t$, H_p is written in terms of a dimensionless real parameter λ which is very small compared with one (1).

$$\hat{H}_p = \lambda \hat{H}_t \tag{3.4.3}$$

Where $\lambda << 1$ and $\hat{H}_t$ is a perturbation part and is include both hopping terms and transverse spin fluctuation. The Eigen value problem for (3.4.2) becomes:

$$\hat{H} \mid \psi\rangle = (\hat{H}_0 + \lambda\hat{H}_t) \mid \psi_n\rangle = E_n \mid \psi_n\rangle \tag{3.4.4}$$

The total energy E_n can be approximate using the ground state E_n^0 energy. To do this we need to calculate the energy shift $\triangle E$ due to perturbation. This is;

$$\triangle E = E_n - E_n^0$$

and then

$$E_n = \triangle E + E_n^0$$

Now (3.4.4) can be written as;

$$(\hat{H}_0 + \lambda\hat{H}_t)|\psi_n\rangle = (\triangle E + E_n^0)|\Psi_n\rangle$$

The above equation can be rearranged as;

$$(E_n^0 - H_0)|\psi_n\rangle = (\lambda\hat{H}_t - \triangle E)|\psi_n\rangle \tag{3.4.5}$$

projecting (3.4.5) on to k we have;

$$\langle k|(E_n^0 - H_0)|\psi_n\rangle = \langle k|(\lambda\hat{H}_t - \triangle E)|\psi_n\rangle$$

$$\langle k|(E_n^0)|\psi_n\rangle - \langle k|H_0|\psi_n\rangle = \langle k|\lambda\hat{H}_t|\psi_n\rangle - \triangle E|\psi_n\rangle$$

Now,

$$\langle k|(E_n^0)|\psi_n\rangle = 0$$

and

$$\langle k|H_0|\psi_n\rangle = 0$$

then

$$\langle k|(\lambda\hat{H}_t|\psi_n\rangle - \triangle E|\psi_n\rangle) = 0$$

From this the energy shift $\triangle E$ is given by;

$$\triangle E = \lambda\frac{\langle k|H_t|\psi_n\rangle}{\langle k|\psi_n\rangle} = \lambda\langle k|H_t|\psi_n\rangle$$

because $\langle k|\psi_n\rangle = 1$. Since λ is a very small parameter ($\lambda << 1$). We can expand using taylors series expansion for the eigenstate $|\Psi_n\rangle$ and total energy E_n,

$$| \psi\rangle = (\lambda^0 \mid \phi_0\rangle + \lambda \mid \psi_n^1\rangle + \lambda^2 \mid \psi_n^2\rangle + ...) \tag{3.4.6}$$

$$E_n = \lambda^0 E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + ... \tag{3.4.7}$$

The level shift interims of the above expansion can be written as

$$\triangle E = E_n - E_n^0 = \lambda^0 E_n^0 + \lambda^1 E_n^1 + \lambda^2 E_n^2 + \lambda^3 E_n^3 + ... - E_n^0 = \lambda^1 E_n^1 + \lambda^2 E_n^2 + \lambda^3 E_n^3 + ... \tag{3.4.8}$$

By considering the non-degenerate or degenerate separate cases, we can find the exact solutions of equa(3.4.4).

Let us calculate the non-degenerate energy eigenvalue and eigenstates. According to the perturbation theory, the eigenvalues and eigenstates are the linear combination of the ground energy(E_n^0) and the ground state $\mid \Phi_0\rangle$ respectably. $E_k^1, E_k^2, E_k^3...$ and $\mid \psi_n^1\rangle$, $\mid \psi_n^2\rangle \dots$ are calculated interims of the (E_n^0) and $\mid \Phi_0\rangle$. So for determine the dispersion of E_k^n, and Eigen state$\mid \psi^n\rangle$, we need first to evaluateE_q^0 and $\mid \Phi_0\rangle$.

Substituting equa(3.4.6) in equa(3.4.4) gives,

$$(H_0 + \lambda H_t) \mid \psi\rangle = (H_0 + \lambda H_t)[\lambda^0 \mid \phi_0\rangle + \lambda \mid \psi_n^1\rangle + \lambda^2 \mid \psi_n^2\rangle + ..] =$$

$$(E_k^0 + \lambda^1 E_k^1 + \lambda^2 E_k^2 + ...)[\lambda^0 \mid \phi_0\rangle + \lambda \mid \psi_n^1\rangle + ...]$$

project to the momentum space ($|k\rangle$) we have;

$$\langle k|(E_q^0 - H_0)|\psi_k\rangle = \langle k|(\lambda H_t - \triangle E_k)|\psi_k\rangle$$

the RHS of the above is zero. From this

$$\langle k|\{\lambda H_t - \triangle E_k\}|\psi_k\rangle = 0$$

then we obtain;

$$\triangle E_k = \frac{\lambda\langle k|H_t|\psi_k\rangle}{\langle k|\psi_k\rangle} = \lambda\langle k|H_t|\psi_k\rangle \tag{3.4.9}$$

By substituting (3.4.9) in (3.4.8) and collecting terms of the same order in λ, we get

$$E_k^n = \lambda\langle k|H_t|\psi_k^{n-1}\rangle \tag{3.4.10}$$

Equa (3.4.10) helps us to find the energy at all orders in terms of the lowest order of eigenstate $\langle k|$.

To find $H_t|\psi_k^{n-1}\rangle$, we need a projector. Let say this projector S^k and is defined as

$$S^k = 1 - |k\rangle\langle k| = \sum_{k\neq q}|q\rangle\langle q|$$

For all $|\psi_k\rangle$, we denote and define the projected state $|\Psi\rangle$ as

$$|\Psi\rangle = S^k|\psi\rangle$$

The above equation can be re-write as

$$\langle k|\Psi\rangle = \langle k|S^k|\psi\rangle = \langle k|\psi\rangle - \langle k|k\rangle\langle k|\psi\rangle = 0 \tag{3.4.11}$$

equa. (3.4.11) is zero because $\langle k|\psi\rangle$ is zero. Now using the projector, we get

$$S^k|\psi\rangle = (E_q^0 - H_0)^{-1}\{\lambda H_t - \triangle E_k\}|\psi\rangle = |\psi_k\rangle - |k\rangle$$

We use the normalization condition $\langle k|\psi\rangle = 1$ for the above equation. We finally obtained

$$|\psi\rangle = |k\rangle + (E_q^0 - H_0)^{-1}S^k(\lambda H_t - \triangle E_k)|\psi\rangle \tag{3.4.12}$$

By letting $(E_q^0 - H_0)^{-1}S^k = Q_k$ and then expanding in series expansion equa. (3.4.12) becomes

$$|k\rangle + \lambda|\psi_k^1\rangle + \lambda^2|\psi_k^2\rangle + ... = |k\rangle + Q_k\lambda(H_t - E_k^1 - \lambda E^2 - ...)[|k\rangle + \lambda|\psi^1\rangle + \lambda^2|\psi^3\rangle + ...]$$

Solving the above equation term by term we obtain the following orders for eigenstates; zero order perturbed of eigenstates

$$|\psi^0\rangle = |k\rangle$$

first order perturbed eigenstate

$$|\psi^1\rangle = Q_kH_t|k\rangle$$

second order perturbed eigenstate

$$|\psi^2\rangle = Q_k H_t Q_k H_t |k\rangle$$

third order perturbed eigenstate

$$|\psi^3\rangle = Q_k H_t Q_k H_t Q_k H_t |k\rangle$$

etc

Similarly for the eigen value

first order correction eigen value

$$E_k^1 = \langle k|H_t|k\rangle = 0$$

second order correction eigen value

$$E_k^2 = \langle k|H_t|\psi^1\rangle = \langle k|H_t Q_k H_t k\rangle = \sum_{k\neq q} \frac{|H_{t(kq)}|^2}{E^0 - E_q^0}$$

thirdorder cotrrection eigen value

$$E_k^3 = \langle k|H_t|\psi^2\rangle = \langle k|H_t Q_k H_t Q_k H_t Q_k H_t|k\rangle = \sum_{kq} \frac{|H_{t(kq)}|^2}{(E^0 - E_q^0)} \sum_{kq} \frac{|H_{t(kq)}|^2}{E^0 - E_q^0}$$

Generally we can derive a formal solution for the wave function interims of the compound projection vector Q_k is;

$$|\psi_k\rangle = |k\rangle + Q_k(\lambda H_t - \triangle E_k)|\psi_k\rangle = Q_k H_1|\psi_k\rangle$$

where$H_1 = \lambda H_t - \triangle E_k$.using series expansion;

$$|\psi_k\rangle = |k\rangle + Q_k H_1\{|k\rangle + Q_k H_!|\psi_k\rangle\} = |k\rangle + Q_k H_1|k\rangle + Q_k H_! Q_k H_1|\psi_k\rangle$$

In short we can write it as;

$$|\psi_k\rangle = |k\rangle + Q_k H_1\{|k\rangle + Q_k H_!|\psi_k\rangle\} = |k\rangle + Q_k H_1|k\rangle + Q_k H_! Q_k H_1|k\rangle + ... + (Q_k H_1)^n|k\rangle + ... \tag{3.4.13}$$

Equa(3.4.13) is a form of geometric series with a formal solution given by,

$$|\psi\rangle = (1 - Q_k H_1)^{-1}|k\rangle \tag{3.4.14}$$

AS we have seen equa(3.4.15), it tells us the n^{th} eigen state order is the linear combination of the unperturbed(ground state)function $|k\rangle$.

For general derivation we introduce a non-canonical normalization $\langle k|\psi_k\rangle = 1$. This implies that the perturbed state $|\psi_k\rangle$ is not normalized.

