Spin-Wave Excitations in Quantum Heisenberg Models

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Certificate of Examination

This is to certify that the dissertation titled **Spin-Wave Excitations in Quantum Heisenberg Models** submitted by **Ashish Verma** (Reg. No. MS09029) for the partial fulfillment of BS-MS dual degree programme of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

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Dated: April 25, 2014

Declaration

The work presented in this dissertation has been carried out by me under the guidance of Dr. Sanjeev Kumar at the Indian Institute of Science Education and Research Mohali.

This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Ashish Verma
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Dated: April 25, 2014

In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. Sanjeev Kumar
(Supervisor)

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Abstract

Spin waves are low energy collective excitations in exchange coupled magnetic systems. They determine the reduction of the order parameter by quantum fluctuations and constitute the ground state of ordered magnetic systems. In this thesis, we study the linear spin wave theory with the techniques of Holstein-Primakoff and Dyson-Maleev bosonization with Bogoliubov transformations. Linear spin wave theory is applied to different magnetic systems such as Heisenberg model and its anisotropic variants and the magnon dispersion relations have been derived. We also explore spin wave theory with a self consistent mean field method to account for higher order corrections which are not included in its linear variety.

Chapter 1

Introduction

1.1 Heisenberg Exchange Interaction

In case of ferromagnetism, the existence of spontaneous magnetic moment can be explained by postulating the existence of an internal field called the Weiss field (denoted by H_E) which causes the magnetic moments of the atoms to align.
The origin of Weiss field lies in the interaction between electrons on different atoms. We will derive the expression for this interaction for the case of two electrons (spin-$\frac{1}{2}$ particles). Consider two neighboring atoms A and B and assume that each electron has one electron. Let wavefunctions of the electrons on atom A and B be denoted by Ψ_a and Ψ_b respectively.
According to Pauli exclusion principle,
the total wavefunction for the pair of electrons is antisymmetric under the exchange of the two electrons which means that if the two electrons are labeled as electron 1 and electron 2,

$$\Psi(1,2) = -\Psi(2,1) \tag{1.1}$$

The wavefunction for an electron consists of two parts:
a spatial part (denoted by Φ) and,
a spin part (denoted by χ).
Let Φ_S and Φ_A denote the symmetric and antisymmetric spatial parts of the wavefunction respectively. Also, let χ_S and χ_A denote the symmetric and antisymmetric spin parts of the wavefunction. Then the total wavefunction for the pair of electrons can be written in the following two ways

[0]This section is adapted from [1]

$$\Psi_I = \Phi_S(r_1, r_2)\chi_A(1,2) \tag{1.2}$$

$$\Psi_{II} = \Phi_A(r_1, r_2)\chi_S(1,2) \tag{1.3}$$

such that both Ψ_I and Ψ_{II} are antisymmetric wavefunctions.

For Ψ_I, the spatial part (which is symmetric) can be written as

$$\Phi_S(r_1, r_2) = \frac{1}{\sqrt{2}}[\Psi_a(1)\Psi_b(2) + \Psi_a(2)\Psi_b(1)] \tag{1.4}$$

where $\Psi_a(i)$ ($\Psi_b(i)$) denotes that electron i is in state Ψ_a (Ψ_b). Similarly for Ψ_{II} the antisymmetric spatial part can be written as

$$\Phi_A(r_1, r_2) = \frac{1}{\sqrt{2}}[\Psi_a(1)\Psi_b(2) - \Psi_a(2)\Psi_b(1)] \tag{1.5}$$

For Ψ_I, the antisymmetric spin part can be written as

$$\chi_A(1,2) = \frac{1}{\sqrt{2}}[\eta_{1\uparrow}\eta_{2\downarrow} - \eta_{1\downarrow}\eta_{2\uparrow}] \tag{1.6}$$

where $\eta_{i\uparrow}$ and $\eta_{i\downarrow}$ denote that the electron i is in spin-up state and spin-down state respectively. This is wavefunction for the singlet ($S = 0$) spin state.
Similarly for Ψ_{II}, the symmetric spin part can be written as

$$\chi_S(1,2) = \begin{cases} \eta_{1\uparrow}\eta_{2\uparrow} \\ \frac{1}{\sqrt{2}}[\eta_{1\uparrow}\eta_{2\downarrow} - \eta_{1\downarrow}\eta_{2\uparrow}] \\ \eta_{1\downarrow}\eta_{2\downarrow} \end{cases}$$

Note that this is the wavefunction for the triplet (S=1) spin state.

Now, we will consider the Coulombic electron-electron interactions,

$$V = \frac{e^2}{r_{12}} \tag{1.7}$$

where r_{12} is the distance between the two electrons. The expectation value of V can be calculated in state Ψ_I and state Ψ_{II} ,
Expectation value of V in state Ψ_I,

$$\begin{aligned}
\langle\Psi_I|\,V\,|\Psi_I\rangle &= \langle\Phi_S|\,V\,|\Phi_S\rangle \\
&= \frac{1}{2}[\langle\Psi_a(1)\Psi_b(2)+\Psi_a(2)\Psi_b(1)|\,V\,|\Psi_a(1)\Psi_b(2)+\Psi_a(2)\Psi_b(1)\rangle] \\
&= \frac{1}{2}[\langle\Psi_a(1)\Psi_b(2)|\,V\,|\Psi_a(1)\Psi_b(2)\rangle+\langle\Psi_a(1)\Psi_b(2)|\,V\,|\Psi_a(2)\Psi_b(1)\rangle \\
&+ \langle\Psi_a(2)\Psi_b(1)|\,V\,|\Psi_a(1)\Psi_b(2)\rangle+\langle\Psi_a(2)\Psi_b(1)|\,V\,|\Psi_a(2)\Psi_b(1)\rangle] \\
&= [\langle\Psi_a(1)\Psi_b(2)|\,V\,|\Psi_a(1)\Psi_b(2)\rangle+\langle\Psi_a(1)\Psi_b(2)|\,V\,|\Psi_a(2)\Psi_b(1)\rangle] \quad (1.8)
\end{aligned}$$

where the first equality holds because V is independent of spin.
The first one of these two terms on the RHS is called the **direct** term and is labeled V_d. The second term is called the **exchange** term and is denoted by J.

Similarly, on calculating the expectation value of V in state Ψ_{II}, we obtain

$$\begin{aligned}
\langle\Psi_{II}|\,V\,|\Psi_{II}\rangle &= \langle\Phi_A|\,V\,|\Phi_A\rangle \\
&= [\langle\Psi_a(1)\Psi_b(2)|\,V\,|\Psi_a(1)\Psi_b(2)\rangle-\langle\Psi_a(1)\Psi_b(2)|\,V\,|\Psi_a(2)\Psi_b(1)\rangle] \quad (1.9)
\end{aligned}$$

Therefore the expectation value of the Coulomb interaction between two electrons is:

For the Ψ_I state (in which the spatial part is symmetric and spin part is antisymmetric)

$$\begin{aligned}
\langle V\rangle &= V_d+J \qquad \text{for the spin singlet state}(S=0) \\
&= V_d+J(1-\mathbf{S}^2) \\
&= V_d+J(1-S(S+1)) \quad (1.10)
\end{aligned}$$

For the Ψ_{II} state,

$$\begin{aligned}
\langle V\rangle &= V_d-J \qquad \text{for the spin triplet state}(S=1) \\
&= V_d+J(1-\mathbf{S}^2) \\
&= V_d+J(1-S(S+1)) \quad (1.11)
\end{aligned}$$

Now consider the following operators,

$$\mathbf{S}=\hat{s_1}+\hat{s_2} \quad (1.12)$$

and

$$\mathbf{S}^2 = (\hat{s_1} + \hat{s_2})^2 \tag{1.13}$$

Using the identity,

$$(\hat{s_1} + \hat{s_2})^2 = \hat{s_1}^2 + \hat{s_2}^2 + 2\hat{s_1}.\hat{s_2}$$

On rearranging,

$$\begin{aligned} \hat{s_1}.\hat{s_2} &= \frac{1}{2}[(\hat{s_1} + \hat{s_2})^2 - \hat{s_1}^2 - \hat{s_2}^2] \\ &= \frac{1}{2}[\mathbf{S}^2 - \frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}(\frac{1}{2}+1)] \\ &= \frac{1}{2}[S(S+1) - (\frac{3}{2})] \end{aligned}$$

where we have used the eigenvalues of the operator $\mathbf{S}^2$ (i.e. $S(S+1)$) and operator $\hat{s_i}^2$ (i.e. $s(s+1)$ with $s = \frac{1}{2}$). Therefore, $S(S+1)$ can be expressed as

$$S(S+1) = 2\hat{s_1}.\hat{s_2} + \frac{3}{2} \tag{1.14}$$

Using this in equations (1.10) and (1.11)

$$\begin{aligned} \langle V \rangle &= V_d + J(1 - S(S+1)) \\ &= V_d - \frac{1}{2}J - 2J\hat{s_1}.\hat{s_2} \end{aligned} \tag{1.15}$$

Here, the third term on the RHS represents the contribution to the Coulombic interaction energy due to a pair of neighboring atoms (or ions). For a large number of atoms the total contribution to the interaction energy can be obtained by summing over all such pairs of electrons,

$$E = \text{constant term } - \sum_{<i,j>} (2J_{ij}\hat{s_i}.\hat{s_j}) \tag{1.16}$$

This interaction term can be thought of as the source of the Weiss internal field which gives rise to ferromagnetism.

1.2 Spin Waves

Consider the isotropic Heisenberg FM Hamiltonian. In the ground state all the spins are aligned along the same direction. Suppose that the system is in the following excited state: all the spins S (at each site) are aligned along the same direction except for one. This state is not the eigenstate of the Hamiltonian. The eigenstate of the system is the one in which this single spin deviation is coherently distributed over the entire lattice, and is called a spin wave. Spin Waves are low energy excitations above the ground state in exchange coupled magnetic systems.

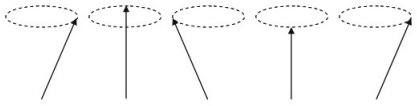

Figure 1.1: Spin waves on a linear ferromagnetic chain

1.2.1 A brief history of spin wave theory [1]

Spin wave theory provides a good description of ferromagnetic and antiferromagnetic substances at low temperatures. In 1930, Felix Bloch [4] invented the concept of a spin wave and formulated the spin wave theory. He was first to show that low-lying excitations of a ferromagnet would be of this nature. He also showed that at low temperatures, the thermodynamic properties of a ferromagnet obtained from this consideration were consistent with experimental results. It was assumed that the no. of of spin wave excitations (or the density of reversed spins) is small and thus the effects of interactions between spin-waves can be neglected. This assumption is good at sufficiently low temperatures and becomes less accurate as higher temperatures are considered. Under this approximation, Bloch's spin-wave theory becomes linear in spin wave amplitudes.

Later, in 1940, a new approach to spin-wave theory was introduced by Holstein and Primakoff[11]. As graduate students, Henry Primakoff and Ted Holstein were studying the low temperature field dependence of the intrinsic magnetization of a ferromagnet. They got the clever idea of expressing spin operators of the Heisenberg model in terms of bosonic creation and annihilation operators. In terms of these new operators, the Hamiltonian splits into two parts: one part is quadratic and the other is of higher

[1] From Ref.[6] and Ref.[15]

order in these operators. The higher order terms of the Hamiltonian represent the effect of interactions between spin waves and are usually called dynamical interaction terms. Considering only the quadratic part of the Hamiltonian gives a theory of non-interacting spin-waves. With some suitable approximations, they could diagonlize the Hamiltonian. Their approximations turned out to be equivalent to those used by F. Bloch who originally proposed the concept of spin waves. Their approach is currently one of the most used approaches to spin wave theory.

1.2.2 Spin Wave Theory

In spin wave theory, the starting point is a classical assumption in which the spin operators are treated as classical vectors of length S. This classical assumption makes the Hamiltonian an energy functional that can be minimized to determine the ground state.[2] The quantum corrections to this classical ground state are then calculated. There are two ways to apply spin wave theory to ordered magnetic systems with non-collinear ground states. One method is to use a local rotating coordinate system for each site such that the local magnetization direction at each site is along the local z-axis (quantization direction) i.e. a rotating local coordinate system is used in which the quantization axis is chosen toward the spin directions. in the classical ground state. The second approach is to consider different types of bosons for different types of sites such that each type of boson has its own ground state corresponding to the local spin orientation. The Hamiltonian is then expressed in terms of bosonic operators using either Holstein-Primakoff transformations or Dyson-Maleev tranformations. It is then diagonalized, in linear spin wave approximation, with a combination of Fourier and Bogoliubov tranformations to obtain the dispersion relation for the spin waves. The diagonalized Hamiltonian can then be used to calculate different physical properties of interest.

1.3 Spin wave analysis of isotropic Heisenberg AFM using two boson approach[2]

1.3.1 Introduction

Consider the Heisenberg AFM model with nearest neighbour interactions.

$$H = \sum_{<i,j>} (J\vec{S}_i.\vec{S}_j) \tag{1.17}$$

Note that $J > 0$ for antiferromagnetic interaction.

1.3.2 Ground State of Heisenberg AFM

One crucial aspect of Heisenberg AFM is that the classical Néel state is not the quantum mechanical ground state. It can be demonstrated as follows:
The energy of the Néel state (in which two nearest neighbour spins point in opposite directions, $|S\rangle_i| - S\rangle_j$) can be calculated from the energy of the repeating nearest neighbours spins. Clearly, for two spins, the energy in this state is

$$E_{ij} = -JS^2. \tag{1.18}$$

Quantum mechanically, the energy of two nearest neighbour spins will be

$$E_{ij} = J\langle S_i.S_j\rangle$$

Now note that,

$$\langle(\hat{S}_i + \hat{S}_j)^2\rangle = \langle\hat{S}_i^2\rangle + \langle\hat{S}_j^2\rangle + 2\langle\hat{S}_i\hat{S}_j\rangle \tag{1.19}$$

$$\Rightarrow \langle\hat{S}_i.\hat{S}_j\rangle = \frac{1}{2}\langle(\hat{S}_i + \hat{S}_j)^2\rangle - \frac{1}{2}\langle\hat{S}_i^2\rangle - \frac{1}{2}\langle\hat{S}_J^2\rangle = \frac{1}{2}\langle(\hat{S}_i + \hat{S}_j)^2\rangle - S(S+1)$$

Therefore, the energy of the bond is:

$$E_{ij} = -JS(S+1) + \frac{J}{2}\langle(\hat{S}_i + \hat{S}_j)^2\rangle$$

[2]Ref.[7]

This is minimum when the spins form a singlet pair, i.e. $(\hat{S}_i + \hat{S}_j) = 0$ and consequently the minimum energy should be

$$E_{min} = -JS(S+1) \tag{1.20}$$

This is less than than the energy in (1.18) (by JS). Néel state, therefore, does not have the lowest energy, i.e. antiparallel spin orientations do not have the lowest energy.

Further, $|S\rangle_i|-S\rangle_j$ can not be the ground state because it is not an eigenstate of the Hamiltonian.

1.3.3 Linear Spin wave analysis

The classical picture of an antiferromagnet is the Néel state, in which the lattice is bipartite. This means that all the lattice points can be categorised into one of the two groups or sublattices(say A and B), such that there are no interactions between spins in the same sublattice and all the antiferromagnetic interactions are between spins one from each A and B.
Spin wave theory is based on the notion that continuation from classical spins to quantum spins is possible. It is expected that the two-sublattice structure persists even in presence of quantum fluctuations.

The Hamiltonian is

$$H = \sum_{<i,j>} (J\vec{S}_i.\vec{S}_j)$$

Writing in terms of spin projection operators,

$$H = J \sum_{<i,j>} [S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z]$$

The Hamiltonian can be written in terms of spin raising and lowering operators which are defined as :

$$S^+ = S^x + iS^y$$

$$S^- = S^x - iS^y$$

Then

$$\begin{aligned} H &= J \sum_{<i,j>} [(\frac{1}{2})^2 (S_i^+ + S_i^-)(S_j^+ + S_j^-) + (\frac{-i}{2})^2 (S_i^+ - S_i^-)(S_j^+ - S_j^-) + S_i^z S_j^z] \\ &= J \sum_{<i,j>} [(\frac{1}{2})\{S_i^+ S_j^- + S_i^- S_j^+\} + S_i^z S_j^z] \end{aligned} \tag{1.21}$$

Holstein-Primakoff Transformation

Holstein-Primakoff transformations transcribe the spin operators in terms of bosonic quasi-particle operators. The main idea is that quantum fluctuations (or spin-deviations from the classical orientation) can be expressed as bosonic quasiparticles (called magnons). Holstein-Primakoff Transformation equations are:

$$S_i^- = \sqrt{2S}\sqrt{(1 - \frac{a_i^\dagger a_i}{2S})}\, a_i^\dagger \tag{1.22}$$

which under the approximation that number density of magnons is small reduces to

$$S_i^- = \sqrt{2S} a_i^\dagger \tag{1.23}$$

i.e. decreasing the eigenvalue of S^z operator for a spin corresponds to creating a boson (called magnon). Further,

$$S_i^+ = \sqrt{2S}\sqrt{(1 - \frac{a_i^\dagger a_i}{2S})}\, a_i \tag{1.24}$$

can be aproximated as

$$S_i^+ = \sqrt{2S} a_i \tag{1.25}$$

i.e. increasing the eigenvalue of S^z operator for a spin corresponds to annihilating a boson.

$$S_i^z = S - a^\dagger a_i \tag{1.26}$$

states that the total number of magnons at a site is equal to the total number of spin deviations at that site.

Two types of bosons

In case of AFM, we need to introduce two types of bosonic operators for the two kinds of spin deviations. First, consider sublattice A. On sublattice A, in classical

orientation, spins are pointing 'up' and lowering of eigenvalue of S_z operator (S^-) corresponds to creation ($a^\dagger$) of a magnon and vice versa (as in case of above transformations).
On the other hand, on sublattice B, in classical configuration, spins are pointing 'down' and increasing of eigenvalue of S_z operator (S^+) corresponds to creation ($b^\dagger$) of a magnon. Therefore,
for sublattice A,

$$\begin{aligned} S_i^- &= \sqrt{2S} a_i^\dagger \\ S_i^+ &= \sqrt{2S} a_i \\ S_i^z &= S - a^\dagger a_i \end{aligned} \tag{1.27}$$

and for sublattice B,

$$\begin{aligned} S_j^- &= \sqrt{2S} b_j \\ S_j^+ &= \sqrt{2S} b_j^\dagger \\ S_j^z &= -S + b_j^\dagger b_j \end{aligned} \tag{1.28}$$

These transformations can be substituted in (1.21) to obtain

$$\begin{aligned} H &= J \sum_{<i,j>} [\frac{1}{2}(2S)\{a_i b_j + a_i^\dagger b_j^\dagger\} + (S - a_i^\dagger a_i)(-S + b_j^\dagger b_j)] \\ &= J \sum_{<i,j>} [-S^2] + J \sum_{<i,j>} [S(a_i b_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i) - a_i^\dagger a_i b_j^\dagger b_j] \\ &= \frac{-JNzS^2}{2} + J \sum_{<i,j>} [S(a_i b_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i) - \text{higher order term(s)}] \end{aligned} \tag{1.29}$$

Note that the Hamiltonian consists of two parts: quadratic part and higher order part. The quadratic part gives the theory of non-interacting spin waves. The higher order part corresponds to theory of interacting spin waves.
Linear spin wave approximation involves neglecting terms of order higher than 2 so that the resultant Hamiltonian describes non-interacting spin waves.

$$H_1 = \frac{-JNzS^2}{2} + J \sum_{<i,j>} [S(a_i b_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i)] \tag{1.30}$$

Fourier Transformation: k-space operators We will use the transformed operators c_k, $c_k^\dagger$, d_k, $d_k^\dagger$. Hamiltonian can be expressed in terms of these operators using

the following transformations:

$$a_i = \sqrt{\frac{2}{N}} \sum_k e^{-i\vec{k}.\vec{r_i}} c_k \tag{1.31}$$

$$a_i^\dagger = \sqrt{\frac{2}{N}} \sum_k e^{i\vec{k}.\vec{r_i}} c_k^\dagger \tag{1.32}$$

$$b_j = \sqrt{\frac{2}{N}} \sum_k e^{-i\vec{k}.\vec{r_j}} d_k \tag{1.33}$$

$$b_j^\dagger = \sqrt{\frac{2}{N}} \sum_k e^{i\vec{k}.\vec{r_j}} d_k^\dagger \tag{1.34}$$

On substituting these operators in the Hamiltonian along with the identity

$$\sum_i e^{i(\vec{k}-\vec{k'}).\vec{r_i}} = N\delta_{kk'}$$

$$H_1 = \frac{-JNzS^2}{2} + JS \sum_k [\sum_{\vec{d}} (e^{i\vec{k}.\vec{d}} c_k d_{-k}) + \sum_{\vec{d}} (e^{-i\vec{k}.\vec{d}} c_k^\dagger d_{-k}^\dagger) + c_k^\dagger c_k) + d_k^\dagger d_k] \tag{1.35}$$

Let

$$\frac{1}{z} \sum_{\vec{d}} (e^{-i\vec{k}.\vec{d}}) = \gamma_k$$

where z is the number of nearest neighbour sites.

Bogoliubov Transformation: Diagonalizing a quadratic Hamiltonian

We introduce new operators α_k and β_k with Bogoliubov Valatin (BV) transformation to diagonalize the Hamiltonian.

$$c_k = (u_k)\alpha_k + (v_k)\beta_{-k}^\dagger \tag{1.36}$$

$$d_k = (u_k)\beta_k + (v_k)\alpha_{-k}^\dagger \tag{1.37}$$

$$c_k^\dagger = (u_k)\alpha_k^\dagger + (v_k)\beta_{-k} \tag{1.38}$$

$$d_k^\dagger = (u_k)\beta_k^\dagger + (v_k)\alpha_{-k} \tag{1.39}$$

The conditions that the coefficient of off-diagonal terms be equal to zero and the transformations should preserve the canonical commutation relations determine the

values of paramaters u_k and v_k. The second condition is obtained by making the coefficient of off-diagonal terms equal to zero. The diagonalized Hamiltonian can be easily obtained:

$$H_1 = \frac{-JzN}{2}S(S+1) + JzS\sum_k \left[\sqrt{1-{\gamma_k}^2}\{({\alpha_k}^\dagger\alpha_k + \frac{1}{2}) + ({\beta_k}^\dagger\beta_k + \frac{1}{2})\}\right] \quad (1.40)$$

The dispersion relation is then,

$$\omega_k = JzS\sqrt{1-{\gamma_k}^2} \quad (1.41)$$

It should be noted that ω_k (which represents the energy of bosons) is always positive. This means that the boson vacuum (of α_k and β_k bosons) is the ground state.

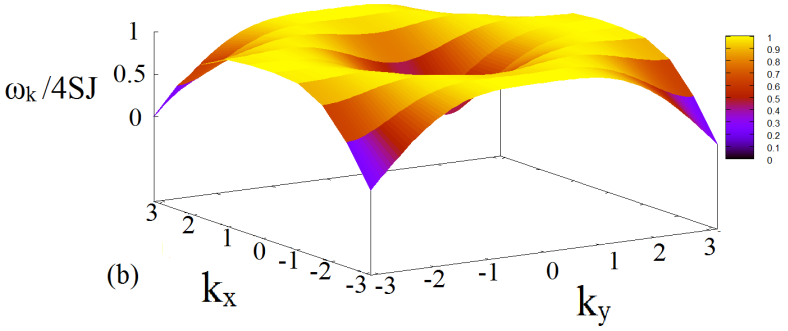

Figure 1.2: Linear spin-wave result Eq. (1.41) for the magnon spectrum of 2D quantum Heisenberg. antiferromagnet

1.4 Spin wave analysis of Heisenberg AFM using local rotating coordinate frame approach

1.4.1 Model

Again consider the Heisenberg AFM model with nearest neighbour interactions.

$$H = \sum_{<i,j>}(J\vec{S}_i.\vec{S}_j) \quad (1.42)$$

with $J > 0$ for antiferromagnetic interaction.

1.4.2 Linear Spin wave analysis

The classical picture of an antiferromagnet is the Néel state. The Hamiltonian is

$$H = \sum_{<i,j>} (J\vec{S}_i.\vec{S}_j)$$

Writing in terms of spin projection operators,

$$H = J \sum_{<i,j>} [S_i^x S_j^{x'} + S_i^y S_j^{y'} + S_i^z S_j^{z'}]$$

We will use a local rotated frame for sublattice B, with the following transformations:

$$\begin{aligned} S^{x'} &= S^x \\ S^{y'} &= -S^y \\ S^{z'} &= -S^z \end{aligned} \tag{1.43}$$

This allows us to a single boson representation for the two sublattices. The Hamiltonian can be written in terms of spin raising and lowering operators which are defined as :

$$S^+ = S^x + iS^y$$

$$S^- = S^x - iS^y$$

With the above transformations, the Hamiltonian can be rewritten as:

$$H = J \sum_{<i,j>} [(\frac{1}{2})\{S_i^+ S_j^+ + S_i^- S_j^-\} - S_i^z S_j^z] \tag{1.44}$$

Holstein-Primakoff Transformation

Holstein-Primakoff transformations (with 'small spin-wave density'approximation) are:

$$\begin{aligned} S_i^- &= \sqrt{2S} a_i^\dagger \\ S_i^+ &= \sqrt{2S} a_i \\ S_i^z &= S - a^\dagger a_i \end{aligned} \tag{1.45}$$

These transformations can be substituted in (1.44) to obtain

$$\begin{aligned} H &= J\sum_{<i,j>}[\frac{1}{2}(2S)\{a_i a_j + a_i^\dagger a_j^\dagger\} - (S - a_i^\dagger a_i)(S - a_j^\dagger a_j)] \\ &= \frac{-JNzS^2}{2} + J\sum_{<i,j>}[S(a_i a_j + a_i^\dagger a_j^\dagger + a_i^\dagger a_i + a_j^\dagger a_j) - \text{higher order term(s)}] \end{aligned} \tag{1.46}$$

Linear spin wave approximation involves neglecting terms which contain products of more than two bosonic operators,

$$H_1 = \frac{-JNzS^2}{2} + J\sum_{<i,j>}[S(a_i b_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i)] \tag{1.47}$$

Fourier Transformation: We will use the transformed operators c_k, $c_k^\dagger$ with the follwing transformations:

$$a_i = \sqrt{\frac{1}{N}}\sum_k e^{-i\vec{k}.\vec{r_i}} c_k \tag{1.48}$$

$$a_i^\dagger = \sqrt{\frac{1}{N}}\sum_k e^{i\vec{k}.\vec{r_i}} c_k^\dagger \tag{1.49}$$

On substituting these opearators in the Hamiltonian along with the identity

$$\sum_i e^{i(\vec{k}-\vec{k'}).\vec{r_i}} = N\delta_{kk'}$$

we obtain,

$$H_1 = \frac{-JNzS^2}{2} + 4JS\sum_k[(\gamma_k c_k c_{-k}) + (\gamma_k c_k^\dagger c_{-k}^\dagger) + c_k^\dagger c_k + c_k^\dagger c_k] \tag{1.50}$$

where

$$\gamma_k = \frac{1}{z}\sum_{\vec{d}}(e^{-i\vec{k}.\vec{d}})$$

with z (= 4 for 2D lattice) being the number of nearest neighbour sites.