To make it a normalized state, we need a new state $|\varphi\rangle$ defined as

$$|\varphi\rangle = \frac{\psi_k\rangle}{\sqrt{\langle\psi|\psi\rangle}}$$

We now;

$$\langle\psi|\psi\rangle = \langle k + \lambda\psi_k^1 + \lambda^2\psi_k^2 + ...|k + \lambda\psi_k^1 + \lambda^2\psi_k^2 + ...\rangle$$

$$\langle\psi|\psi\rangle = 1 + \lambda^2\langle\psi^1|\psi^1\rangle + \lambda^4\langle\psi^2|\psi^2\rangle + \lambda^6\langle\psi^3|\psi^3\rangle + ...$$

Rearranging the above equation the normalization factor $\langle\psi|\psi\rangle$ for n^{th} order is given by

$$\langle\psi|\psi\rangle = 1 + \lambda^2\frac{\sum_{k,q}|H_t(kq)|^2}{E_k^0 - E_{q_1}^0} + ...$$

Therefore, the normalized perturbed state is given by

$$\begin{aligned} |\varphi\rangle &= \frac{|\psi_k\rangle}{\sqrt{\langle\psi|\psi\rangle}} \\ &= \frac{|\psi_k\rangle}{\sqrt{1 + \lambda^2\frac{\sum_{k,q}|H_t(kq)|^2}{E_k^0 - E_q^0} + ...}} \end{aligned} \tag{3.4.15}$$

Taking

$$\sqrt{\langle|\ \psi\ |\ \psi\rangle} = \sqrt{1 + \lambda^2\frac{\sum_{k,q}\mid H_t(kq)\mid^2}{E_k^0 - E_q^0} + ...}$$

as a normalization constant$\frac{1}{\sqrt{N}}$, we can write (3.4.15) as,

$$|\varphi\rangle = a_k^0 h^+|k\rangle + \frac{1}{\sqrt{N}}\sum_{q_1} a^1_{(k,q_1)} h^+_{(k-q_1)} h_k \alpha_{q_1}|k\rangle + \frac{1}{N}\sum_{q_2} a^2_{(k,q_2)} h^+_{(k-q_1-q_2)} h_k \alpha^+_{q_1}\alpha^+_{q_2}|k\rangle... \tag{3.4.16}$$

where $a^n_{(k,q)}$ is constant coefficient to be determined further.

In a simple form to determine the energy eigenvalue to n order and eigenstates to the zero order for f fold excitation, we use the following steps:

- First we must determine for each "f"fold excitation levels of the "$f \times f$" matrix of the perturbation $\hat{H}_p$. i.e

$$H_p = \begin{vmatrix} H_{p11} & H_{p12} & H_{p13}\cdots \\ H_{p21} & H_{p22} & H_{p23}\cdots \\ H_{p31} & H_{p32} & H_{p33}\cdots \\ \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots. \\ \cdots & \cdots & \cdots. \end{vmatrix}.$$

  where

$$H_p = \langle k|H_p|\psi_n\rangle$$

- Diagonalizing the matrix given in step 1 just to f fold eigen values. As we know H_0 and H_t are initially diagonalizing using Bogilbouv transformation. So that:

$$(H_0 + \lambda H_t)|\psi_n\rangle = E_n|\psi_n\rangle \tag{3.4.17}$$

This leads to

$$H_0|\psi_n\rangle + \lambda H_t|\psi_n\rangle = E_n|\psi_n\rangle$$

where:

$$H_0|\psi_n\rangle = \omega|\psi_n\rangle = -\frac{1}{2N}JS^2|\psi_n\rangle$$

But the eigen function $|\psi_n\rangle$ is the linear combination of the ground state $|k_n\rangle$ i.e

$$|\psi_n\rangle = \sum_{k,q} a_{k,q}|k_n\rangle \tag{3.4.18}$$

the state $|k_n\rangle$ is orthogonal with respect to k. i.e.,

$$\langle k_{n\alpha}||k_{n\beta}\rangle = \sigma_{\alpha\beta}$$

and $|psi_n\rangle$ to be normalized ($\langle\psi_n|\psi_n\rangle = 1$). the coefficient a_α obeys the relation

$$\langle\psi_n|\psi_n\rangle = \sum_{\alpha\beta} a^*_\alpha a_\beta \sigma_{\alpha\beta} = \sum_{\alpha\beta} |a_\alpha|^2 = 1 \tag{3.4.19}$$

To find the coefficients and the first order correction to the energy let's substitute equ((3.4.18)) in equ((3.4.17)) and results in,

$$\sum_\alpha [E^0_n|k_{n\alpha}\rangle + H_p|k_{n\alpha}\rangle]a_\alpha = E_n \sum_{\alpha=1} a_\alpha|k_{n\alpha}\rangle$$

multiplying the above equation both sides by $\langle k_{n\alpha}$ leads to

$$\sum_\alpha [E^0_n\sigma_{\alpha\beta} + \langle k_{n\alpha}|H_p|k_{n\alpha}\rangle] = E_n \sum_{\alpha=1} a_\alpha\sigma_{\alpha\beta}$$

or

$$a_\beta E_n = a_\beta E^0_n + \sum_{\alpha=1}^{f} a_\alpha\langle k_{n\alpha}|H_p|k_{n\alpha}\rangle \tag{3.4.20}$$

Using $\langle k_{n\alpha}|H_p|k_{n\alpha}\rangle = \sigma_{\alpha\beta}$ we can rewrite eq. (3.4.20) as,

$$\sum_{\alpha=1}^{f} [H_{p\alpha\beta} - (E_n - E^0_n)\sigma_{\alpha\beta}]a_\alpha = 0 \tag{3.4.21}$$

Where, $(\beta = 1, 2, 3, ...)$.

The above equation is a system of homogenous linear equation for the coefficient a_α. This coefficient is non-vanishing only when the determinant is zero. i.e.,

$$|H_{p\alpha\beta} - (E_n - E^0_n)\sigma_{\alpha\beta}| = 0$$

This means;‘

$$\begin{vmatrix} H_{p11} - E^0_n & H_{p12} & H_{p13}... \\ H_{p21} & H_{p22} - (E_n - E^0_n) & H_{p23}... \\ H_{p31} & H_{p32} & H_{p33} - (E_{n2} - E^0_q)... \\ .... & ... & .... \\ ..... & .... & .... \\ ..... & .... & .... \end{vmatrix} = 0$$

The above equation hasf^{th} degree equation and and then has f different real roots. These roots are from the first order correction to the eigen value $E_{n\alpha}$ of $\hat{H}$ to find the coefficients a_α we need simply substitute these roots in to equ((3.4.21)) and then solving the resulting expression.knowing these coefficients, it helps us to determine the eigen function $|\psi_n\rangle$ of the Hamiltonian H.

As a result of the diagonalization of the matrix in step 1, we can write the energy eigen value as,

$$E_{n\alpha} = E_{n_1} + E_{n_2} + E_{n_3} + E_{n_4} + ... \tag{3.4.22}$$

3.4.2 Effective Hamiltonian via canonical transformation

As we have seen from the results of the perturbation calculation, the roots of the "$f \times f$" matrix for the total energy or Hamiltonian results a divergent terms. So through perturbation process o we can't get a convergent results. Due to this we need an additional transformation method to obtain a convergent result. This method of diagonalization a resulting Hamiltonian is Bogoliubov transformation. To do this, we need to leave the old Hamiltonian equation by transforming to a new invariant Hamiltonian.This activity is Canonical transformation.

Bogoliubov transformation helps to avoid perturbation theory. This transformation avoids the divergent term by exactly diagonalizing the higher terms.

Due to the perturbable nature of the hole motion,and due to the rotational symmetry (d-orbital in magnetic ions) i.e the translational symmetry lattice, the hopping of hole (3.4.1) causes to interact with the spins waves (magnons). when

$$\langle\alpha|H|\beta\rangle \neq 0$$

we have degenerate first order perturbation and H_t splits the states by a comparable energy and no longer perturbation. As a result of this we need to apply the method of canonical transformation.

Let this term is "U". Imagine "U" is a unitary transforming. So the hamiltonian gets converters in to H effective Hamiltonian. And is given by;

$$H = U(H_J + H_t)U^+$$

Now choose "U" so that H has no terms first order inH_t. That is, to the lowest order it is non-interacting. Now, we simply write U as $U = e^{is}$ with certain operator S. The first order in H_t is

$$i[H, S] = H_t$$

So we propose a general form of transforming generator S. Such transformation is given as

$$S = \sum \sum_{k,q} F_{k,q}[h^{+}_{k-q} h_k \alpha^{+}_{q} - h.c]$$

where $F_{k,q}$ is the perturbation parameter. We can relate this parameter with the kinematic factor $M_{k,q}$ as

$$F_{k,q} = f_{k,q} M_{k,q}$$

where $f_{k,q}$ is a free transformation parameter. To find the effective Hamiltonian of the system, we can use the usual commutation expansion,

$$H_{eff} = e^{-s} H e^{s}$$

Using series expansion

$$e^{-s} = 1 - s + \frac{1}{2}s^2 - \frac{1}{6}s^3 + \frac{1}{24}s^4 - \frac{1}{120}s^5 \ldots$$

$$e^{s} = 1 + s + \frac{1}{2}s^2 + \frac{1}{6}s^3 + \frac{1}{24}s^4 + \frac{1}{120}s^5 \ldots$$

Then,

$$H_{eff} = e^{-s} H e^{s} = (1 - s + \frac{1}{2}s^2 - \frac{1}{6}s^3 + \frac{1}{24}s^4 - \frac{1}{120}s^5 \ldots.) H.(1 + s + \frac{1}{2}s^2 + \frac{1}{6}s^3 + \frac{1}{24} + \frac{1}{120} \ldots..)$$

$$H_{eff} = H + [H, s] + \frac{1}{2}[[H, s], s] + \frac{1}{6}[[[H, s], s], s] + \ldots..$$

$$H_{eff} = H - SH + HS + (\frac{1}{2}S^2 H - SHS + \frac{1}{2}HS^2) + \ldots. \qquad (3.4.23)$$

We know that

$$H = H_0 + \lambda H_t$$

Then,

To solve the commutation relation for the effective Hamiltonian we use the following three conditions for any given inner product of operates $[C, C^{+}]$:

$$1.\ \ |(\lambda_0\hat{A} + \lambda_1\hat{B}), C^{+}| = \lambda_0|\hat{A}, C^{+}| + \lambda_1|\hat{B}, C^{+}|$$

where λ_0 and λ_1 are any given arbitrary numbers.

$$2.\ \ |[A, H], B^{+}| = |A[H, B^{+}]|$$

$$3. |A, B^{+}| = |B, A^{+}|^{*}$$

Based on these equ((3.4.23)) can be reduced to:

$$H_{eff} = e^{s}(H_0 + \lambda H_t)e^{-s} = H_0 + \lambda H_t + [H_0, S] + \lambda[H_t, S] + \frac{1}{2}[[H_0, S], S] + \frac{1}{2}[[\lambda H_t, S], S] + ... \tag{3.4.24}$$

where

$$[H, S] = [(H_0 + \lambda H_t), S] = [H_0, S] + \lambda[H_t, S]$$

If S is chosen, so that the effective Hamiltonian (H_{eff}) has no terms of first order in H_t. Then this point is to the lowest order that results H_0 and H_t are not interacting. So for S in the first order in H_t. As a result of this (3.4.24) above satisfying the following relation;

$$\lambda H_t + [H_0, S] = 0$$

$$\lambda H_t + H_0 S - S H_0 = 0 \tag{3.4.25}$$

From (3.4.25) we understand that $|S| \approx \lambda$. So all the terms in H_{eff} are either of the order of λ^0 or λ^n, for which $n > 1$. Re-writing equa(3.4.24) as:

$$H_{eff} = H_0 + \frac{\lambda}{2}[H_t, S] + \lambda[H_t, S] + \sum_{k,q}[H_{t(kq)} + h.c] \tag{3.4.26}$$

where

$$H_0 = \sum_{q} \omega_q \alpha_q^{+} \alpha_q$$

$$\frac{\lambda}{2}[H_t, S] + \lambda[H_t, S] = \sum_k E_k h_k^+ h_k$$

And:

$$\sum_{k,q}[H_{t(kq)} + h.c] = t\sqrt{\frac{2}{N}}\sum_{kq}[M_{kq}h_{k-q}^+ h_k \alpha_q^+ + h_c]$$

. Inserting the value of the above given, the effective Hamiltonian is;

$$H_{eff} = \sum_k E_k h_k^+ h_k + \sum_q \omega_q \alpha_q^+ \alpha_q - t\sqrt{\frac{2}{N}}\sum_{kq}[M_{kq}h_{k-q}^+ h_k \alpha_q^+ + h_c] \tag{3.4.27}$$

The hole-magnon interaction adds another mechanism for the charge career motion which is magnon assisted condition. The hole-magnon interaction is responsible for the formation of spin polaron. A hole is injected in a non-frustrated. Now our intension focuses on the hole-magnon part of the effective hamiltonian located in equ((3.4.27))

$$H_{hm} = -t\sqrt{\frac{2}{N}}\sum_{kq}[M_{kq}h_{k-q}^+ h_k \alpha_q^+ + h_c] \tag{3.4.28}$$

where

$$M_{kq} = -i\cos\theta(\beta_k \nu_{-q} - \beta_{k-q}U_q)$$

which is defined as the hole-magnon vertex interaction.

$$\beta_k = \sum_\sigma Sink_\sigma$$

Chapter 4

SPECTRAL FUNCTION OF HOLE AND MAGNON DISTRIBUTION FUNCTION

4.1 The Hole Energy Dispersion

As we have seen in the preceding chapter, we carry out the diagonalization method for the equation of motion for hole dynamics and for spin wave exchange interaction to make easy for the divergent terms in high orders of the perturbation calculation. Exact value for the divergent terms could be obtained a convergent result through Bogoliubou transformation by avoiding perturbation theory by diagonalizing exactly to reduce a convergent Hamiltonian.

This method of diagonalization leads to use a systematic ways of transformation. This transformation, we preferred is canonical transformation. It helps us to produced full equation of motion with no derivation as stated in equa.(3.4.23) for the projection operator S.

But from Heisenberg equation of motion

$$\frac{i}{\hbar}\frac{dS}{dt} = [H_0, S] = -\lambda H_t = H_0 S - S H_0 \tag{4.1.1}$$

Now we need to solve the Heisenberg equation of motion of the above equation first.

$$\frac{i}{\hbar}\frac{dS}{dt} = \frac{i}{\hbar}\frac{d}{dt}\{\sum_{kq} f M_{kq}(h^{+}_{k-q} h_k \alpha^{+}_q - h.c)\}$$

After some technical usage of mathematical approach, the above equation reduced to

$$\frac{i}{\hbar}\frac{dS}{dt} = fM_{kq}E_K\alpha_q^+ \tag{4.1.2}$$

and

$$\frac{i}{\hbar}\frac{dS^+}{dt} = -fM_{kq}E_K\alpha_q \tag{4.1.3}$$

Also solving the RHS of equa. (4.1.1) gives

$$\langle n|SH_0|m\rangle - \langle n|H_0S|m\rangle = \langle n|\lambda H_t|m\rangle$$

$$\langle n|S|m\rangle[H_0|m\rangle - H_0|n\rangle] = \lambda\langle n|H_t|m\rangle$$

then

$$\langle n|S|m\rangle = \frac{\lambda\langle n|H_t|m\rangle}{\omega_m - \omega_n} \tag{4.1.4}$$

where H_0 is the Heisenberg Hamiltonian which is taken as unperturbed hamiltonian. the Hamiltonian of equ(3.4.23) can be re-write as:

$$H_0 = \sum_{kq} H_{kq} + constant \tag{4.1.5}$$

by relating equa. (4.1.2), equa.(4.1.3) and equa.(4.1.4) gives, for $H_t = H_{kq}$,

$$H_{kq} = \lambda_0(a_k^+a_q + a_{-k}^+a_{-q}) + \lambda_1(a_ka_{-q} + a_{-k}^+a_q^+) \tag{4.1.6}$$

with $\lambda_0 = E_k - \omega$, and $\lambda_1 = -t\sqrt{\frac{2}{N}\frac{fM_{kk'}}{(\omega-\omega_q)}}$.

Note that this activity shows how the coupling of a_k and a_q^+ for the magnon operators $\alpha_{k'}^+$ and α_k. These new magnon operators are transformed to new boson variables as in the following equations.

$$\alpha_k = \upsilon_k a_k - \nu_k a_k^+; \alpha_k^+ = \upsilon_k a_k^+ - \nu_k a_{-k} \tag{4.1.7}$$

Where υ_k and ν_k are real functions of k and there commutation relation is:

$$[\alpha^+_{q'}, \alpha_q] = \upsilon_k^2 - \nu_k^2 = 1$$

With this choice we can solve for a_k and a_k^+,

$$a_k^+ = \upsilon_k \alpha_k^+ + \nu_k \alpha_{-k}$$

and

$$a_k = \upsilon_k \alpha_k + \nu_k \alpha^+_{-k}$$

. Using (4.1.4) and (4.1.6) we have

$$[\alpha_k^+, H_k] = \upsilon_k(-\lambda_0 a_k^+ - \lambda_1 a_{-k}) - \nu_k(\lambda_0 a_k + \lambda_1 a_k^+). \tag{4.1.8}$$

Observing equa. (4.1.4) and equa.(4.1.8) they are equal to each other. So we obtain two linear equations as shown below:

$$\lambda_0 \upsilon_k + \lambda_1 \nu_k = E_n \upsilon_k$$

$$\lambda_1 \upsilon_k + \lambda_0 \nu_k = -E_n \nu_k$$

. The equation shown above are form of linear function. So we can find it's solution as

$$\begin{vmatrix} \lambda_0 - E_n & \lambda_1 \\ \lambda_1 & \lambda_0 + E_n \end{vmatrix} = 0$$

$$(\lambda_0 - E_n)(\lambda_0 + E_n) = (\lambda_1)(\lambda_1)$$

Or

$$E_n^2 = \lambda_0^2 - \lambda^2 1 = (E_k + \omega)^2 - (-t\sqrt{\frac{2}{N}}\frac{fM_{kk'}}{(\omega - \omega_q)})^2$$

.

$$E_n = \sqrt{(E_k + \omega)^2 - [-t\sqrt{\frac{2}{N}}\frac{fM_{kk'}}{(\omega - \omega_q)}]^2}$$

$$E_n = (E_k + \omega)\sqrt{1 - [-t\sqrt{\frac{2}{N}}\frac{fM_{kk'}}{(E_k + \omega)(\omega - \omega_q)}]^2} \tag{4.1.9}$$

Where $E_k = -2t\cos\theta\sin k$, $\omega = \frac{1}{2N}S^2J^2$ and $\omega_q = -2JS\sqrt{(1+\gamma_q)(1-\cos\theta\gamma_q)}$

We get the energy dispersion for a single hole after we use Ising Limit for the vertex interaction:

4.1.1 Ising Limit

The general spin-hole Hamiltonian formalism, for the t-J model, it can be solved using momentum independent of ω_q in the Ising limit. According to this limit $\omega_q = U_q = 1$ and $V_q = 0$ The Hamiltonian referred in equa. (3.4.23) for the hole-magnon interaction becomes in the Ising limit as:

Where

$$M^I_{k,q} = iCos\theta(\beta_{k-q})$$

$\beta_{k-q} = \sum_\sigma \sin{(k-q)} = \begin{bmatrix} 0 & \sin{(k-q)} \\ \frac{1}{2} & 0 \end{bmatrix} = \begin{bmatrix} 0 & \sin{(k)} \\ \frac{1}{2} & 0 \end{bmatrix} \begin{bmatrix} 0 & \cos{(q)} \\ \frac{1}{2} & 0 \end{bmatrix} + \begin{bmatrix} 0 & \sin{(q)} \\ \frac{1}{2} & 0 \end{bmatrix} \begin{bmatrix} 0 & \cos{(k)} \\ \frac{1}{2} & 0 \end{bmatrix}$

$\beta_{k-q} = \beta_{(k)}\beta_{(q)} + \bar{\beta}_{(k)}\bar{\beta}_{(q)} = \frac{1}{4}\sin(k-q)$ Then,

$$M^I_{k,q} = \frac{-i}{4}\cos\theta\sin(k-q)$$

Using the analogy with the transformation:

$$S = f\sum_{(k,q)} M^I_{k,q}(h^+_{k-q}h_k\alpha^I_q - H) \tag{4.1.10}$$

The equation shown in equa.(4.1.9) is a form of $f(x) = \sqrt{1-x^2}, x << 1$ which is a decreasing function we need to expand using Taylor series expansion.

$$f(x) = f(0) + f'(0) + \frac{f''(0)}{2!} + \frac{f'''(0)}{3!} + ...$$

$$f(x) = 1 + \frac{1}{2}x - \frac{1}{8}x^2 - \frac{1}{48}x^3 + ... + ...$$

Then

$$E_n = (f(x)) = 1 + \frac{x}{2} - \frac{1}{8}x^2 - \frac{1}{48}x^3 + ... \tag{4.1.11}$$

Now the one hole energy E^h_n can be calculated for the fourth order expansion of the transformation as:

$E^h_n = 8tf\cos\theta\sin{(k-q)} + 8jf^2\cos^2\theta\sin^2{(k-q)} - \frac{32}{3}tf^3\cos^3\theta\sin^3{(k-q)} -$
$\frac{16}{3}Jf^4\cos^4\theta\sin^4{(k-q)}$

Taking the minimization of the hole energy provides an equation for f,

$$\begin{aligned}\frac{\partial E_h}{\partial f} =&8t\cos\theta\sin(k-q)+16Jf\cos^2\theta\sin^2(k-q)\\&-32tf^2\cos^3\theta\sin^3(k-q)-\frac{64}{3J}f^3\cos^4\theta\sin^4(k-q)=0\end{aligned}\tag{4.1.12}$$

$$\begin{aligned}8\cos\theta\sin(k-q)(t+2Jf\cos\theta\sin(k-q)-4tf^2\cos^2\theta\sin^2(k-q)\\-\frac{8}{3}Jf^3\cos^3\theta\sin^3(k-q))=0\end{aligned}\tag{4.1.13}$$

hence,

$$t+2Jf\cos\theta\sin(k-q)-4tf^2\cos^2\theta\sin^2(k-q)-\frac{8}{3}Jf^3\cos^3\theta\sin^3(k-q)=0$$

Solving for the parameter f for which $\frac{t}{J} << 1$ gives:

$$f=(\frac{-t}{2J})\cos(\theta)\sin(k-q)\tag{4.1.14}$$

The solution for f in (4.1.14) can be done based on the strength of t and J interaction energies. First let rearrange the equa.(4.1.14) as:

$$\frac{t}{2J}\cos(\theta)\sin(k-q)+f-\frac{2t}{J}\cos(\theta)\sin(k-q)f^2-\frac{4}{3}f^3=0$$

For $\frac{t}{J} << 1$, $-\frac{2t}{J}\cos(\theta)\sin(k-q)f^2$ and $-\frac{4}{3}f^3$ becomes vanish because they are very small. Therefore

$$f=\frac{-t}{2J}\cos(\theta)\sin(k-q)$$

For $\frac{t}{J} << 1$, $f=(\frac{-t}{2J})\cos(\theta)\sin(k-q)$ then,

$$\begin{aligned}\frac{E_t}{J}&=-8t^2\frac{\cos\theta\sin(k-q)}{2J}-\frac{4t}{3}(\frac{\cos\theta\sin(k-q)}{2J})^3\\&+\frac{2J}{t}(\frac{-t}{2}(\frac{\cos(\theta)\sin(k-q))}{2J})^2-\frac{1}{3}\frac{-t\cos\theta)\sin(k-q)}{2J}\\&=8t\Bigg[\frac{-t\cos(\theta)\sin(k-q)}{2J}\frac{-4t}{3}(\frac{\cos\theta\sin(k-q)}{2J})^3\\&-\frac{2J\cos\theta\sin(k-q)}{2t}(\frac{-t\cos\theta\sin(k-q)}{4J})^2-\frac{t\cos\theta\sin(k-q)}{6J}\Bigg]\\&=-2t^2(\frac{\cos\theta\sin(k-q)}{J})+\frac{1}{8}(\frac{t\cos\theta\sin(k-q)}{J})^3\end{aligned}\tag{4.1.15}$$

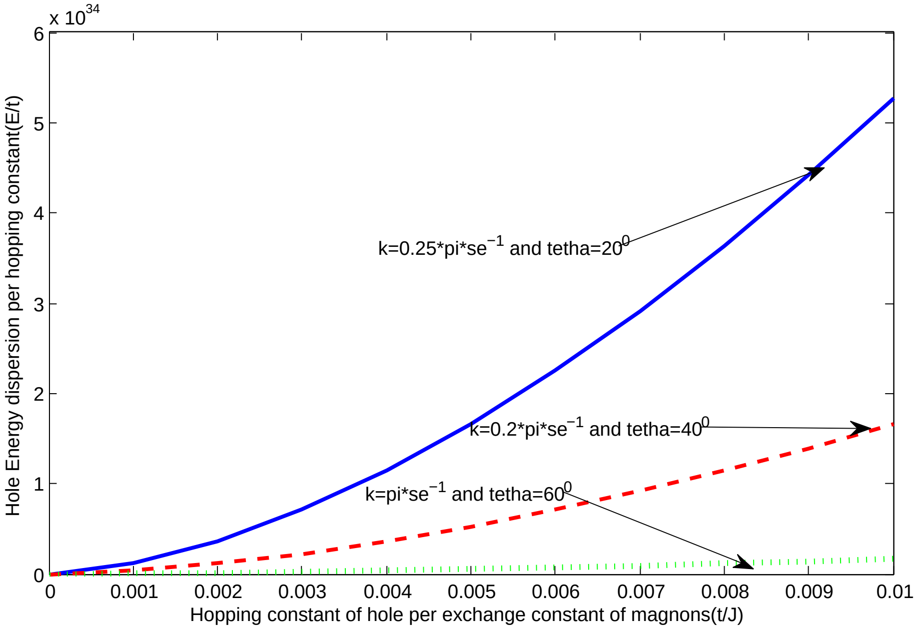

Figure 4.1: plot of hole energy dispersion per hopping constant versus (t/J)

.

$$\frac{E}{t} = -2(\frac{t}{J})\cos(\theta)\sin(k-q) + (\frac{t}{J})^3(\cos(\theta)\sin(k-q))^3 \tag{4.1.16}$$

Using equa. (4.1.16), we have drawn Fig 4.1. As we have observed, the energy of the hole per t ($\frac{E}{t}$) decreases with increasing $\frac{t}{J}$. This is the case for $t << J$. This situation shows there is a free like motion of hole. Based on this phenomena observed, we can say that there is an increment of the FM property of the system with increasing θ and k from 0^0 to 90^0.

4.2 Spectral Function of Hole

A freely hopping hole implies a finite probability of movements with out interaction to magnons (no emission and no absorptions of magnons by hole). This situation shows the direct consequence of the underlying non-collinear of the magnetic structure of the FM or AF order.

To derive the spectral density for studying the property of hole motion in the presence of anti-ferromagnetic long range order, we use the perturbed wave function we derived in equa. (3.4.16). This wave function is written in the form:

$$|\psi\rangle = z_k[h_k^+ + \frac{1}{\sqrt{N^n}}\sum_{k,q} R^2_{(k_n,q_{n+1})} h^+_{(k-q_n)}\alpha^+_{q_n} + ...]|k\rangle \tag{4.2.1}$$

Where $z_k = |\langle k|h^+|k\rangle|^2 = \sum_k |a_k^0|^2 = 1$,

$R^2_{(k_n,q_{n+1})} = M_{(k_n,q_{n+1})} G_{(k_{n+1},\omega-\omega(q_1...q_{n+1}))} = a^n_{(k_n,q_{n+1})}$, $G_{(k,\omega)} = [\omega - E_k - \Sigma_{(k,\omega)}]^{-1}$ is called Green's function, $M_{(k_n,q_{n+1})} = -i\cos\theta\sum_{k,q}\sin(k-q)$ is called hole-magnon vertex interaction, and finally $\Sigma_{(k,\omega)} = \frac{1}{N}\sum_{k,q}|M(k,q)|^2 G(k,\omega-\omega_q)$ is the self energy of hole.

The spectral function of hole can be now defined as:

$$A^h(k,\omega) = -\frac{1}{\pi} Im G(k,\omega) \tag{4.2.2}$$

The main features of this spectra are clearly differentiated and therefore easier to identify the underlying mechanisms for the hole motion. We have seen the hole green function as shown above which can be written as

$$G^h(k,\omega) = \frac{1}{\omega - E_k - \Sigma(k,\omega)} \tag{4.2.3}$$

The imaginary part of the Greens function is due to the complex value of the self-energy resulting from the complex propagation of the wave vector **k**. Hence,

$$\Sigma(k,\omega) = \Sigma_1(k,\omega) + i\Sigma_2(k,\omega) \tag{4.2.4}$$

Where $\Sigma_1(k,\omega) = Re\Sigma(k,\omega)$ and $\Sigma_2(k,\omega) = Im\Sigma(k,\omega)$ are the real and imaginary parts of the self-energy $\Sigma(k,\omega)$. After we determined the self-energy usually by solving iteratively of the equation (4.2.4), We can solve the spectral function$A^h(k\omega)$ and quasi-particle weight (Z_k). The self energy ($\Sigma(k,\omega)$) ,the free hole energy(E_k) and quasi-particle(Qp) energy ($\epsilon(k,q)$) are related as

$$\epsilon_{(k,q)} = E_k - \Sigma(E) \tag{4.2.5}$$

Where E_k is the bare(free) Hole energy, which is equal to

$$E_k = -2t(\cos k_x + \cos k_y)\cos\theta = -4tcos\theta\cos k$$

.

Before we evaluate the self energy, let's first rearrange equ.(4.2.3) as follow:

$$G^h(k,\omega) = \frac{(\omega - \omega_q - E_k + Re(k,\omega) + iI(k,\omega))}{(\omega - \omega_q - E_k + Re(k,\omega) + iI(k,\omega))^2 + I^2(k,\omega)} \tag{4.2.6}$$

Now the imaginary part of $G^h_{(k,\omega)}$ is

$$ImG^h_{(k,\omega)} = \frac{I_{(k,\omega)}}{(\omega - \omega_q - E_k + Re(k,\omega) + iI(k,\omega))^2 + I^2(k,\omega)} \tag{4.2.7}$$

The spectral density function for a single hole is in general given by

$$A^h_{(k,\omega)} = \sum n, m|\langle\psi_n|\psi_n\rangle|^2 e^{-\beta E}(e^{i\beta E} + 1)\sigma[\omega - (E_n - E_m)]$$

By observing the above equation $A^h_{(k,\omega)}$ is non-negative for all k and ω. Also $I(k,\omega) \leq 0$ for the imaginary party of the self energy of the hole. The quasiparticle energy ϵ_k is given as

$$\epsilon_k = E_k - Re\Sigma_{(k\omega)}$$

By assuming the imaginary part of the self energy is different from zero (Ik,ω)). For this case $|I_{k,\omega)}| << |E_k - Re\Sigma(k\omega)|$ is valid within a certain neighborhood of the resonance $\epsilon_{i(k)}$.so we can expect a prominent maximum at the energy $\omega = \epsilon_{i(k)}$. to see this we expand the expression $F_{i(k,\omega)} = E_k - Re\Sigma_{(k,\omega)}$ around the resonance position and terminate the series expansion after the linear term.