Bogoliubov Transformation: Diagonalizing a quadratic Hamiltonian

We introduce new operators α_k and β_k with Bogoliubov-Valatin (BV) transformation to diagonalize the Hamiltonian.

$$c_k = (u_k)\alpha_{-k} - (v_k)\alpha_k^\dagger \tag{1.51}$$
$$c_{-k} = (u_k)\alpha_k - (v_k)\alpha_{-k}^\dagger \tag{1.52}$$
$$c_k^\dagger = (u_k)\alpha_{-k}^\dagger - (v_k)\alpha_k \tag{1.53}$$
$$c_{-k}^\dagger = (u_k)\alpha_k^\dagger - (v_k)\alpha_{-k} \tag{1.54}$$

The conditions that the coefficient of off-diagonal terms be equal to zero and the transformations should preserve the canonical commutation relations determine the values of paramaters u_k and v_k. The second condition is obtained by making the coefficient of off-diagonal terms equal to zero.

$$\begin{aligned} H_1 = \frac{-JNzS^2}{2} &+ zJS\sum_k[({u_k}^2\gamma_k + {v_k}^2\gamma_k - 2u_kv_k)(\alpha_{-k}^\dagger\alpha_k^\dagger + \alpha_{-k}\alpha_k)] \\ &+ zJS\sum_k[({u_k}^2 + {v_k}^2 - 2u_kv_k\gamma_k)(\alpha_{-k}^\dagger\alpha_{-k} + \alpha_k^\dagger\alpha_k)] \\ &+ zJS\sum_k[2{v_k}^2 - 2\gamma_k u_k v_k)] \end{aligned} \tag{1.55}$$

For the Hamiltonian to be diagonal,

$${u_k}^2\gamma_k + {v_k}^2\gamma_k - 2u_kv_k = 0 \tag{1.56}$$

i.e. the coefficient of off-diagonal terms should be equal to zero. Further, the 'new'operators should obey the bosonic canonical commutation relations. This implies,

$${u_k}^2 - {v_k}^2 = 0 \tag{1.57}$$

Combining the two conditions in eqn.(1.56) and eqn.(1.56), one can easily find that,

$$\begin{aligned} u_k &= \left[\frac{1}{2}\left(\frac{1}{\sqrt{1-{\gamma_k}^2}}+1\right)\right]^{\frac{1}{2}} \\ v_k &= \left[\frac{1}{2}\left(\frac{1}{\sqrt{1-{\gamma_k}^2}}-1\right)\right]^{\frac{1}{2}} \end{aligned} \tag{1.58}$$

The diagonalized Hamiltonian can then be easily obtained:

$$H_1 = \frac{-JzN}{2}S(S+1) + zJS\sum_k \left[\sqrt{1-{\gamma_k}^2}\{\alpha_k^\dagger\alpha_k + \alpha_{-k}^\dagger\alpha_{-k} + 1\}\right] \tag{1.59}$$

The dispersion relation is then,

$$\omega_k = JzS\sqrt{1-{\gamma_k}^2} \tag{1.60}$$

These are the same results as obtained with the two boson approach in the previous section.

Chapter 2

Application of SWT to an AF-DM-field model

2.1 AF-DM-field model

We study the spin-S antiferromagnetic Heisenberg model with nearest-neighbor interactions on a square lattice with the DM interaction in an external magnetic field following Ref.[12].

$$H = \sum_{<i,j>} (J\vec{S}_i.\vec{S}_j + \vec{D}.(\vec{S}_i \times \vec{S}_j)) - \sum_i \vec{H}.\vec{S}_i \tag{2.1}$$

where, $\sum_{<i,j>}$ denotes summation over nearest neighbour pairs of spins on the lattice. This Hamiltonian is written as a sum of three terms:

$$H = H_0 + H_{DM} + H_H \tag{2.2}$$

The different terms in the above Hamiltonian are:

Heisenberg Exchange (H_0): Exchange interaction is bilinear in spins and has a scalar product form. It is isotropic under rotations and is represented by J times $\vec{S}_i.\vec{S}_j$, the scalar product of classical spin angular momentum vectors, with i, j denoting the indices of two nearest neighbour spins and represents the Heisenberg exchange energy. The coefficient J denotes the exchange coupling constant. A negative J means parallel orientation of neighboring spins will be favored and results in ferromagnetic order while a positive J means antiparallel orientation of neighboring spins will be favored

and results in antiferromagnetic order.

Dzyaloshinskii-Moriya interaction (H_{DM}): Antisymmetric exchange or Dzyaloshinskii-Moriya interaction [8, 9, 10] is represented by $\vec{D}.(\vec{S_i} \times \vec{S_j})$, the cross product of classical spin angular momentum vectors, with i, j denoting the indices of two nearest neighbour spins.
$\vec{D}$ is called the DM vector. The direction of DM vector is fixed by the microscopic arrangement of atoms and orbitals. In the following analysis, we have assumed the direction of DM vector to be along $\hat{z}$ with a constant magnitude.

Magnetic feld coupling (H_H): An external magnetic field $\vec{H}$ couples as [17]

$$H_H = -\vec{H}.\sum_i g_i \mu_B \vec{S_i} \tag{2.3}$$

It is convenient to rewrite H_H as

$$H_H = -\vec{H}.\sum_i \vec{S_i} \tag{2.4}$$

absorbing $g_i \mu_B$ into the magnetic field H, so that the field $\vec{H}$ has the units of energy.

2.2 Finding the classical ground state

The model Hamiltonian (1) consists of three terms:

- Heisenberg term
- DM term
- Magnetic field coupling

The effect of Heisenberg term alone is that the nearest neighbor spins tend to align antiparallel to each other and thus tend to produce antiferromagnetic order. Therefore, in the presence of Heisenberg term alone, the ground state would look like in Fig. 2.1,

The DM interaction energy is minimized when nearest neighbor spins stay in plane perpendicular to $\vec{D}$ and make 90 degrees angle with each other. Therefore, in the presence of DM term alone, the ground state would look like in Fig.2.2, The additional

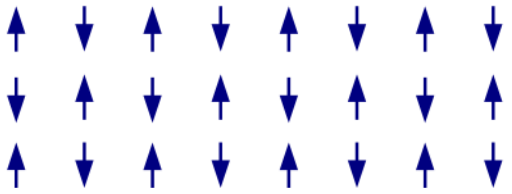

Figure 2.1: Classical spin pattern that corresponds to lowest total energy for Heisenberg term alone ($D = 0$ and $H = 0$). All global rotations of this pattern will also lead to the same total energy.

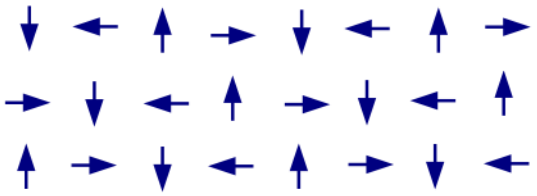

Figure 2.2: Classical spin configuration that minimizes the total energy for Dzyaloshinskii-Moriya interacting term ($J = 0$ and $H = 0$). Nearest neighbour spins are mutually perpendicular and lie in plane perpendicular to DM vector.

effect of DM interaction to pure AFM Heisenberg Hamiltonian would be to make previously antiparallel nearest neighbor spins cant toward each other so that the angle α between any two nearest neighbor spins is such that:

$$\frac{\pi}{2} < \alpha < \pi \tag{2.5}$$

where the limiting angles $\alpha = \frac{\pi}{2}$ and $\alpha = \pi$ are obtained when $J = 0$ and $D = 0$ respectively. In presence of both Heisenberg term and DM term, the classical ground state would look like in Fig. 2.3

If an external magnetic field is applied to the system, then all the spins will tend to orient maximally toward the magnetic field direction under the constraint due to the other two terms. As a result, the above configuration will make a global rotation toward the direction of external magnetic field, and the angle between any two nearest neighbor spins will decrease depending on the strength of the applied magnetic field.

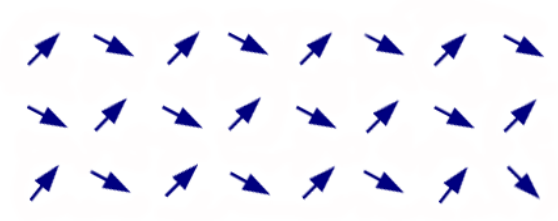

Figure 2.3: In the presence of both exchange interaction ($J \neq 0$) and Dzyaloshinskii-Moriya interaction ($\vec{D} \neq 0$), the nearest neighbour spins cant toward each other. The canting angle is determined by the strength of applied magnetic field.

2.3 Application of Spin Wave Theory to this model

The Hamiltonian is:

$$H = \sum_{<i,j>} (J\vec{S}_i.\vec{S}_j + \vec{D}.(\vec{S}_i \times \vec{S}_j)) - \sum_i \vec{H}.\vec{S}_i \tag{2.6}$$

It can be rewritten in terms of spin projection operators S_x, S_y, S_z so that:

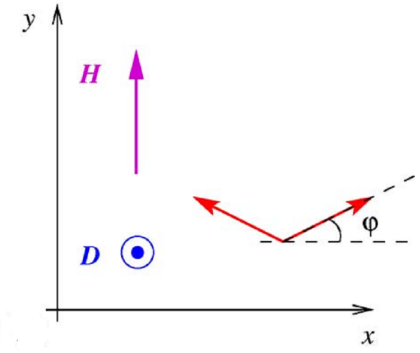

Figure 2.4: Spin configuration that minimizes the classical energy for AFM-DM-field model.(Figure from Ref. [12])

$$H = J \sum_{<i,j>} [S_i^x.S_j^x + S_i^y.S_j^y + S_i^z.S_j^z] + D \sum_{<i,j>} [(S_i^x S_j^y - S_i^y S_j^x)] - \sum_i \vec{H}.\vec{S}_i \tag{2.7}$$

2.3.1 Transformation from lab frame to rotating frame

- We want to choose quantization axes (z-axis) for spins along their classical GS directions.
- Every spin on the lattice does not have the same orientation.

- There are 2 possible orientations.
- Therefore, we need to choose a rotating coordinate frame such that at every lattice site, the quantization axis (z-axis) points along the local spin direction.
- This allows us to use a single boson operator.

Effectively, there are two sublattices: A and B (say).
To get the required ground state spin orientations:
Spin Rotation Operators:
If (x, y, z) are the axes of the original frame and (x_0, y_0, z_0) are the axes of the rotated coordinate frame, then we get the following transformation equations:

- ***For sublattice A:***
  $S_i^x = -S_i^{x_0}(sin(\phi)) + S_i^{z_0}(cos(\phi))$
  $S_i^y = S_i^{z_0}(sin(\phi)) + S_i^{x_0}(cos(\phi))$
  $S_i^z = S_i^{y_0}$

- ***For sublattice B:***
  $S_j^x = -S_j^{x_0}(sin(\phi)) - S_j^{z_0}(cos(\phi))$
  $S_j^y = S_j^{z_0}(sin(\phi)) - S_j^{x_0}(cos(\phi))$
  $S_j^z = S_j^{y_0}$

The Hamiltonian (in the original coordinate frame) is:

$$H = \sum_{<i,j>} [J\{S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z\}] - \sum_{<i,j>} [D\{S_i^x S_j^y - S_i^y S_j^x\}] + \sum_i [\vec{H}.\vec{S}]$$

On writing original frame projection operators S^x, S^y, S^z in terms of rotated frame projection operators $S^{x_0}, S^{y_0}, S^{z_0}$, we get:

$$\begin{aligned}
H = J \sum_{<i,j>} & [\{-S_i^{x_0}(\sin\phi) + S_i^{z_0}(\cos\phi)\}.\{-S_j^{x_0}(\sin\phi) - S_j^{z_0}(\cos\phi)\} \\
& +\{S_i^{z_0}(\sin\phi) + S_i^{x_0}(\cos\phi)\}.\{S_j^{z_0}(\sin\phi) - S_j^{x_0}(\cos\phi)\} + S_i^{y_0} S_j^{y_0}] \\
+D \sum_{<i,j>} & [\{-S_i^{x_0}(\sin\phi) + S_i^{z_0}(\cos\phi)\}.\{S_j^{z_0}(sin(\phi)) - S_j^{x_0}(cos(\phi))\} \\
& +\{S_i^{z_0}(sin(\phi)) + S_i^{x_0}(cos(\phi))\}.\{S_j^{z_0}(-S_j^{x_0}(sin(\phi)) - S_j^{z_0}(cos(\phi))\} \\
& -\sum_i \vec{H}.\vec{S}_i
\end{aligned}$$

Expanding the products,

$$\begin{aligned}
H = J \sum_{<i,j>} & [\{S_i^{x_0} S_j^{x_0}(\sin^2\phi) + S_i^{x_0} S_j^{z_0}(\sin\phi\cos\phi) - S_i^{z_0} S_j^{x_0}(\cos\phi\sin\phi) - S_i^{z_0} S_j^{z_0}(\cos^2\phi)\} \\
& +\{S_i^{z_0} S_j^{z_0}(\sin^2\phi) - S_i^{z_0} S_j^{x_0}(\sin\phi\cos\phi) + S_i^{x_0} S_j^{z_0}(\cos\phi\sin\phi) - S_i^{x_0} S_j^{x_0}(\cos^2\phi)\} \\
& +S_i^{y_0} S_j^{y_0}] \\
+D \sum_{<i,j>} & [\{-S_i^{x_0} S_j^{z_0}(\sin^2\phi) + S_i^{x_0} S_j^{x_0}(\sin\phi\cos\phi) + S_i^{z_0} S_j^{z_0}(\cos\phi\sin\phi) - S_i^{z_0} S_j^{x_0}(\cos^2\phi)\} \\
& -\{-S_i^{z_0} S_j^{x_0}(\sin^2\phi) - S_i^{z_0} S_j^{z_0}(\sin\phi\cos\phi) - S_i^{x_0} S_j^{x_0}(\cos\phi\sin\phi) - S_i^{x_0} S_j^{z_0}(\cos^2\phi)\} \\
& -\sum_i \{\vec{H}.\vec{S}_i\}
\end{aligned}$$

Collecting the terms with same spin operators,

$$\begin{aligned}
H = J \sum_{<i,j>} & [\{S_i^{x_0} S_j^{x_0}(\sin^2\phi - \cos^2\phi) + S_i^{x_0} S_j^{z_0}(2\sin\phi\cos\phi) - S_i^{z_0} S_j^{x_0}(2\cos\phi\sin\phi) \\
& -S_i^{z_0} S_j^{z_0}(\cos^2\phi - \sin^2\phi)\} + S_i^{y_0} S_j^{y_0}] \\
+D \sum_{<i,j>} & [\{-S_i^{x_0} S_j^{z_0}(\sin^2\phi - \cos^2\phi) + S_i^{x_0} S_j^{x_0}(2\sin\phi\cos\phi) + S_i^{z_0} S_j^{z_0}(2\cos\phi\sin\phi) \\
& -S_i^{z_0} S_j^{x_0}(\cos^2\phi - \sin^2\phi)\} \\
& -\sum_i \{\vec{H}.\vec{S}_i\}
\end{aligned}$$

The above expression is equivalent to,

$$H = J \sum_{<i,j>} [\{-S_i^{x_0} S_j^{x_0} (\cos 2\phi) + S_i^{x_0} S_j^{z_0} (\sin 2\phi) - S_i^{z_0} S_j^{x_0} (\sin 2\phi) - S_i^{z_0} S_j^{z_0} (\cos 2\phi)\} + S_i^{y_0} S_j^{y_0}]$$
$$+D \sum_{<i,j>} [S_i^{x_0} S_j^{z_0} (\cos 2\phi) + S_i^{x_0} S_j^{x_0} (\sin 2\phi) + S_i^{z_0} S_j^{z_0} (\sin 2\phi) - S_i^{z_0} S_j^{x_0} (\cos 2\phi)]$$
$$- \sum_i \{\vec{H}.\vec{S}_i\}$$

2.3.2 Using Spin raising and lowering operators

Now, spin projection operators can be written in terms of spin raising S^+ and lowering S^- operators,

Spin raising and lowering operators are defined as :

$S^+ = S^x + iS^y$

$S^- = S^x - iS^y$

Using these to write,

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

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

The Hamiltonian can now be written in the following form:

$$H = J \sum_{<i,j>} [-\{(\frac{1}{2})^2 (S_i^+ + S_i^-)(S_j^+ + S_j^-)(\cos 2\phi)\}$$
$$+\{\frac{1}{2}(S_i^+ + S_i^-) S_j^z (\sin 2\phi)\} - \{S_j^z (\frac{1}{2})(S_j^+ + S_j^-)\}(\sin 2\phi)\}$$
$$-\{S_i^z S_j^z (\cos 2\phi)\} + (\frac{-i}{2})^2 (S_i^+ - S_i^-)(S_j^+ + S_j^-)]$$
$$+D \sum_{<i,j>} [\{(\frac{1}{2})(S_i^+ + S_i^-)(S_j^z)(\cos 2\phi)\} + \{(\frac{1^2}{2})(S_i^+ + S_i^-)(S_j^+ + S_j^-)(\sin 2\phi)\}$$
$$+\{S_i^z S_j^z (\sin 2\phi)\} - \{S_i^z (\frac{1}{2})(S_j^+ + S_j^-)(\cos 2\phi)\}] - \sum_i [\vec{H}.\vec{S}_i]$$

$$\Rightarrow H = J\sum_{<i,j>}[-\frac{1}{4}\{S_i^+S_j^+ + S_i^+S_j^- + S_i^-S_j^+ + S_i^-S_j^-\}(\cos 2\phi)$$
$$+\frac{1}{2}\{(S_i^+ + S_i^-)(S_j^z)\}(\sin 2\phi) - \frac{1}{2}(S_i^z)(S_j^+ + S_j^-)(\sin 2\phi)$$
$$-S_i^zS_j^z(\cos 2\phi) - \frac{1}{4}\{S_i^+S_j^+ - S_i^+S_j^- - S_i^-S_j^+ + S_i^-S_j^-\}]$$
$$+D\sum_{<i,j>}[\{\frac{1}{2}\{(S_i^+ + S_i^-)(S_j^z)\}(\cos 2\phi)\} + \frac{1}{4}\{S_i^+S_j^+ + S_i^+S_j^- + S_i^-S_j^+ + S_i^-S_j^-\}(\sin 2\phi)$$
$$+S_i^zS_j^z(\sin 2\phi) - \frac{1}{2}(S_i^z)(S_j^+ + S_j^-)(\cos 2\phi)] - \sum_i[\vec{H}.\vec{S}_i]$$

2.3.3 Holstein-Primakoff Transformation

Holstein-Primakoff Transformation Holstein-Primakoff Transformation equations are:

$$S_i^- = \sqrt{2S}a_i^\dagger \tag{2.8}$$

$$S_i^+ = \sqrt{2S}a_i \tag{2.9}$$

$$S_i^z = S - a^\dagger a_i \tag{2.10}$$

Application of H-P tranformations equation gives us the following expression for Hamiltonian:

$$H = J\sum_{<i,j>}[\frac{-1}{4}\{(2S)a_ia_j + (2S)a_ia_j^\dagger + (2S)a_i^\dagger a_j + (2S)a_i^\dagger a_j^\dagger\}(\cos 2\phi)$$
$$+\frac{1}{2}\{(\sqrt{2S})(a_i + a_i^\dagger)(S - a_j^\dagger a_j)\}((\sin 2\phi)) - (\frac{1}{2})\{(S - a_i^\dagger a_i)\sqrt{2S}(a_j + a_j^\dagger)\}$$
$$-\{(S - a_i^\dagger a_i)(S - a_j^\dagger a_j)(\cos 2\phi) - \frac{1}{4}\{(2S)a_ia_j - (2S)a_ia_j^\dagger - (2S)a_i^\dagger a_j + (2S)a_i^\dagger a_j^\dagger\}]$$
$$+D\sum_{<i,j>}[\frac{1}{2}(\cos 2\phi)\{(\sqrt{2S})(a_i + a_i^\dagger)(S - a_j^\dagger a_j)\}$$
$$+\frac{1}{4}(\sin 2\phi)\{(2S)a_ia_j + (2S)a_ia_j^\dagger + (2S)a_i^\dagger a_j + (2S)a_i^\dagger a_j^\dagger\}$$
$$+\{(\sin 2\phi)(S - a_i^\dagger a_i)(S - a_j^\dagger a_j)\} - (\frac{1}{2})(\cos 2\phi)\{(S - a_i^\dagger a_i)\sqrt{2S}(a_j + a_j^\dagger)\}]$$
$$-\sum_i[\vec{H}.\vec{S}_i]$$

This gives,

$$H = J\sum_{<i,j>}[\frac{-S}{2}\{a_ia_j + a_ia_j^\dagger + a_i^\dagger a_j + a_i^\dagger a_j^\dagger\}(\cos 2\phi) + \frac{2S}{\sqrt{2}}\{Sa_i - a_ia_j^\dagger a_j + Sa_i^\dagger - a_i^\dagger a_i a_j^\dagger\}(\sin 2\phi)$$
$$-\frac{S}{\sqrt{2}}\{Sa_j + Sa_j^\dagger - a_i^\dagger a_i a_j - a_i^\dagger a_i a_j^\dagger\}(\sin 2\phi) - \{S^2 - Sa_j^\dagger a_j - Sa_i^\dagger a_i + a_i^\dagger a_i a_j^\dagger a_j\}(\cos 2\phi)$$
$$-\frac{S}{2}\{a_ia_j - a_ia_j^\dagger - a_i^\dagger a_j + a_i^\dagger a_j^\dagger\}$$
$$+D\sum_{<i,j>}[\frac{S}{\sqrt{2}}\{Sa_i - a_ia_j^\dagger a_j + Sa_i^\dagger - a_i^\dagger a_j^\dagger a_j\}(\cos 2\phi) + \frac{S}{2}\{a_ia_j + a_ia_j^\dagger + a_i^\dagger a_j + a_i^\dagger a_j^\dagger\}(\sin 2\phi)$$
$$+\{S^2 - Sa_j^\dagger a_j - Sa_i^\dagger a_i + a_i^\dagger a_i a_j^\dagger a_j\}(\sin 2\phi) - \frac{2S}{\sqrt{2}}\{Sa_j + Sa_j^\dagger - a_i^\dagger a_i a_j - a_i^\dagger a_i a_j^\dagger\}(\cos 2\phi)$$
$$-\vec{H}.\sum_i \vec{S}_i$$

Taking the linear spin wave approximation, i.e. neglecting the terms of order 3 or higher in boson operators,

$$H = J\sum_{<i,j>}[\frac{-1}{4}(2S)\{a_ia_j + a_ia_j^\dagger + a_i^\dagger a_j + a_i^\dagger a_j^\dagger\}(\cos 2\phi)$$
$$+\frac{1}{2}\sqrt{2S}\{Sa_i + Sa_i^\dagger\}(\sin 2\phi) - \frac{1}{2}\sqrt{2S}\{Sa_j + Sa_j^\dagger\}(\sin 2\phi)$$
$$-\{S^2 - Sa_j^\dagger a_j - Sa_i^\dagger a_i\}(\cos 2\phi) - \frac{1}{4}(2S)\{a_ia_j - a_ia_j^\dagger - a_i^\dagger a_j + a_i^\dagger a_j^\dagger\}$$
$$+D\sum_{<i,j>}[\frac{1}{2}\sqrt{2S}\{Sa_i + Sa_i^\dagger\}(\cos 2\phi) + \frac{1}{4}(2S)\{a_ia_j + a_ia_j^\dagger + a_i^\dagger a_j + a_i^\dagger a_j^\dagger\}(\sin 2\phi)$$
$$+\{S^2 - Sa_j^\dagger a_j - Sa_i^\dagger a_i\}(\sin 2\phi) - \frac{1}{2}\sqrt{2S}\{Sa_j + Sa_j^\dagger -\}(\cos 2\phi)$$
$$-\vec{H}.\sum_i \vec{S}_i$$

2.3.4 Fourier Transformation

The Fourier transformed operators are defined as:

$$a_i = \frac{1}{\sqrt{N}}\sum_k e^{-i\vec{q}.\vec{r}_i}a_k \tag{2.11}$$

$$a_i^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{i\vec{q}.\vec{r}_i}a_k^\dagger$$

Using these operators in the above Hamiltonian along with the identity

$$\sum_i e^{i(\vec{k}-\vec{k'}).\vec{r_i}} = N\delta_{kk'}$$

gives the Hamiltonian in the k-space

$$\begin{aligned} H = 4S\sum_k[(a_k a_{-k} + a_k^\dagger a_{-k}^\dagger)(\gamma_k \frac{C_3}{2}) + (a_k^\dagger a_k)(C_2\gamma_k + C_1)] \\ -J(2NS^2)(\cos 2\phi) + D(2NS^2)(\sin 2\phi) - \sum_i HS_i \sin\phi \end{aligned} \tag{2.12}$$

where $\gamma_k = \frac{\cos k_x + \cos k_y}{2}$.
Hamiltonian constitutes of two terms:

$$H = E_{cl} + H_{LSWT} \tag{2.13}$$

where,

$$H_{LSWT} = 4S\sum_k[(a_k a_{-k} + a_k^\dagger a_{-k}^\dagger)(\gamma_k \frac{C_3}{2}) + (a_k^\dagger a_k)(C_2\gamma_k + C_1)] \tag{2.14}$$

$$E_{cl} = -J(2NS^2)(\cos 2\phi) + D(2NS^2)(\sin 2\phi) - \sum_i HS_i \sin\phi \tag{2.15}$$

E_{cl} is exactly the classical energy which is obtained by substituting classical spin angular momentum vectors $\vec{S}$ in the original Hamiltonian model expression.

$$C_1 = J(\cos 2\phi) - D(\sin 2\phi)$$

$$C_2 = \frac{J}{2}(-\cos 2\phi + 1) + \frac{D}{2}(\sin 2\phi)$$

$$C_3 = \frac{J}{2}(-\cos 2\phi - 1) + \frac{D}{2}(\sin 2\phi)$$

2.3.5 Diagonalizing the Hamiltonian: Bogoliubov tranformation

A Hamiltonian expressed as:

$$H = f()a_k^\dagger a_k$$

is diagonalized. The Hamiltonian H_{LSWT} above contains terms in which there are products of the form $a_k a_k$ and $a_k^\dagger a_k^\dagger$. It is not in diagonal form and can be diagonalized by using Bogoliubov transformation.

Bogoliubov Valatin (B-V) Transformation: A linear transformation to diagonalize the quantum quadratic Hamiltonian in creation and annihilation operators. This tranformation defines new bosonic operators in terms of variable parameters.The value of these parameters can be found so that when the Hamiltonian is expressed in terms of these new bosonic operators, it becomes diagonal.

We use the following tranformation:

$$a_k = \{(cosh\theta_k)\alpha_{-k} - (sinh\theta_k)\alpha_k^\dagger\} \tag{2.16}$$

$$a_{-k} = \{(cosh\theta_k)\alpha_k - (sinh\theta_k)\alpha_{-k}^\dagger\} \tag{2.17}$$

$$a_k^\dagger = \{(cosh\theta_k)\alpha_{-k}^\dagger - (sinh\theta_k)\alpha_k\} \tag{2.18}$$

$$a_{-k}^\dagger = \{(cosh\theta_k)\alpha_k^\dagger - (sinh\theta_k)\alpha_{-k}\} \tag{2.19}$$

where the coefficients are determined by two conditions:

- Transformations should preserve canonical commutation relations , and
- Hamiltonian should be diagonal in terms of 'new'operators.

Now, these transformations can be used in the Hamiltonian. We collect the coefficients of terms containing products of two creation and two annihilation operators $\alpha_k^\dagger \alpha_{-k}^\dagger$ and $\alpha_k \alpha_{-k}$ and use the condition that,

$$\text{coefficients of } \alpha_k^\dagger \alpha_{-k}^\dagger \text{ and } \alpha_k \alpha_{-k} = 0 \tag{2.20}$$

We get the following resultant equation:

$$\{-(C_2\gamma_k + C_1)(A_k B_k) + (\gamma_k \frac{C_3}{2})(A_k^2 + B_k^2)\} = 0 \tag{2.21}$$

where, $A_k = (cosh\theta_k)$ and $B_k = (sinh\theta_k)$.