$F_{i(k,\omega)} = F_{(k-\epsilon_{i(k)})} + (E_{i(k)})\frac{\partial F}{\partial\omega}|_{\omega=\epsilon_{i(k)}} + ...$

$F_{i(k,\omega)} = \epsilon_{i(k)} + (\omega - \epsilon_{i(k)})\frac{\partial Re\Sigma_{(k,\omega)}}{\partial\omega}|_{\omega=\epsilon_{(k)}} + ...$

This means,

$$\begin{aligned}(\omega - \epsilon_{i(k)} - Re\Sigma_{(k,\omega)})^2 &= (\omega - \epsilon_{i(k)})^2(1 - \frac{\partial Re\Sigma_{(k,\omega)}}{\partial\omega}|_{\omega=\epsilon_{i(k)}})^2 \\ &= Z_k^{-2}(\omega - \epsilon_{i(k)})^2 \end{aligned} \tag{4.2.8}$$

Inserting of equa (4.2.8) in equa.(4.2.2) and by further assuming that $I_{(k,\omega)}$ in the neighbor of the resonance $\epsilon_{i(k)}$ is a continues, only weakly varying function of ω. So that to a good approximation in the energy region of interest, we can set: $I_{(k,\omega)} = I_{(k,\epsilon_{i(k)})} = I_{(k)}$. Then the spectral density function can be approximated as follows:

$$A^{h}_{(k,\omega)} \approx -\frac{1}{\Pi}[\frac{Z^{2}_{(k)}I_{(k)}}{(\omega-\epsilon_{i(k)})^{2}+(Z_{(k)}I_{(k)})^{2}}] \tag{4.2.9}$$

To find the value of I_k we let the maximum energy of the free hopping hole is given by:

$$E_k = \frac{\hbar^2 k^2}{2m^*}$$

Using the Q_p energy definition, we obtain:

$$\frac{\hbar^2 k^2}{2m^*} = \epsilon_{i(k)} - \Sigma(k,\omega)$$

$$k = \frac{2m^*}{\hbar^2}\sqrt{\epsilon_{i(k)} - \Sigma_{(k,\omega)}} \tag{4.2.10}$$

The complex propagation k is written as:

$$k = k_1 + ik_2 \tag{4.2.11}$$

From free motion of hole E_k can be re-write

$$E_k = \frac{\hbar^2 k^2}{2m^*} = -4t\cos\theta\cos(k) \tag{4.2.12}$$

From equa.(4.2.12) we have:

$$k = \sqrt{\frac{2m^*}{\hbar^2}(E_k - \Sigma_k)} \tag{4.2.13}$$

Substituting equa. (4.2.13) in equa.(4.2.11), the resulting value becomes:

$$k_1 + ik_2 = \sqrt{\frac{2m^*}{\hbar^2}(E_k - \Sigma_k)}$$

Squaring both sides of the above equation gives:

$$k_1^2 + 2ik_1k_2 - k_2^2 = \frac{2m^*}{\hbar^2}(E_k - \Sigma_k)$$

This shows:

$$k_1 = \frac{2m^*}{\hbar^2}|E_k - \Sigma_{1(k)}|$$

and

$$k_2 = \frac{m^*}{\hbar^2}\frac{|\Sigma_{2(k)}|}{k_1}$$

By using the value of k_1:

$$k_2 = \frac{|\Sigma_{2(k)}|}{\hbar v} \tag{4.2.14}$$

where v is group velocity and is given as $v = \frac{R}{\tau} = \frac{\hbar k_1}{m^*}$ at any energyE_k. So

$$k_2 = \frac{|\Sigma_{2(k)}|}{\hbar}\frac{\tau}{R}$$

$\Sigma_{1(k)}$ and $\Sigma_{2(k)}$ indicates the real and imaginary part of $\Sigma_(k)$,R-is mean free path and τ is the relaxation time. The limiting expression for the equation to be valid are,

$$|\Sigma_{2(k)}| << |E_k - \Sigma_{1(k)}|$$

From equation of k_1 and K_2, we see that the real part of k of the propagation constant is re-normalized because of the presence of the self-energy. But the imaginary part of k of the propagation would lead to the decay of the average of the off-diagonal matrix element of the Green's function:$G(n, m, E)$ as $|n - m| \to \infty$. So that in simple expression the energy dispersion approaches to the free hole energy

$$E_{(k)} = -4t \cos\theta \sin k$$

.

Remember that,

$$G(r, r', E) = \sum_i \frac{\psi(r)\psi^*_(r')}{E - E_i}$$

$$G(r, r', E) = \sum_i \psi(r)\psi_i^*(r')e^{i\frac{\psi_(r)-\psi_(r')}{E-E_i}}$$

For this situation the quantum average Green's function shall have;

$$< G(n, m, E) >= G_0(n, m, E) = \frac{m^* a^2}{2\pi\hbar^2}(\frac{e^{ia(k1|n-m|-k2|n-m|)}}{|n-m|}) \tag{4.2.15}$$

Where a- is the lattice constant. From the mean free path R and the relaxation time τ, we can relate, the energy dependent relaxation time is related as the inverse of the imaginary part $\Sigma(E)$. The normalized wave length λ corresponding to the energy E_k is given as

$$\lambda = \frac{2\pi}{k_1} = \frac{2\pi\hbar}{\sqrt{\frac{2m^*}{\hbar^2}[(E_k - \Sigma_k)]}} \tag{4.2.16}$$

equ (4.2.15) shows that the average Green function $G(r, r', E)$ decaying for large $|r-r'|$ that means $|r - r'| >> R$, R-is mean free path: the mean free path R is defined through the decay of average Green's function

$$G(r, r', E) \sim e^{\frac{-|r-r'|}{2R}}$$

for large value of $|r - r'|$, and comparing this equation with equ. (4.2.15), we found,

$$\lambda = \frac{1}{2k_2} = \frac{\hbar v}{2\Sigma_{2(k)}|}$$

From this equation and mean free path, we calculate the relaxation time τ,

$$\tau = \frac{\hbar}{2\Sigma_{2(k)}|}$$

From this, the imaginary part of $\Sigma(k)$ is inversely proportional to the energy dependent relaxation time.

When we average over all configurations of the random variables involved in the Hamiltonian, the phase difference $\langle\psi(r) \mid \psi(r')\rangle$ oscillate strongly for large $|r-r'|$ and as a result, it contribute to the decay of $< G(r, r', E) >$ for $|r - r'| >> R$ The spectral function of a hole is

$$A^h(k, \omega) = -\frac{i}{\pi} I_m G^h(k, \omega)$$

$= \frac{-i}{\pi} \sum_i \frac{\psi(r)\psi^*_(r')}{E-E_i} = \frac{-i}{\pi} \frac{2\Pi\hbar}{\sqrt{\frac{2m^*}{\hbar^2}[(E_k-\Sigma_k)]}} e^{\frac{-(r-r')}{2R}}$

This can be put easily as;

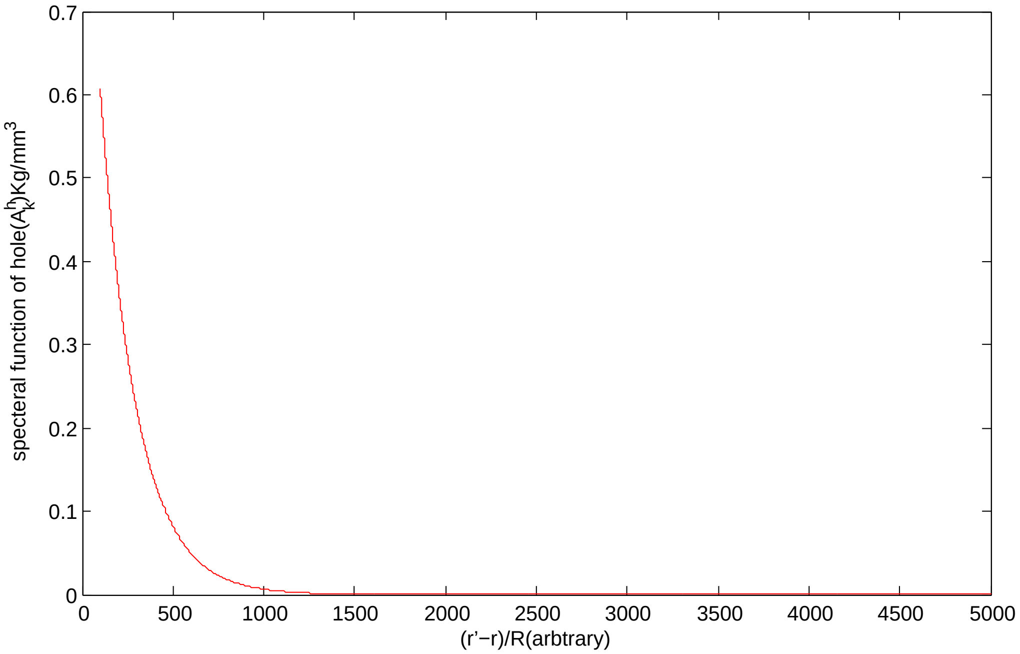

Figure 4.2: spectral density of hole verses $(r - r')$ hopping distance between two sites

$$A^h(k,\omega) \sim e^{\frac{-|r-r'|}{2R}} \tag{4.2.17}$$

Spectral function $A_{(k)}$ is an important tool in describing the behavior of propagation of hole in an AF background. It is dependent on the self energy. Self energy is a complex function of hole propagation in the field of spin wave. From the result of equa (4.2.17) above, A_k depends on the factor of $e^{\frac{-|r-r'|}{2R}}$ and consequently, it's characteristic is shown in the fig(4.2). This shows the existence of interference between hole in motion and magnons.

The exponential decaying of the A_k with increasing of mean distance (R) is due to the relaxation time τ and is inversely proportional to the hopping constant t (i.e $\tau \sim \frac{1}{t}$). This is happen when $J >> t(\frac{t}{J} << 1)$.

This phenomena indicates the hole moves easily due to the increasing magnetic ordering coming from the hole motion causes disturbance on the AF background.

4.3 Quasiparticle Excitations(Quasi Particle Weight)

In this section we analyze the quasi particle excitation in the low energy spectra. This can be quantified by the quasi particle weight (Z_k) which is given by:

$$Z_k = |\langle\phi_n|h^+|\phi_n\rangle|^2 = \sum_k |a^n(k,q)|^2 = 1 \tag{4.3.1}$$

The effective Hamiltonian in equ(3.4.27) leads to an analytical expression for the Qp wave function. This takes to an account to the contribution of different numbers of magnons involved in the formation of the Qp. The equation shown in equ.(4.2.1) indicate the number of magnon contributed in the interaction.

Generally the number of magnons necessary in the Quasiparticle wave function is obtained by normalization condition.

$$\langle\psi|\psi\rangle = z_k = \sum_{m=0}^{n} |a^m(k,q)|^2 = 1$$

The number $a^m(k,q)$ in the above equation is given from (4.2.1) by

$$a^m(k,q) = \frac{Z_k}{N^m} \sum_{q_1 \cdots q_n} R^2_{k,q_1} R^2_{k_1,q_2} R^2_{k_2,q_3} \dots . R^2_{k_{n+1},q_n} \tag{4.3.2}$$

For $m = 0$,$a^{(0)}_{k,q} = z_k$. a^0_k stands for the bare hole operator without magnon, and $a^1(k,q)$ indicates one magnon is interacting with the hole and so on. From the Schrodinger equation, we obtain the following equation for the expansion coefficients of one magnon contribution as:

$$\omega a^0(k) - \frac{1}{N} \sum_{q_1} a^1(k,q_1) M_{k,q_1} = 0 \tag{4.3.3}$$

And for two magnons

$$(\omega - \omega_{q_1}) a^1(k,q_1) - a^0(k) M_{k,q_1} - \frac{1}{N} \sum_{q_2} a^2(k_1,q_1,q_2) M_{(k-q_1-q_2)} = 0 \tag{4.3.4}$$

Using the contradiction rule, the general equation for $n > 0$ becomes:

$$(\omega - \omega_{(q_n)}) a^n(k,q_n) - a^{(n-1)}(k,q_n) M_{(k,q_n)} - \frac{1}{N} \sum_{(k_n,q_{(n+1)})} a^{n+1}(k,q_{n+1}) M(k_n,q_{n+1}) = 0 \tag{4.3.5}$$

where

$$k_n = k - q_1 - q_2 - q_3 \dots q_{(n+1)}$$

.

The equations shown above have a general solution:

$$a^{n+1}(k, q_1 - \cdots - q_{(n+1)}) = a^n(k, q_1 - \cdots - q_n)M(k_n, q(n+1)) \tag{4.3.6}$$

From equa (4.3.3) we have a relation:

$$\omega a^0(k) = \frac{1}{N}\sum_{q_1} a^1(k, q_1)Mk, q_1 \tag{4.3.7}$$

Using relation of equa (4.3.3) and equa (4.3.5) we obtain:

$$a^0(k)(\omega - E_k) = 0 \tag{4.3.8}$$

Equa. (4.3.8) has a solution for $a^0(k)$, which is different from zero at Quasiparticle (Qp) energy ($\omega - E_{(k)}$). The coefficient $a^0(k)$ determine the bare quasi particle weight (z_k).

$$z_k = \sum |a^0(k)|^2 \tag{4.3.9}$$

Equa. (4.3.9) follows from the normalization of wave function.

$$< \psi_k|\psi_k >= \sum_{(n=0)}^{\infty} |a^n_{(k,\dots qn)}|^2 = 1 \tag{4.3.10}$$

Using the equa (4.2.8), and it reduced to:

$$Z_k = (1 - \frac{\partial\Sigma(k,\omega)}{\partial\omega})^{-1}|_{\omega=E_k}$$

But:

$$\frac{\partial\Sigma(k,\omega)}{\partial\omega}\ |_{\omega=E_k} \approx -(\frac{t}{J})^2 m^* E_k$$

Therefore:

$$Z_k \approx (1 + (\frac{t}{J})^2 m^* E_k)^{-1} \tag{4.3.11}$$

Where:-$E_k = -2t\cos\theta\cos(k)$. For $Z_k \to 1$ means the hole moves freely by the FM order.

As we have seen in the figures the quasi particle weight (Z_k) increases or decrease