This condition can be used to find the values of parameters A_k andB_k such that the Hamiltonian when expressed in terms of the new bosonic operators is diagonalized.

The diagonalized Hamiltonian is finally found to be:

$$H_{LSWT} = \delta E + \sum_k (\omega_k \alpha_k^\dagger \alpha_k) \tag{2.22}$$

where,

$$\delta E = \frac{1}{2}\sum_{k}(\omega_k - 4SC_1) \tag{2.23}$$

The expression for ω_k gives the dispersion relation,

$$\omega_k = 4S\sqrt{(C_1 + C_2\gamma_k)^2 - (C_3\gamma_k)^2} \tag{2.24}$$

2.4 Results and Discussion

2.4.1 Spontaneously Broken Symmetry and Goldstone modes[1]

A pure isotropic Heisenberg Hamiltonian is invariant under rotation, making the ensemble averages of magnetization equal to zero. But, we know that magnets possess a non-zero magnetization and therefore this ensemble average does not represent a physically correct picture. Even though the Hamiltonian exhibits rotational symmetry, this symmetry is spontaneously broken by the ground state. In the ground state the system acquires a specific configuration, which no longer has the symmetry present in the Hamiltonian. There are infinite number of possible degenerate ground states, which in totality can recover the symmetry. But once the spins are in a particular configuration, the system can not make transition from one such ground state to another becuase all the spins would have to rotate spontaneously by the same amount in the same direction, for which the probability is almost zero. The symmetry is restored by the wave-like excited states in the sense that (local) ground states vary over space. These are the Goldstone excitations.

2.4.2 Zero anisotropic exchange case ($\vec{D} = 0$)

If the DM-term in Hamiltonian (with staggered DM vector) is neglected and $J = 1$ is assumed, the following expression for the spin-wave spectrum can be calculated [12]:

$$\omega_k^{D=0} = 4S\sqrt{(1 + \gamma_k)(1 - \cos 2\phi_0\gamma_k)} \tag{2.25}$$

where

$$\cos 2\phi_0 = 1 - 2(\frac{H}{H_S})^2$$

[1] See Chap.7 in Ref.[13]

and $H_S = 8S$ is the saturation field at which spins become fully polarized in the direction of the magnetic field.

Magnon spectrum ($D = 0$) for $H = 0$, $H = 0.707H_S$ and $H = H_S$:

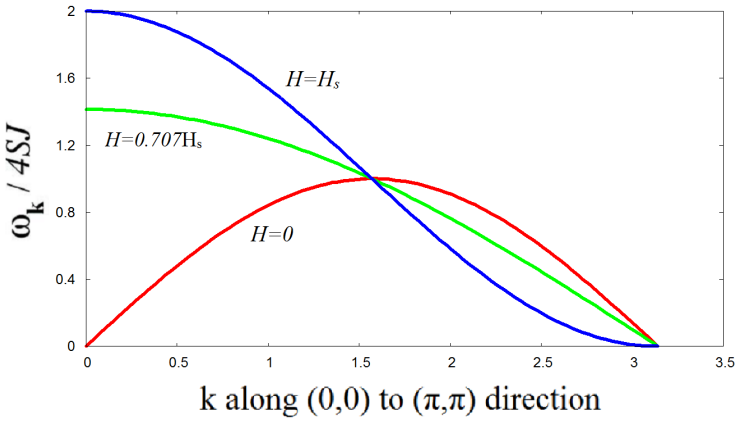

Figure 2.5: $\omega_k^{D=0}$ Eq.(2.25) magnon spectrum for $H = 0$, $H = 0.707H_S$ and $H = H_S$ along $(0, 0)$ to (π, π) direction

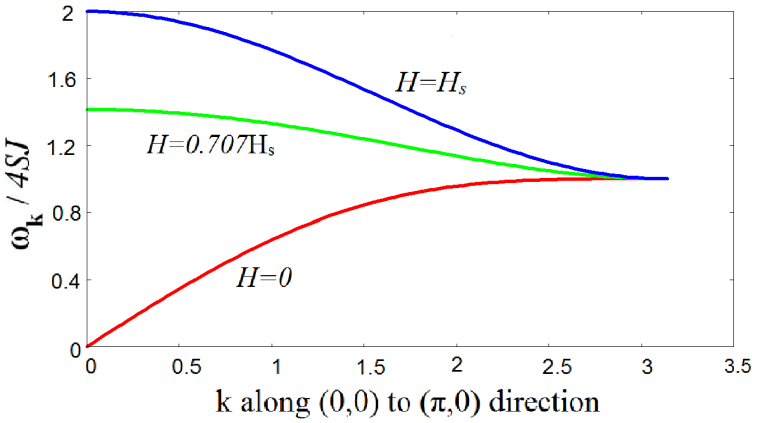

Figure 2.6: $\omega_k^{D=0}$ magnon spectrum Eq.(2.25) for $H = 0$, $H = 0.707H_S$ and $H = H_S$ along $(0, 0)$ to $(\pi, 0)$ direction

Why $k = (\pi, \pi)$ mode remains gapless ?

A mode remains gapless if it corresponds to the Goldstone mode related to the spontaneous symmetry breaking (of the Hamiltonian by the ground state). There should be a continuous symmetry present in the Hamiltonian which should be spontaneously broken by the ground state. For $D = 0$ case, i.e. only in presence of Heisenberg term and field,

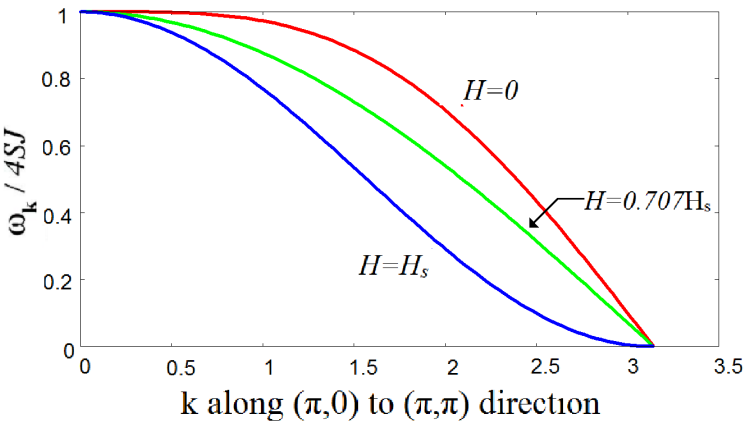

Figure 2.7: $\omega_k^{D=0}$ magnon spectrum Eq.(2.25) for $H = 0$, $H = 0.707H_S$ and $H = H_S$ along $(\pi, 0)$ to (π, π) direction

the continuous symmetry present in the Hamiltonian is the $O(2)$ symmetry of spins (the symmetry present in Hamiltonian) in plane perpendicular to field. This continuous symmetry is spontaneously broken by the ground state(as a specific orientation is assumed by the spins in the ground state).
$k = (\pi, \pi)$ mode corresponds to the Goldstone mode related to spontaneous symmetry breaking, $k = (\pi, \pi)$ mode remains gapless (even in the presence of field).

2.4.3 Zero field ($H = 0$) case

If we neglect the field coupling-term in the Hamiltonian (with staggered DM vector) and take $J = 1$, the following expression for the spin-wave spectrum is obtained [12]:

$$\omega_k^{H=0} = 4S\sqrt{1+D^2}\sqrt{(1-\gamma_k)(1+\frac{\gamma_k}{\sqrt{1+D^2}})} \tag{2.26}$$

$H = 0$ magnon spectrum for $D = 0.04$, $D = 0.4$ and $D = 1.0$:

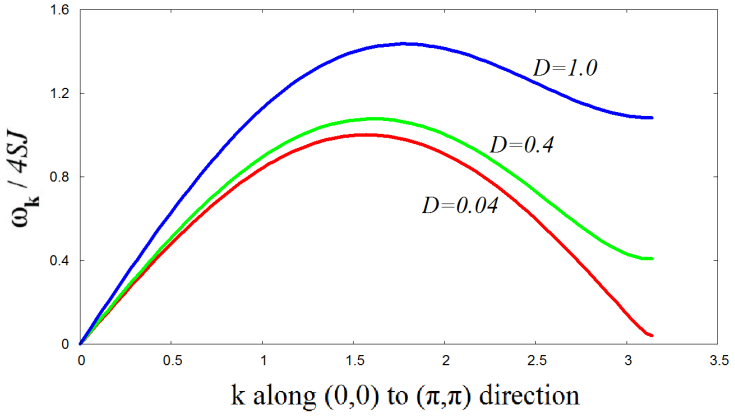

Figure 2.8: $\omega_k^{H=0}$ magnon spectrum Eq.(2.26) for $D = 0.04$, $D = 0.4$ and $D = 1.0$ along $(0, 0)$ to (π, π) direction

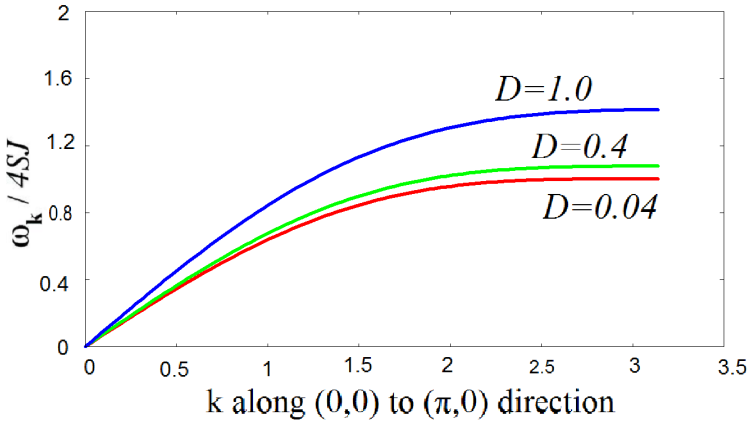

Figure 2.9: $\omega_k^{H=0}$ magnon spectrum Eq.(2.26) for $D = 0.04$, $D = 0.4$ and $D = 1.0$ along $(0, 0)$ to $(\pi, 0)$ direction

Why $k = (0, 0)$ mode remains gapless ?

Again, a mode remains gapless if it corresponds to the Goldstone mode related to

the spontaneous symmetry breaking (of the Hamiltonian by the ground state). There should be a continuous symmetry present in the Hamiltonian which should be spontaneously broken by the ground state. Here, for $H = 0$ case, i.e. only in presence of Heisenberg term and DM interaction,
the continuous symmetry present in the Hamiltonian is related to the choice of the direction of DM-induced (ferromagnetic) magnetization. This continuous symmetry is spontaneously broken by the ground state(as a specific orientation is assumed by the DM-induced magnetization vector in the ground state).
Since here $k = (0, 0)$ mode corresponds to the Goldstone mode related to this spontaneous symmetry breaking, $k = (\pi, \pi)$ mode remains gapless.

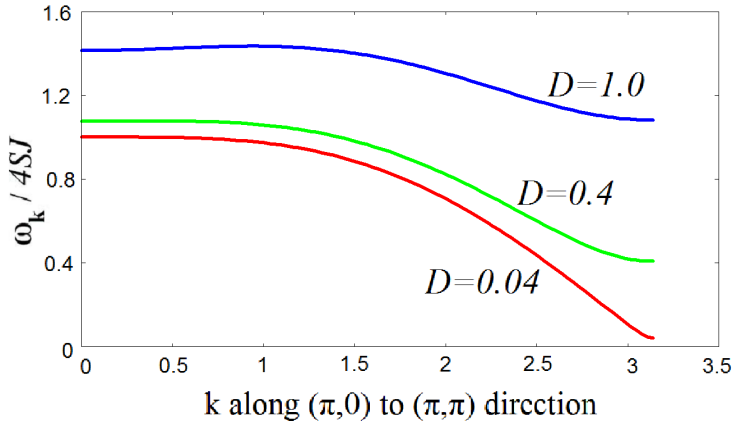

Figure 2.10: $\omega_k^{H=0}$ magnon spectrum Eq.(2.26) for $D = 0.04$, $D = 0.4$ and $D = 1.0$ along $(\pi, 0)$ to (π, π) direction

Chapter 3

Self Consistent Spin Wave Analysis of isotropic Heisenberg AFM

3.1 Model Hamiltonian

$$H = \sum_{<i,j>} (J\vec{S}_i.\vec{S}_j) \tag{3.1}$$

where, $\sum_{<i,j>}$ denotes summation over nearest neighbour pairs of spins on the lattice. S is the magnitude of the spin. Self consistent spin wave theory is studied following Ref.[14].

3.2 Dyson-Maleev transformations

The antiferromagnetic Dyson-Maleev transformations [**?**] are:
For sublattice A,

$$S_i^- = a_i^\dagger \tag{3.2}$$

$$S_i^+ = (2S - a_i a_i^\dagger)a_i \tag{3.3}$$

$$S_i^z = S - a^\dagger a_i \tag{3.4}$$

For sublattice B,

$$S_j^- = b_j \tag{3.5}$$

$$S_j^+ = b_j^\dagger(2S - b_j^\dagger b_j) \tag{3.6}$$

$$S_j^z = -S + b_j^\dagger b_j \tag{3.7}$$

where $a_i^\dagger$ and a_i are respectively the bosonic creation and annihilation operators on sublattice A, $b_j^\dagger$ and b_j are the corresponding operators on sublattice B.

The two sublattices have different vacuum states such that, in vacuum state, sublattices A and B each have zero bosonic excitations implying $S_i^z = S$ or $a_i^\dagger a_i = 0$, and $S_j^z = -S$ or $b_j^\dagger b_j = 0$.