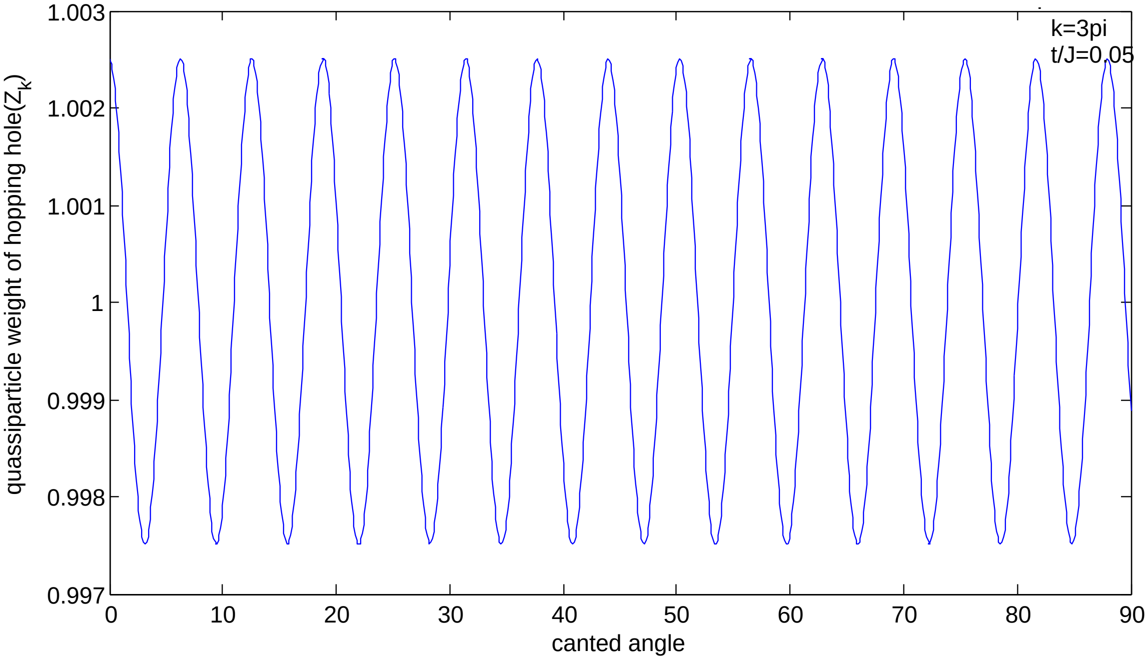

Figure 4.3: Plot of quasiparticle weight versus canted angle θ

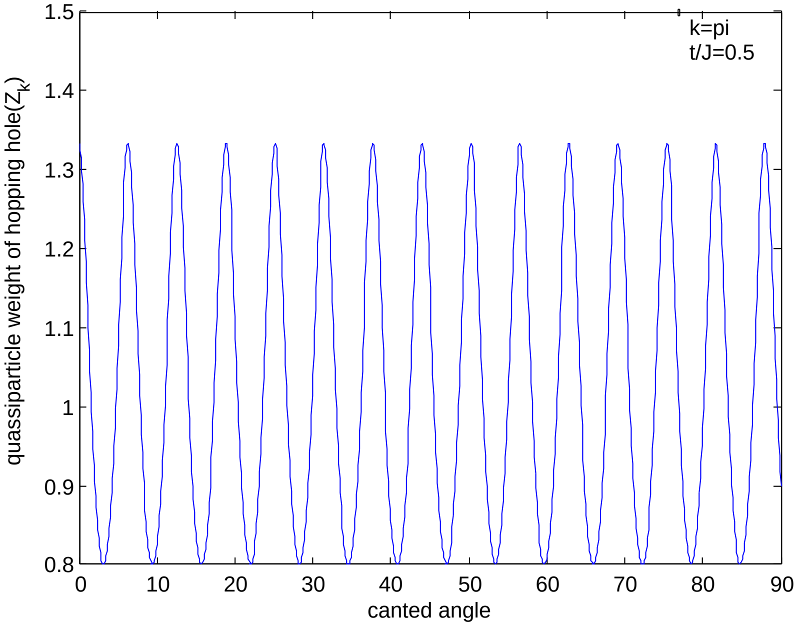

Figure 4.4: Plot of quasiparticle weight versus canted angle θ

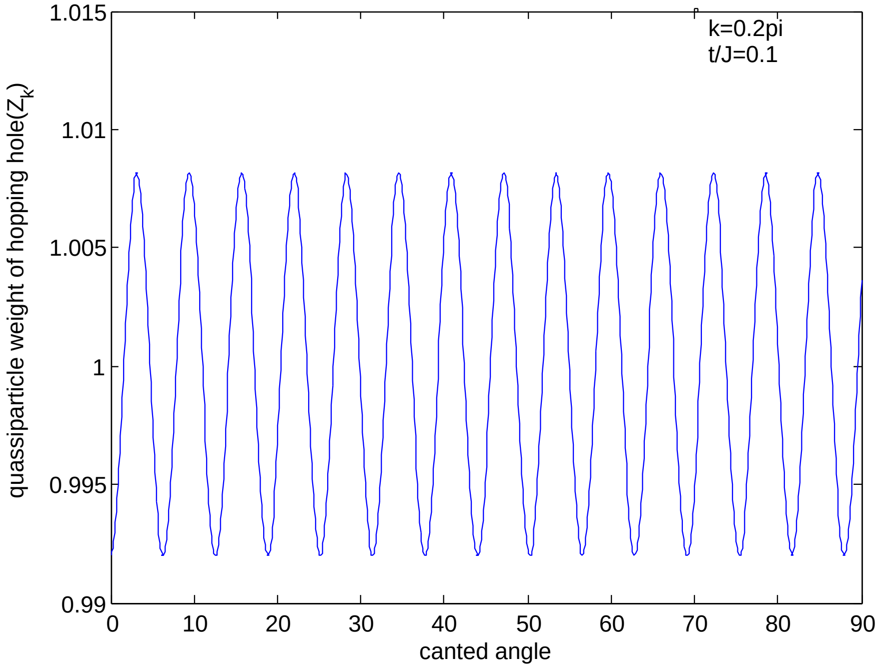

Figure 4.5: Plot of quasiparticle weight versus canted angle θ

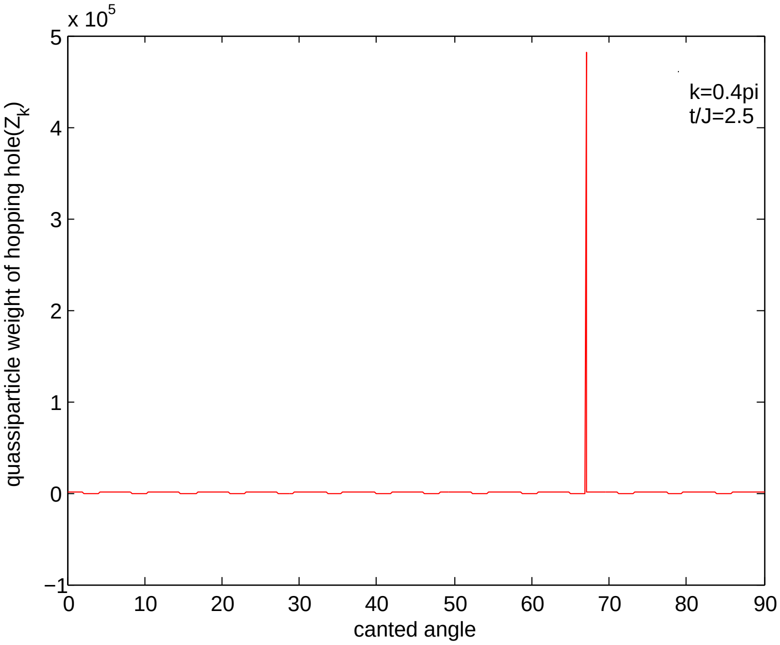

Figure 4.6: Plot of quasiparticle weight versus canted angle θ

quadratically from $\theta = 0$ to $\theta = 90^0$ for a constant k and $\frac{t}{J}$. This shows the quasi particle weight increases outside the magnetic Brillioun zone. On the other hand, the quasi particle weight has a peak at the angle θ and increases for $k = (\frac{\pi}{2}, \frac{\pi}{2})$ inside the magnetic Brillioun zone. It indicates the reduction of the quasi particle weight associated with the vanishing of the coupling (vertex interaction) for hole and magnon, as shown in fig(4.11).

We discuss the evolution of Z_K with respect to the canted angle for some values of k and $\frac{t}{J}$ as shown in the Fig.(4.3), Fig.(4.4), Fig.(4.5), Fig.(4.6), Fig.(4.8), and Fig.(4.7). Here, it appears that a classical ferromagnetic component of characteristic with high peak resonant value is shown. The relative peak of the resonant describes the free hopping mechanism and magnon assisted motion of hole. The fluctuation of the peaks in the figures show the transfer of Z_k from low energy sector to high energy sector that depends on the different value of k and $\frac{t}{J}$.

This is due to the mechanism signatted by a finite life time for hole hopping and $t-$ resonant. On the other hand the evolution of Z_k at a considerable canted angle with respect to wavevector k and $\frac{t}{J}$ shows different existence as in Fig(4.11).

Generally the value of Z_k as the value of canted angle increase from 0^0 to 90^0 determine the probability of finding the motion of hole for a given values of k and $\frac{t}{J}$. The point of peak in the Z_k versus θ graph describes the degree of freely movement along the ferromagnetic order or the magnon assisted movement in the spin fluctuation as we have seen in fig(4.3),fig(4.4), fig(4.5), fig(4.6),fig(4.7), and fig(4.8).

The low and high energy structure of the hole as it hopes from one site to another site in AF background depends on the coupling between the moving hole and the underlying AF order. This low and high energy of the hole is measured in terms of the characteristic relaxation time order. For low energy sector the characteristic relaxation time for the hopping hole is the order of $\frac{1}{t}$ and its spectral density function decaying exponentially as we have seen in Fig(4.2). At this point $J > t$ and the hole is surrounded by the AF cloud energy (quasiparticle excitation). The fluctuation in the length of the peaks for a given k

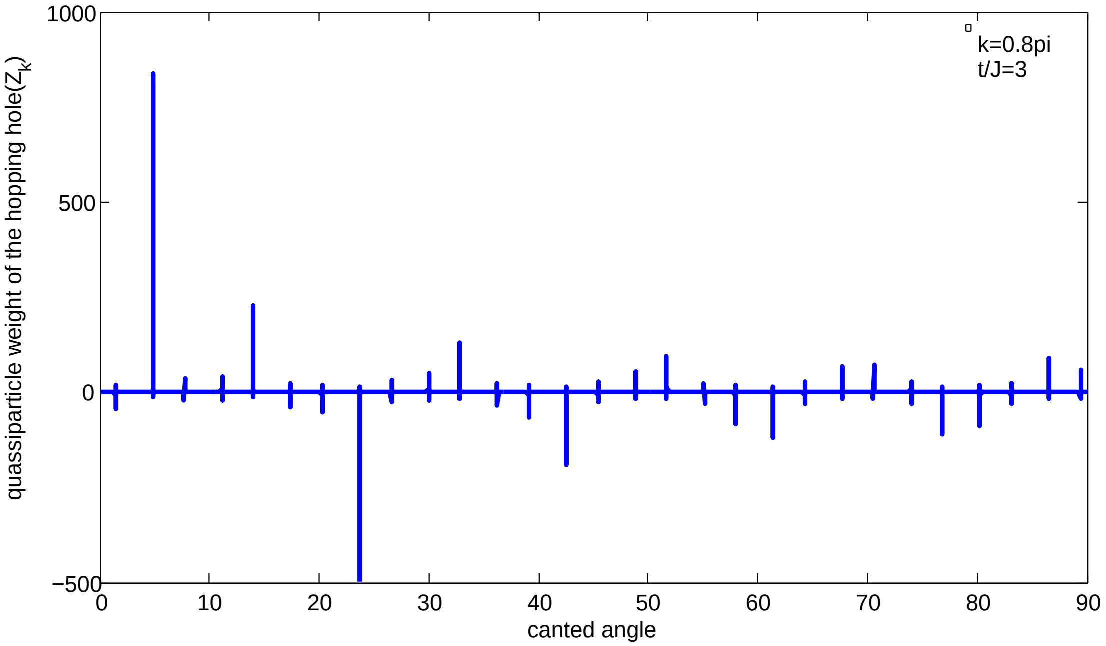

Figure 4.7: Polt of quasiparticle weight versus canted angle θ

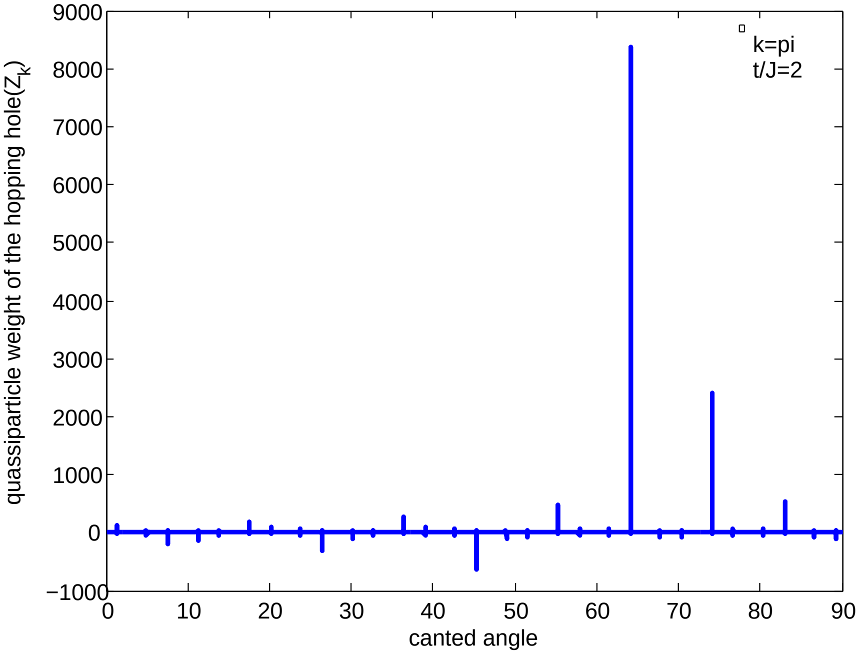

Figure 4.8: Plot of quasiparticle weight versus canted angle θ

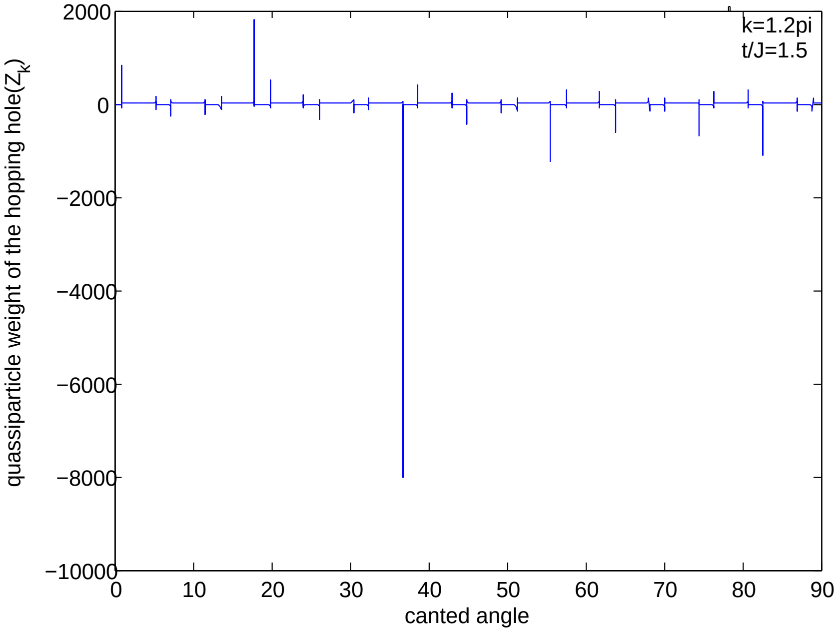

Figure 4.9: Plot of quasiparticle weight versus canted angle θ

and $\frac{t}{J}$ is due to the pair repair spin characteristic of the AF order.