To use the D-M transformations, the hamiltonian should be expressed in terms of spin raising (S^+) and spin lowering (S^-) operators.

$$H = J \sum_{<i,j>} [S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z] \tag{3.8}$$

Spin raising and lowering operators are defined as :

$$S^+ = S^x + iS^y$$

$$S^- = S^x - iS^y$$

Using these to write,

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

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

Substituting into hamiltonian in Eq. (8) ,

$$\begin{aligned} H &= J \sum_{<i,j>} [(\frac{1}{2})^2 (S_i^+ + S_i^-)(S_j^+ + S_j^-) + (\frac{-i}{2})^2 (S_i^+ - S_i^-)(S_j^+ - S_j^-) + S_i^z S_j^z] \\ &= J \sum_{<i,j>} [(\frac{1}{4})\{S_i^+ S_j^+ + S_i^+ S_j^- + S_i^- S_j^+ + S_i^- S_j^-\} \\ &+(\frac{-1}{4})\{S_i^+ S_j^+ - S_i^+ S_j^- - S_i^- S_j^+ + S_i^- S_j^-\} + S_i^z S_j^z] \\ &= J \sum_{<i,j>} [(\frac{1}{2})\{S_i^+ S_j^- + S_i^- S_j^+\} + S_i^z S_j^z] \end{aligned} \tag{3.9}$$

Now, using the D-M transformations from Eqs. (2) – (8),

$$
\begin{aligned}
H &= J \sum_{<i,j>} [\frac{1}{2}\{(2S - a_i^\dagger a_i)a_i b_j + a_i^\dagger b_j^\dagger (2S - b_j^\dagger b_j)\} + (S - a_i^\dagger a_i)(-S + b_j^\dagger b_j)] \\
&= J \sum_{<i,j>} [-S^2] + J \sum_{<i,j>} [S(a_i b_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i) - \frac{1}{2} a_i^\dagger (a_i + b_j^\dagger)^2 b_j] \\
&= -JNzS^2 + J \sum_{<i,j>} [S(a_i b_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i) - \frac{1}{2} a_i^\dagger (a_i + b_j^\dagger)^2 b_j]
\end{aligned} \tag{3.10}
$$

where N is the number of sites on each sublattice and z denotes the number of nearest neighbours.

It can be noted that the last term in the Hamiltonian is not Hermitian, disregarding this, it is treated as any ordinary Hamiltonian following Ref.[15].

3.3 Mean Field Treatment of quartic term

Now, the last (and non-linear) quartic term in the Hamiltonian Eq.(3.10) will be treated with a self-consistent MF theory,

$$
a_i^\dagger (a_i + b_j^\dagger)^2 b_j = a_i^\dagger a_i a_i b_j + a_i^\dagger b_j^\dagger b_j^\dagger b_j + 2 a_i^\dagger a_i b_j^\dagger b_j \tag{3.11}
$$

Neglecting higher energy excitations, following Takahashi in Ref.[18],

$$
< a_i a_i > = < b_j^\dagger b_j^\dagger > = 0, < a_i^\dagger b_j > = < a_i b_j^\dagger > = 0
$$

.

The higher order terms can be decoupled using Mean Field approximation. The terms which can be decoupled in more than one way will be decoupled using a Lagrangian multiplier (weight factor) λ. The value of parameter λ signifies the extent of competition between diagonal and off-diagonal terms. It can be later determined by minimizing the energy of the ground state.

Term 1

$$
a_i^\dagger a_i a_i b_j \simeq < a_i^\dagger a_i > a_i b_j + a_i^\dagger a_i < a_i b_j > - < a_i^\dagger a_i >< a_i b_j > \tag{3.12}
$$

This term can be decoupled in a single unique way.

Note: All possible ways in which a term can be decoupled can be seen by noting

the number of ways in which operators can be paired up next to one another in the four operator term, given that that such a rearrangement of terms is allowed by the commutation relations[Write eqn number here].

Term 2

$$a_i^\dagger b_j^\dagger b_j^\dagger b_j \simeq < a_i^\dagger b_j^\dagger > b_j^\dagger b_j + a_i^\dagger b_j^\dagger < b_j^\dagger b_j > - < a_i^\dagger b_j^\dagger >< b_j^\dagger b_j > \tag{3.13}$$

This term can be decoupled in a single unique way.

Term 3

$$a_i^\dagger a_i b_j^\dagger b_j = < a_i^\dagger a_i > b_j^\dagger b_j + a_i^\dagger a_i < b_j^\dagger b_j > - < a_i^\dagger a_i >< b_j^\dagger b_j > \tag{3.14}$$

This term can be written (and therefore decoupled) in two ways:

- $a_i^\dagger a_i b_j^\dagger b_j \simeq < a_i^\dagger a_i > b_j^\dagger b_j + a_i^\dagger a_i < b_j^\dagger b_j > - < a_i^\dagger a_i >< b_j^\dagger b_j >$
- $a_i^\dagger b_j^\dagger a_i b_j \simeq < a_i^\dagger b_j^\dagger > a_i b_j + a_i^\dagger b_j^\dagger < a_i b_j > - < a_i^\dagger b_j^\dagger >< a_i b_j >$

These two forms of decouplings can be combined in the following ways using the parameter λ:

$$\begin{aligned} a_i^\dagger a_i b_j^\dagger b_j \simeq & (1-\lambda)(a_i^\dagger a_i b_j^\dagger b_j) + \lambda(a_i^\dagger b_j^\dagger a_i b_j) \\ \simeq & (1-\lambda)(< a_i^\dagger a_i > b_j^\dagger b_j + a_i^\dagger a_i < b_j^\dagger b_j > - < a_i^\dagger a_i >< b_j^\dagger b_j >) \\ & + \lambda(< a_i^\dagger b_j^\dagger > a_i b_j + a_i^\dagger b_j^\dagger < a_i b_j > - < a_i^\dagger b_j^\dagger >< a_i b_j >) \end{aligned} \tag{3.15}$$

Now, here onwards the following definitions for averages will be used:

$$\langle D \rangle = < a_i^\dagger a_i >_{T=0} = < b_j^\dagger b_j >_{T=0} \tag{3.16}$$

$$\langle O \rangle = < a_i^\dagger b_j^\dagger >_{T=0} = < a_i b_j >_{T=0} \tag{3.17}$$

so that the Hamiltonian becomes:

$$H == -JNzS^2 + J \sum_{<i,j>} [S(a_i b_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i) - \frac{1}{2}(a_i^\dagger a_i a_i b_j + a_i^\dagger b_j^\dagger b_j^\dagger b_j + 2a_i^\dagger a_i b_j^\dagger b_j)] \tag{3.18}$$

Using the notation from (3.16), (3.17) and using the decoupling expressions from (3.12), (3.13) and (3.15)

$$\begin{aligned}
H &= -JNzS^2 + J\sum_{<i,j>}[S(a_ib_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i)] \\
&\quad -\frac{1}{2}J\sum_{<i,j>}[(a_i^\dagger a_i a_i b_j + a_i^\dagger b_j^\dagger b_j^\dagger b_j + 2a_i^\dagger a_i b_j^\dagger b_j)] \\
&= -JNzS^2 + J\sum_{<i,j>}[S(a_ib_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i)] \\
&\quad -\frac{1}{2}J\sum_{<i,j>}[\{\langle D\rangle a_ib_j + a_i^\dagger a_i\langle O\rangle - \langle D\rangle\langle O\rangle\} \\
&\qquad +\{\langle O\rangle b_j^\dagger b_j + a_i^\dagger b_j^\dagger\langle D\rangle - \langle O\rangle\langle D\rangle\} \\
&\qquad +2\{(1-\lambda)(\langle D\rangle b_j^\dagger b_j + a_i^\dagger a_i\langle D\rangle - \langle D\rangle\langle D\rangle) \\
&\qquad +\lambda(\langle O\rangle a_ib_j + a_i^\dagger b_j^\dagger\langle O\rangle - \langle O\rangle\langle O\rangle)\}
\end{aligned}$$

Collecting the coefficients in second term,

$$\begin{aligned}
H &= -JNzS^2 + J\sum_{<i,j>}[S(a_ib_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i)] \\
&\quad -\frac{1}{2}J\sum_{<i,j>}[\{(\langle D\rangle + 2\lambda\langle O\rangle)a_ib_j + (\langle D\rangle + 2\lambda\langle O\rangle)a_i^\dagger b_j^\dagger \\
&\qquad +(\langle O\rangle + 2(1-\lambda)\langle D\rangle)a_i^\dagger a_i + (\langle O\rangle + 2(1-\lambda)\langle D\rangle)b_j^\dagger b_j]
\end{aligned}$$

$$\begin{aligned}
H &= -JNzS^2 + J\sum_{<i,j>}[S(a_ib_j + a_i^\dagger b_j^\dagger + b_j^\dagger b_j + a_i^\dagger a_i)] \\
&\quad -\frac{1}{2}J\sum_{<i,j>}[\{(P)a_ib_j + (P)a_i^\dagger b_j^\dagger + (Q)a_i^\dagger a_i + (Q)b_j^\dagger b_j] \\
&\qquad -2\langle D\rangle\langle O\rangle - 2(1-\lambda)\langle D\rangle^2 - 2\lambda\langle O\rangle^2]
\end{aligned}$$

where $\langle D\rangle + 2\lambda\langle O\rangle = P$ and $\langle O\rangle + 2(1-\lambda)\langle D\rangle = Q$

This can be further rewritten as:

$$\begin{aligned} H = -JNzS^2 + J\sum_{<i,j>}[(a_i^\dagger a_i)(S-\frac{1}{2}Q) + (b_j^\dagger b_j)(S-\frac{1}{2}Q) \\ +(a_i b_j)(S-\frac{1}{2}P) + (a_i^\dagger b_j^\dagger)(S-\frac{1}{2}P)] \\ +J\sum_{<i,j>}[\langle D\rangle\langle O\rangle + (1-\lambda)\langle D\rangle^2 + \lambda\langle O\rangle^2] \end{aligned}$$

The operators in momentum space are defined as follows:
For sublattice A,

$$\begin{aligned} a_i &= \frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}.\vec{r_i}}a_k \\ a_i^\dagger &= \frac{1}{\sqrt{N}}\sum_k e^{-i\vec{k}.\vec{r_i}}a_k^\dagger \end{aligned} \tag{3.19}$$

For sublattice B,

$$\begin{aligned} b_j &= \frac{1}{\sqrt{N}}\sum_k e^{-i\vec{k}.\vec{r_j}}b_k \\ b_j^\dagger &= \frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}.\vec{r_j}}b_k^\dagger \end{aligned} \tag{3.20}$$

where (again), N is the number of sites on each sublattice. The various terms in the hamiltonian can be written after the Fourier Transformation as:

$$\sum_{<i,j>} a_i b_j \longrightarrow z\sum_k[\gamma_k a_k b_k] \tag{3.21}$$

$$\sum_{<i,j>} a_i^\dagger b_j^\dagger \longrightarrow z\sum_k[\gamma_k a_k^\dagger b_k^\dagger] \tag{3.22}$$

$$\sum_{<i,j>} b_j^\dagger b_j \longrightarrow z\sum_k[b_k^\dagger b_k] \tag{3.23}$$

$$\sum_{<i,j>} a_i^\dagger a_i \longrightarrow z\sum_k[a_k^\dagger a_k] \tag{3.24}$$

where, again z is the no. of nearest neighbours
and $\gamma_k = \frac{1}{z}\sum_{\vec{d}} e^{i\vec{k}.\vec{d}}$ with $\vec{d}$ being the vector connecting to all nn sites.

Using these operators, the Hamiltonian can be expressed in terms of momentum space operators

$$\begin{aligned} H = -JNzS^2 + J\sum_k [z(a_k^\dagger a_k)(S - \frac{1}{2}Q) + z(b_k^\dagger b_k)(S - \frac{1}{2}Q) \\ + z(a_k b_k)(S - \frac{1}{2}P) + z(a_k^\dagger b_k^\dagger)(S - \frac{1}{2}P)] \\ + J\sum_{<i,j>} [\langle D\rangle\langle O\rangle + (1-\lambda)\langle D\rangle^2 + \lambda\langle O\rangle^2] \end{aligned} \tag{3.25}$$

3.4 Bogoliubov Valatin (BV) transformation

Next, we introduce the new operators α_k and β_k with Bogoliubov Valatin (BV) transformation

$$\begin{aligned} a_k &= u_k\alpha_k + v_k{\beta_k}^\dagger \\ b_k &= u_k\beta_k + v_k{\alpha_k}^\dagger \end{aligned} \tag{3.26}$$

Corresponding expressions for hermitian conjugate operators are:

$$\begin{aligned} a_k^\dagger &= u_k\alpha_k^\dagger + v_k\beta_k \\ b_k^\dagger &= u_k\beta_k^\dagger + v_k\alpha_k \end{aligned} \tag{3.27}$$

The various terms in the hamiltonian can be written after the BV transformation as

$$\begin{aligned} a_k^\dagger a_k =& (u_k\alpha_k^\dagger + v_k\beta_k)(u_k\alpha_k + v_k{\beta_k}^\dagger) \\ =& (({u_k}^2)\alpha_k^\dagger\alpha_k + (u_kv_k)\alpha_k^\dagger{\beta_k}^\dagger + (u_kv_k)\beta_k\alpha_k + ({v_k}^2)\beta_k{\beta_k}^\dagger) \end{aligned} \tag{3.28}$$

$$\begin{aligned} b_k^\dagger b_k =& (u_k\beta_k^\dagger + v_k\alpha_k)(u_k\beta_k + v_k{\alpha_k}^\dagger) \\ =& (({u_k}^2)\beta_k^\dagger\beta_k + (u_kv_k)\beta_k^\dagger{\alpha_k}^\dagger + (u_kv_k)\alpha_k\beta_k + ({v_k}^2)\alpha_k{\alpha_k}^\dagger) \end{aligned} \tag{3.29}$$

$$\begin{aligned} a_k b_k =& (u_k\alpha_k + v_k{\beta_k}^\dagger)(u_k\beta_k + v_k{\alpha_k}^\dagger) \\ =& (({u_k}^2)\alpha_k\beta_k + (u_kv_k)\alpha_k{\alpha_k}^\dagger + (u_kv_k)\beta_k^\dagger\beta_k + ({v_k}^2)\beta_k^\dagger{\alpha_k}^\dagger) \end{aligned} \tag{3.30}$$

$$\begin{aligned} a_k^\dagger b_k^\dagger =&(u_k\alpha_k^\dagger + v_k\beta_k)(u_k\beta_k^\dagger + v_k\alpha_k) \\ =&((u_k{}^2)\alpha_k^\dagger\beta_k^\dagger + (u_kv_k)\alpha_k^\dagger\alpha_k + (u_kv_k)\beta_k\beta_k^\dagger + (v_k{}^2)\beta_k\alpha_k) \end{aligned} \tag{3.31}$$

Substituting in the hamiltonian,

$$\begin{aligned} H = -JNzS^2 + J\sum_k [&z((u_k{}^2)\beta_k^\dagger\beta_k + (u_kv_k)\beta_k^\dagger\alpha_k{}^\dagger + (u_kv_k)\alpha_k\beta_k + (v_k{}^2)\alpha_k\alpha_k{}^\dagger)(S-\frac{1}{2}Q) \\ &+z((u_k{}^2)\beta_k^\dagger\beta_k + (u_kv_k)\beta_k^\dagger\alpha_k{}^\dagger + (u_kv_k)\alpha_k\beta_k + (v_k{}^2)\alpha_k\alpha_k{}^\dagger)(S-\frac{1}{2}Q) \\ &+z((u_k{}^2)\alpha_k\beta_k + (u_kv_k)\alpha_k\alpha_k{}^\dagger + (u_kv_k)\beta_k^\dagger\beta_k + (v_k{}^2)\beta_k^\dagger\alpha_k{}^\dagger)(S-\frac{1}{2}P) \\ &+z((u_k{}^2)\alpha_k^\dagger\beta_k^\dagger + (u_kv_k)\alpha_k^\dagger\alpha_k + (u_kv_k)\beta_k\beta_k^\dagger + (v_k{}^2)\beta_k\alpha_k)(S-\frac{1}{2}P)] \\ +J\sum_{<i,j>}&[\langle D\rangle\langle O\rangle + (1-\lambda)\langle D\rangle^2 + \lambda\langle O\rangle^2] \end{aligned} \tag{3.32}$$

Gathering the coefficients of different terms

$$\begin{aligned} H = -JNzS^2 + Jz\sum_k [&(\alpha_k^\dagger\alpha_k)\{(u_k{}^2)(S-\frac{1}{2}Q) + \gamma_ku_kv_k(S-\frac{1}{2}P)\} \\ &+(\beta_k^\dagger\beta_k)\{(u_k{}^2)(S-\frac{1}{2}Q) + \gamma_ku_kv_k(S-\frac{1}{2}P)\} \\ &+(\alpha_k\alpha_k^\dagger)\{(v_k{}^2)(S-\frac{1}{2}Q) + \gamma_ku_kv_k(S-\frac{1}{2}P)\} \\ &+(\beta_k\beta_k^\dagger)\{(v_k{}^2)(S-\frac{1}{2}Q) + \gamma_ku_kv_k(S-\frac{1}{2}P)\} \\ &+(\alpha_k^\dagger\beta_k^\dagger)\{2(u_kv_k)(S-\frac{1}{2}Q) + \gamma_k(v_k{}^2)(S-\frac{1}{2}P) + \gamma_k(u_k{}^2)(S-\frac{1}{2}P)\} \\ &+(\alpha_k\beta_k)\{2(u_kv_k)(S-\frac{1}{2}Q) + \gamma_k(u_k{}^2)(S-\frac{1}{2}P) + \gamma_k(v_k{}^2)(S-\frac{1}{2}P)\}] \\ +J\sum_{<i,j>}&[\langle D\rangle\langle O\rangle + (1-\lambda)\langle D\rangle^2 + \lambda\langle O\rangle^2] \end{aligned} \tag{3.33}$$

From the commutation relations, we know that: $\alpha_k\alpha_k^\dagger = 1+\alpha_k^\dagger\alpha_k$ and $\beta_k\beta_k^\dagger = 1+\beta_k^\dagger\beta_k$, therefore

$$\begin{aligned} H = -JNzS^2 + Jz\sum_k [&(\alpha_k^\dagger\alpha_k)\{({u_k}^2+{v_k}^2)(S-\frac{1}{2}Q) + 2\gamma_k u_k v_k(S-\frac{1}{2}P)\} \\ &+\{({v_k}^2)(S-\frac{1}{2}Q) + \gamma_k u_k v_k(S-\frac{1}{2}P)\} \\ &+(\beta_k^\dagger\beta_k)\{({u_k}^2+{v_k}^2)(S-\frac{1}{2}Q) + 2\gamma_k u_k v_k(S-\frac{1}{2}P)\} \\ &+\{({v_k}^2)(S-\frac{1}{2}Q) + \gamma_k u_k v_k(S-\frac{1}{2}P)\} \\ &+(\alpha_k^\dagger\beta_k^\dagger)\{2(u_k v_k)(S-\frac{1}{2}Q) + \gamma_k({u_k}^2+{v_k}^2)(S-\frac{1}{2}P)\} \\ &+(\alpha_k\beta_k)\{2(u_k v_k)(S-\frac{1}{2}Q) + \gamma_k({u_k}^2+{v_k}^2)(S-\frac{1}{2}P)\}] \\ &+JNz[\langle D\rangle\langle O\rangle + (1-\lambda)\langle D\rangle^2 + \lambda\langle O\rangle^2] \end{aligned} \tag{3.34}$$

For the hamiltonian to be diagonal,
Coefficient of $\alpha_k\beta_k$ = Coefficient of $\alpha_k^\dagger\beta_k^\dagger = 0$

$$\Rightarrow 2(u_k v_k)(S-\frac{1}{2}Q) + \gamma_k({u_k}^2+{v_k}^2)(S-\frac{1}{2}P) = 0 \tag{3.35}$$

Also, for commutation relations to be satisfied by the new operators,

$${u_k}^2 - {v_k}^2 = 1$$

$$\Rightarrow u_k = \pm\sqrt{1+{v_k}^2}$$

Using $u_k = +\sqrt{1+{v_k}^2}$ here onwards.

From (3.35),

$$\gamma_k(S-\frac{1}{2}P)({u_k}^2+{v_k}^2) + 2(S-\frac{1}{2}Q)(u_k v_k) = 0$$

$$\gamma_k(S-\frac{1}{2}P)(2{v_k}^2+1) + (2S-Q)(\sqrt{1+{v_k}^2}v_k) = 0$$

$$\Rightarrow \frac{\gamma_k}{2}(\frac{2S-P}{Q-2S})(\frac{2{v_k}^2+1}{v_k}) = \sqrt{1+{v_k}^2}$$

On squaring,

$$(\frac{\gamma_k^2}{4})(\frac{2S-P}{2S-Q})^2(\frac{2{v_k}^2+1}{v_k})^2 = 1+{v_k}^2$$

Let, $(\frac{2S-P}{2S-Q}) = A$ (say),

$$\Rightarrow (\frac{\gamma_k^2}{4})(A^2)(4{v_k}^4 + 1 + 4v_k^2) = {v_k}^2 + {v_k}^4$$

$$\Rightarrow {v_k}^4(1 - A^2\gamma_k^2) + v_k^2(1 - A^2\gamma_k^2) - \frac{A^2\gamma_k^2}{4} = 0$$

$$\Rightarrow v_k^2 = \frac{-(1 - A^2\gamma_k^2) \pm \sqrt{(1 - A^2\gamma_k^2)^2 - 4(1 - A^2\gamma_k^2)(-\frac{A^2\gamma_k^2}{4})}}{2(1 - A^2\gamma_k^2)}$$

$$\Rightarrow v_k^2 = \frac{-1 \pm \sqrt{\frac{1}{1 - A^2\gamma_k^2}}}{2}$$

For v_k^2 to be positive,

$$v_k^2 = \frac{-1}{2} + \frac{1}{2\sqrt{1 - A^2\gamma_k^2}} = \frac{1}{2}(-1 + \frac{1}{\sqrt{1 - A^2\gamma_k^2}}) \tag{3.36}$$

Using ${u_k}^2 - {v_k}^2 = 1$,

$${u_k}^2 = \frac{1}{2}(1 + \frac{1}{\sqrt{1 - A^2\gamma_k^2}}) \tag{3.37}$$

we obtain,

$${u_k}^2 v_k^2 = (\frac{1}{2})^2(1 + \frac{1}{\sqrt{1 - A^2\gamma_k^2}})(-1 + \frac{1}{\sqrt{1 - A^2\gamma_k^2}}) = \frac{1}{4}(\frac{A^2\gamma_k^2}{1 - A^2\gamma_k^2}) \tag{3.38}$$

$$\Rightarrow u_k v_k = (\pm)(\frac{1}{2})(\frac{A\gamma_k}{\sqrt{1 - A^2\gamma_k^2}})$$

(using negative sign)
Then,

$$\begin{aligned} H = -JNzS^2 + Jz\sum_k [(\alpha_k^\dagger \alpha_k)\{(\frac{1}{\sqrt{1 - A^2\gamma_k^2}})(\frac{2S - Q}{2}) + 2\gamma_k(-\frac{1}{2})(\frac{A\gamma_k}{\sqrt{1 - A^2\gamma_k^2}})(\frac{2S - P}{2})\} \\ +(\beta_k^\dagger \beta_k)\{(\frac{1}{\sqrt{1 - A^2\gamma_k^2}})(\frac{2S - Q}{2}) + 2\gamma_k(-\frac{1}{2})(\frac{A\gamma_k}{\sqrt{1 - A^2\gamma_k^2}})(\frac{2S - P}{2})\} \\ +\{(-1 + \frac{1}{\sqrt{1 - A^2\gamma_k^2}})(S - \frac{Q}{2}) + \gamma_k(-1)(\frac{A\gamma_k}{\sqrt{1 - A^2\gamma_k^2}})(S - \frac{1}{2}P)\}] \\ +JNz[\langle D\rangle\langle O\rangle + (1 - \lambda)\langle D\rangle^2 + \lambda\langle O\rangle^2] \end{aligned} \tag{3.39}$$

Now, consider the coefficient of $(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k)$ $(= h\omega_k$ (say)) from above expression:

$$\begin{aligned}
h\omega_k =& \{(\frac{1}{\sqrt{1-A^2\gamma_k^2}})(\frac{2S-Q}{2}) + 2\gamma_k(-\frac{1}{2})(\frac{A\gamma_k}{\sqrt{1-A^2\gamma_k^2}})(\frac{2S-P}{2})\} \\
=& (\frac{1}{\sqrt{1-A^2\gamma_k^2}})(\frac{2S-Q}{2})\{1 - A\gamma_k^2(\frac{2S-P}{2S-Q})\} \\
=& (\frac{1}{\sqrt{1-A^2\gamma_k^2}})(\frac{2S-Q}{2})[1 - A^2\gamma_k^2] \\
=& (S - \frac{Q}{2})(\sqrt{1-A^2\gamma_k^2}) \\
=& S(1 - \frac{Q}{2S})(\sqrt{1-A^2\gamma_k^2}) \\
=& S(1 - \frac{\langle O\rangle}{2S} - \frac{(1-\lambda)\langle D\rangle}{S})\frac{1}{\Delta_k}
\end{aligned} \tag{3.40}$$

where $\Delta_k = \frac{1}{\sqrt{1-A^2\gamma_k^2}}$ and $h\omega_k$ represents the energy of spin wave with momentum $\vec{k}$.

Remaining terms from the Hamiltonian

$$\begin{aligned}
H' =& -JNzS^2 + Jz\sum_k [\{(-1 + \frac{1}{\sqrt{1-A^2\gamma_k^2}})(S - \frac{Q}{2}) + \gamma_k(-1)(\frac{A\gamma_k}{\sqrt{1-A^2\gamma_k^2}})(S - \frac{1}{2}P)\}] \\
&+ JNz[\langle D\rangle\langle O\rangle + (1-\lambda)\langle D\rangle^2 + \lambda\langle O\rangle^2] \\
=& -JNzS^2 + Jz\sum_k [(S(\frac{2 - Q/S}{2})(1 - \sqrt{1-A^2\gamma_k^2})] \\
&+ JNz[\langle D\rangle\langle O\rangle + (1-\lambda)\langle D\rangle^2 + \lambda\langle O\rangle^2] \\
=& -JNzS[S + \sum_k \{(1 - \frac{Q}{2S})(1 - \frac{1}{\Delta_k})(\frac{1}{N})\} - \{\frac{\langle D\rangle\langle O\rangle}{S} + \frac{(1-\lambda)\langle D\rangle^2}{S} + \frac{\lambda\langle O\rangle^2}{S}\}] \\
=& -JNzS[S + (1 - \frac{\langle O\rangle + 2(1-\lambda)\langle D\rangle}{2S})(1 - \frac{1}{N}\sum_k \frac{1}{\Delta_k}) \\
&- \{\frac{\langle D\rangle\langle O\rangle}{S} + \frac{(1-\lambda)\langle D\rangle^2}{S} + \frac{\lambda\langle O\rangle^2}{S}\}] \\
=& -JNzS(S + \theta)
\end{aligned} \tag{3.41}$$

where

$$\theta = (1 - \frac{\langle O\rangle + 2(1-\lambda)\langle D\rangle}{2S})(1 - \frac{1}{N}\sum_k \frac{1}{\Delta_k}) - \{\frac{\langle D\rangle\langle O\rangle}{S} + \frac{(1-\lambda)\langle D\rangle^2}{S} + \frac{\lambda\langle O\rangle^2}{S}\} \tag{3.42}$$

3.5 Results

The dispersion relation obtained for Heisenberg AFM model is:

$$h\omega_k = S(1 - \frac{\langle O\rangle}{2S} - \frac{(1-\lambda)\langle D\rangle}{S})\frac{1}{\Delta_k} \tag{3.43}$$

where $\Delta_k = \frac{1}{\sqrt{1-A^2\gamma_k^2}}$ and $h\omega_k$ represents the energy of spin wave with momentum $\vec{k}$. $\langle D\rangle$ and $\langle O\rangle$ satisfy the following self-consistent equations:

$$\langle D\rangle = \frac{1}{N}\sum_k v_k^2 = \frac{1}{2N}\sum_k(\Delta_k - 1)$$

$$\langle O\rangle = \frac{1}{N}\sum_k \gamma_k u_k v_k = -\frac{1}{2N}\sum_k(A\Delta_k\gamma_k^2)$$

and

$$A = \frac{1 - \frac{\langle D\rangle}{2S} - \frac{\lambda\langle O\rangle}{S}}{1 - \frac{\langle O\rangle}{2S} - \frac{(1-\lambda)\langle D\rangle}{S}}$$

Staggered sublattice magnetization is defined as:

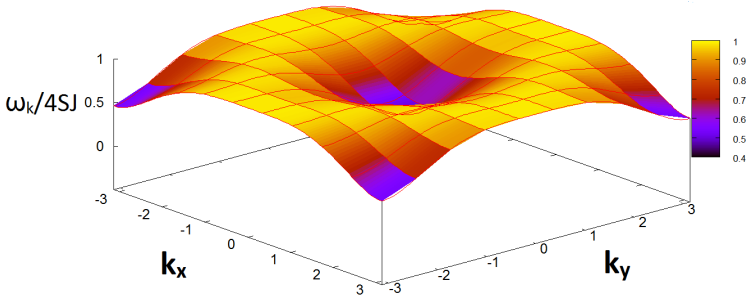

Figure 3.1: Self consistent spin wave theory result with higher order corrections for spin-wave dispersion (3.43) in HAFM.

$$m_0 = |S - \langle D\rangle|$$

In the classical ground state (Néel state), spins on the two sublattices are aligned perfectly antiparallel to each other. Therefore, per site staggered magnetization is equal to the magnitude S of spins. The average value of per site staggered sublattice magnetization is lowered from its classical value ($S = 0.5$) due to the quantum fluctuations in the form of spin wave excitations (coherently distributed spin deviations).