On the other hand for the case $J < t$ the hole couples strongly with the spin cloud in the AF order. The propagation of hole at a finite probability with a considerable high energy at a specific canted angle described by the long peak where as the other resonance shows the string effects of the hole and AF cloud. Based on Fig.(4.3), Fig.(4.4) and Fig.(4.5), the hole is shown propagating with a steady energy at each canted angle but with different oscillating amplitude. This is because inside the BZ for very small value of $\frac{t}{J}$, the motion of hole does not affect the structure of the spin ground. Where as illustrations in Fig.(4.6), Fig.(4.7), Fig.(4.8), Fig.(4.9) and Fig.(4.10) indicate fluctuation in energy of the hopping hole due to the overturned effect of the AF order by the hole motion.

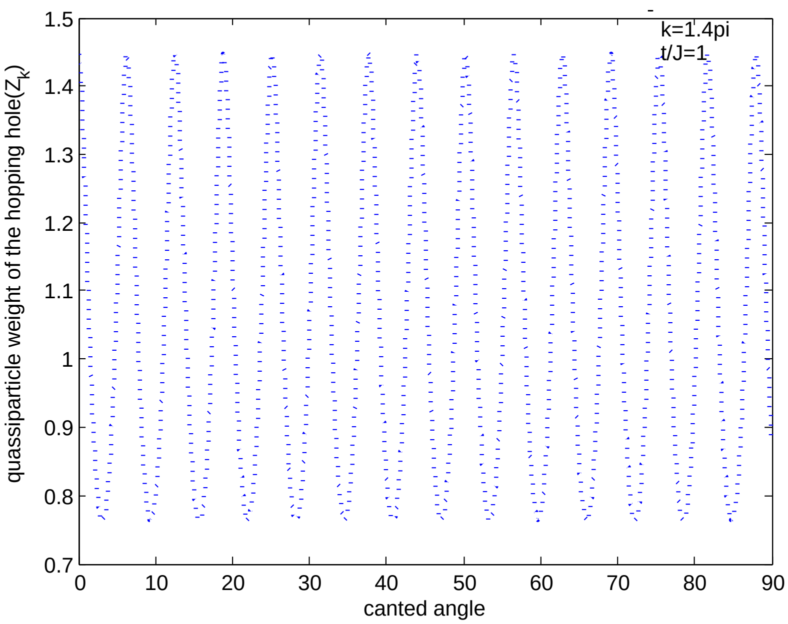

Figure 4.10: Plot of quasiparticle weight versus canted angle θ

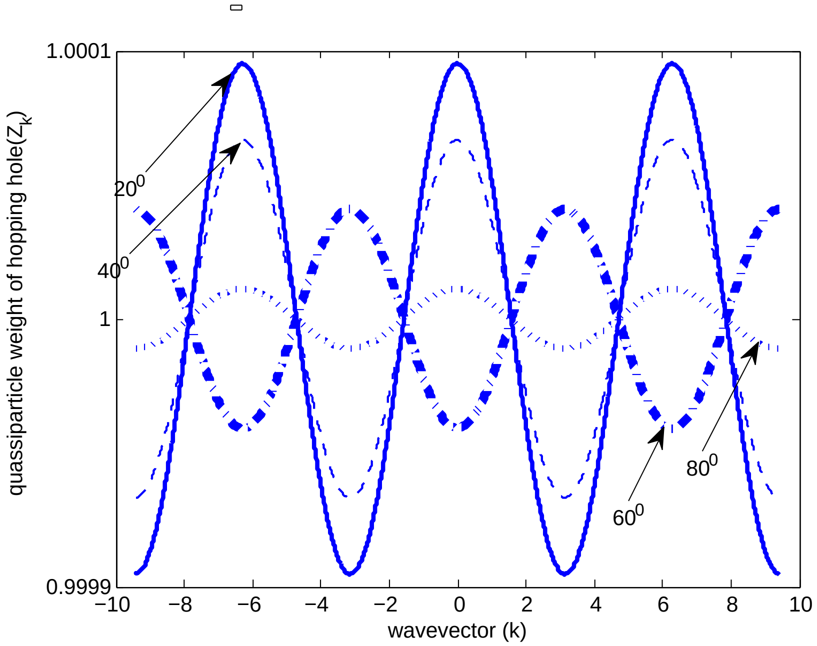

Figure 4.11: plot of quasiparticle weight versus wavevector (k)

Chapter 5

DISCUSSION AND CONCLUSION

We have used a detailed analysis for formulating mathematical mechanism in terms of canonical transformation function for the enhancement of its contribution to the progress of ferromagnetism in diluted magnetic semiconductors. To study this effect, we have explained the motion of a hole in a canted anti ferromagnetic (AF) order by introducing the spineless fermion representation for hole operators with Holstein primalkoff transformation for magnon and hole operators in t-J model Hamiltonian.

The problem that formulated allows us to study the hole dynamics continually from the pure AF background case to the pure ferromagnetic one. As it is well shown in fig. 4.3, Fig.(4.4), Fig.(4.5), Fig.(4.6), Fig.(4.7), Fig.(4.8), Fig.(4.9), and Fig(4.10). A hole can propagate in un frustrated Neel order or state by disturbing the spin alignment of the pure AF order. But the hole moves freely in the ferromagnetic order.

This phenomena can be shown using the hole motion as the function of the canted angle. We call the phenomenon computing of the hole spectral function. For this case we have used a numerical method. We obtain a function with a complex momentum (k, q) and canted angle θ dependent equations shown in Equa((4.3.11)).

The motion of hole in the anti-ferromagnetic and ferromagnetic area can be shown in terms of the comparison of t and J values.

When a hole moves in AF background, the result shows, the motion of a hole has two phases. A free like hopping (propagation) due to the ferromagnetic order and a free restricted like propagation due to a result of AF fluctuation. These two mechanisms for the motion of the hole in the AF background, is due to the interaction of the hole with

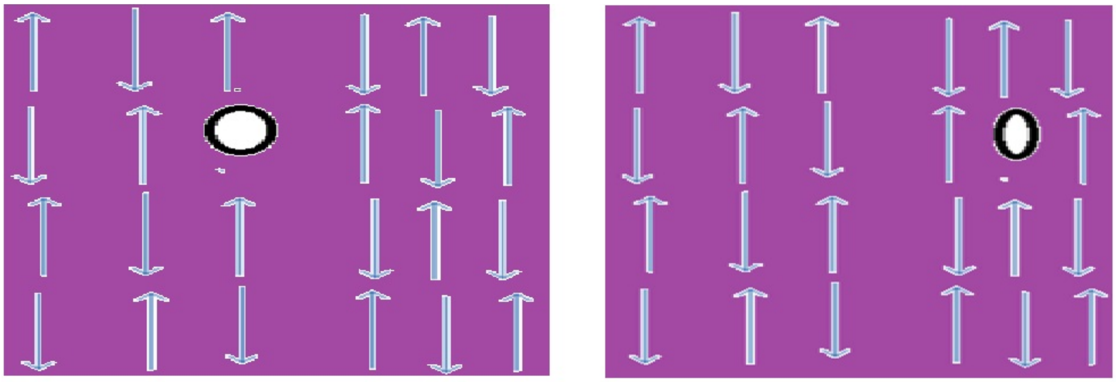

Figure 5.1: (a) The bold spin represents the charge spin disturbed by the hole motion and (b) show the formation of polaron.

the magnon causes to induce ferromagnetic correlation in the system. The restricted and free like propagation of the hole in the AF depends on the comparison value of t and J. For $t > J(\frac{t}{J} >> 1)$ region, the hole moves or propagates at low and high energies.

The low energy is due to the quasi particle polaron and The high energy sector is due to the weakly re normalized magnons that gives a free hopping hole. For $(t/J << 1)$ region, the quasi particle excitation state ends and free hole motion takes place. This is characterized by the high peak value of the resonant figures.

Generally, the coupling between holes and magnons defined on the strength of interaction of spins (J) and the strength of hopping constant of holes (t) describes the following two mechanisms. These two mechanisms for a hole motion in anti-Ferromagnetic background are:

Magnon assisted hoping (hole-magnon interaction)

Consider the illustration shown in Fig.(5.1) for the motion of hole in anti-ferromagnetic background.

As we have seen in Fig.(5.1a), the hole moves only by disturbing the anti-Ferromagnetic order. To this situation $J >> t$ and then $\tau_{exch} \sim \tau_{hop} < J/t$. As a result of this, the hole can propagate easily in anti-ferromagnetic background.

Freely hopping hole with high energy

On the hand for the hole motion in anti-ferromagnetism shown in Fig.(5.1b), the hole and the surrounding cloud of spin flips produce the so called quasi particle polaron (flip cloud). For this to occur, $J << t$ then $\tau_{exch} >> \tau_{hop}$. As a result of this situation the hole will leave behind a string of wrong spins and also causes to increase its effective mass. Where τ_{exch} refers the relaxation time for the exchange interaction (J) among spins and τ_{hop} indicating the relaxation time for the hopping of hole in the AF back ground.

Chapter 6

Summary

Regarding to the hole motion propagating in a canted AF background, we done a detailed analysis of formulating the problem. To study the hole dynamics, we have introduced an approximation methods for suitable reasons. These methods are the spinless fermion representations for hole operators and canonical and Holeistein-Primakoff transformation for the hole and spins for describing it as a bosonic operators in the t-J model. We have modeled the canted AF background by adding a Zeeman term to the t-J model. The effect of Zeeman term is to tilt the AF Neel state to rise the magnetic component. Our aim is to study the motion of the hole starting from the pure AF order to the pure ferromagnetic order continuously.

We found that, the hole moves or propagate with less energy in the AF case due to the coupling of the hole with the spin waves, where as the propagation becomes free with energy of ground state in the pure FM phase. The propagation of the pure AF situation results in FM order with increase in hopping. This is due to to the increase in the kinetic energy of the hole. To show this effect, we computed the spectral function and quasiparticle weight of hole using a reliable numerical method.

For $t > J$, we have obtained a complex function that is dependent on the complex momentum p (wave vector k) and the canted angle θ. This shows that there is strong coupling of the hole with magnons. For the case of $t < J$, the hole moves freely in this region showing the FM order. The increasing of the FM order from the AF background is due to the motion of the hole causing disturbance in anti-spin arrangement in the AF making arrangement of spin in the same direction and hence, the spins in AF order becomes polarized as a result of the hole motion.

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DECLARATION

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

Name: Degefa Mesele

Signature: ____________________

This research thesis has been submitted to for examination with my approval as university advisor.

Name: Dr. Chernet Amente
Signature: ____________________

Place and date of submission:

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May 11, 2014