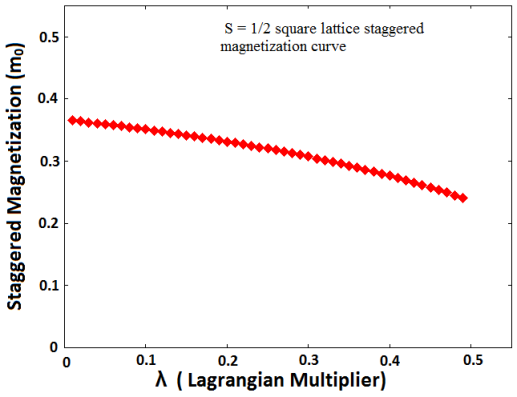

Figure 3.2: Staggered sublattice magnetization (m_0) with λ

Ground state energy is : $E = -JNzS(S+\theta)$ where

$$\theta = (1 - \frac{\langle O\rangle + 2(1-\lambda)\langle D\rangle}{2S})(1 - \frac{1}{N}\sum_k \frac{1}{\Delta_k}) - \{\frac{\langle D\rangle\langle O\rangle}{S} + \frac{(1-\lambda)\langle D\rangle^2}{S} + \frac{\lambda\langle O\rangle^2}{S}\}$$

Then per-site GS energy e_0 is defined with

$$E = 2JNe_0$$

The energy of ground state decreases as λ increases from 0 to 0.5. At $\lambda = 0.5$,

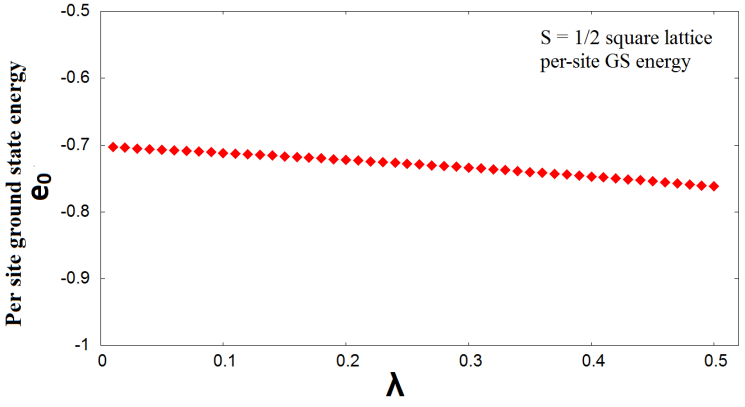

Figure 3.3: Per-site ground state energy (e_0) with λ

when the contribution of diagonal and off-diagonal terms of the quartic term in the

Hamiltonian are equal, the per-site ground state energy is minimized. For $\lambda > 0.5$, non-physical results for energy are obtained and therefore neglected.

Chapter 4

Conclusions and outlook

In this thesis, we explored spin wave theory and its application to different quantum Heisenberg models. The techniques of Holstein-Primakoff (Ref.[11]) were employed to transform the Hamiltonians to bosonic form and subsequent diagonalization was performed with Bogoliubov tranformations in accordance with conventional spin wave theories. In particular, we studied the isotropic Heisenberg AFM using two different approaches namely two boson approach and local rotating coordinate approach. We obtained the same results with the two methods. We also explored Heisenberg model with Dzyaloshinskii-Moriya anisotropy in the presence of magnetic field (Ref.[12]) and obtained the magnon spectrum. Further, we discussed the gapless modes in the spectrum with their correspondence to spontaneous breaking of continuous symmetries present in different limits of the exchange coupling and DM interaction. In addition, we studied spin wave theory with a self-consistent mean field method for Heisenberg AFM (Ref.[14, 18]) and calculated staggered sublattice magnetization and per-site ground state energy.

The original goals of the project were: (1) to understand spin wave theories with their application to different systems and (2) to combine the bosonization methods employed in standard spin wave theories with computational exact diagonalization to improve the mean field approximation with site-dependent averages and apply the method to a general frustrated Heisenberg model with nearest neighbour and next-nearest neighbour interactions. The first part of the project is complete and the second part is partially complete as most required computational schemes have been written and analysis of the referred model is partially finished. The project will be completed by doing the spin wave analysis of the system with the proposed method.

Appendix A

Appendix

A.1 Canonical Transformations

Def. : Linear Canonical Transformations
Linear transformations of creation and annihilation operators which preserve the canonical commutation relations are called linear canonical transformations. These can be categorised on the basis of whether these transformations mix creation and annihilation operators or not.

1. Linear Transformations that **do not mix creation and annihilation operators** correspond to unitary transformations of single particle orbitals(states?).

2. The more general class of linear transformations that **mix creation and annihilation operators** lead to the important concept of a quasiparticle. A particular example of such types of transformations is Bogoliubov transformation.
   In case of AFM spin wave theory it leads to the concept of 'magnon' quasiparticle.

Suppose that the space of single particle states is of finite dimension n. $\{a^\dagger$ and a denote the creation and annihilation operators as usual.$\}$ To write expressions in a compact form, it will be useful to collect the creation and annihilation operators into a column vector as follows:

[0]Adapted from Ref.[19]

$$\alpha \equiv \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \equiv \begin{pmatrix} a_1 \\ a_2 \\ . \\ a_n \\ a_1^\dagger \\ a_2^\dagger \\ . \\ a_n^\dagger \end{pmatrix} \tag{A.1}$$

The corresponding dual vector is the row vector

$$\alpha^\dagger \equiv \left(a^\dagger \, a\right) \equiv \left(a_1^\dagger \, a_2^\dagger \, ... a_n^\dagger \, a_1 \, a_2 \, ... \, a_n\right) \tag{A.2}$$

Consider the (symmetric) matrix γ,

$$\gamma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which will be used to exchange the position of the creation and annihilation operators in vector α.

As an illustration note that to obtain row vector $\alpha^\dagger$ from column vector α (or vice versa), one needs the matrix γ in addition to performing transpose on α ($\alpha^\dagger$) i.e., if $\alpha \equiv \begin{pmatrix} a \\ a^\dagger \end{pmatrix}$ then $\alpha^\dagger = (\gamma(\alpha))^T \equiv \begin{pmatrix} a^\dagger \\ a \end{pmatrix}^T = \left(a^\dagger \, a\right)$.

Consider the following inhomogeneous transformation

$$\begin{pmatrix} b \\ b^\dagger \end{pmatrix} = \begin{pmatrix} U & \varepsilon V \\ \varepsilon Y & X \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} + \begin{pmatrix} c \\ d \end{pmatrix} \tag{A.3}$$

where b and $b^\dagger$ denote 'new' (transformed) boson or fermion operators. Here, $\varepsilon = -1$ for bosons and $\varepsilon = +1$ for fermions. . U, V, X and Y are $n \times n$ matrices (as a and $a^\dagger$ are n-element column vectors).

Note that, in general, b and $b^\dagger$ are not necessarily Hermitian conjugate operators (of

each other). We have, for example, from the above transformation,

$$\begin{pmatrix} b_1 \\ b_2 \\ b_1^\dagger \\ b_2^\dagger \end{pmatrix} = \begin{pmatrix} u_1 & u_2 & \varepsilon v_1 & \varepsilon v_2 \\ u_3 & u_4 & \varepsilon v_3 & \varepsilon v_4 \\ \varepsilon y_1 & \varepsilon y_2 & x_1 & x_2 \\ \varepsilon y_3 & \varepsilon y_4 & x_3 & x_4 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_1^\dagger \\ a_2^\dagger \end{pmatrix} + \begin{pmatrix} c_1 \\ c_2 \\ d_1 \\ d_2 \end{pmatrix} \tag{A.4}$$

This gives for b_1,

$$b_1 = u_1 a_1 + u_2 a_2 + \varepsilon v_1 a_1^\dagger + \varepsilon v_2 a_2^\dagger + c_1 \tag{A.5}$$

taking the Hermitian conjugate,

$$b_1^\dagger = (u_1^*) a_1^\dagger + (u_2^*) a_2^\dagger + \varepsilon (v_1^*) a_1 + \varepsilon (v_2^*) a_2 + c_1^*$$

Comparing it with the expression for $b_1^\dagger$ from the transformation,

$$b_1^\dagger = x_1 a_1^\dagger + x_2 a_2^\dagger + \varepsilon y_1 a_1 + \varepsilon y_2 a_2 + d_1$$

gives the condition for a and $a^\dagger$ to be hermitian conjugate operators,

$$x_i = u_i^*, \;\; v_i = y_i^*, \;\; d_i = c_i^*$$

or equivalently,

$$X = U^*, \;\; V = Y^*, \;\; d = c^*$$

Now if we use the following notation,

$$T = \begin{pmatrix} U & \varepsilon V \\ \varepsilon Y & X \end{pmatrix}, \delta = \begin{pmatrix} c \\ d \end{pmatrix}, \beta = \begin{pmatrix} b \\ b^\dagger \end{pmatrix}$$

the transformation Eq.(A.3) can be re-written as

$$\beta = T\alpha + \delta \tag{A.6}$$

The corresponding transformation for row vector $\beta^\dagger$ will be

$$\beta^\dagger = \tilde{\beta}\gamma = [(\alpha^\dagger \gamma)\tilde{T}\gamma] + \tilde{\delta}\gamma$$

where $\tilde{M}$ denotes the transpose of matrix(or vector) M. Note that in above expression,

$$\alpha^\dagger\gamma = \begin{pmatrix} a^\dagger & a \end{pmatrix}\gamma = \begin{pmatrix} a & a^\dagger \end{pmatrix}$$

$$\tilde{T}\gamma = \begin{pmatrix} U & \varepsilon Y \\ \varepsilon V & X \end{pmatrix}\gamma = \begin{pmatrix} \varepsilon Y & U \\ X & \varepsilon V \end{pmatrix}$$

$$\{(\alpha^\dagger\gamma)\tilde{T}\gamma\} = \begin{pmatrix} a & a^\dagger \end{pmatrix}\begin{pmatrix} \varepsilon Y & U \\ X & \varepsilon V \end{pmatrix} = \begin{pmatrix} (\varepsilon Y)a + (X)a^\dagger & (U)a + (\varepsilon V)a^\dagger \end{pmatrix}$$

and

$$\tilde{\delta}\gamma = \begin{pmatrix} \tilde{c} & \tilde{d} \end{pmatrix}\gamma = \begin{pmatrix} \tilde{d} & \tilde{c} \end{pmatrix}$$

so that

$$\{(\alpha^\dagger\gamma)\tilde{T}\gamma\} + \tilde{\delta}\gamma = \beta^\dagger$$

If the transformation matrix T diagonalizes some matrix M, then it consists of the eigenvectors of the matrix M stored in the columnwise format. Further, the non-zero elements of the diagonalized matrix D(say) are the eigenvalues.

$$\begin{bmatrix} b_1 & b_2 & b_1^\dagger & b_2^\dagger \end{bmatrix}\begin{bmatrix} e_1 & 0 & n & 0 \\ 0 & e_2 & 0 & n \\ n & 0 & e_3 & 0 \\ 0 & n & 0 & e_4 \end{bmatrix}\begin{bmatrix} b_1^\dagger \\ b_2^\dagger \\ b_1 \\ b_2 \end{bmatrix}$$

The numerical diagonalization can be achieved by writing a Hamiltonian in matrix form and diagonalizing the corresponding matrix numerically to solve the eigenvalue problem.

Bibliography

[1] John J. Quinn, Kyung-Soo Yi, Solid State Physics: Principles and Modern Applications. Springer (2009).

[2] M. Y. Veillette, J. T. Chalker, and R. Coldea, Phys. Rev. B 71, 214426 (2005)

[3] Daniel D. Stancil, Anil Prabhakar, Spin Waves: Theory and Applications, Springer (2009).

[4] F. Bloch, Z. Physik 61, 206 (1930).

[5] F. J. Dyson, Phys. Rev. 102, 1217 (1956).

[6] S.P. Rosen, Henry Primakoff : A Biographical Memoir. National Academies Press, Washington D.C. (1995)

[7] Patrik Fazekas, Lecture Notes on Electron Correlation and Magnetism, World Scientific (1999).

[8] I. Dzyaloshinsky, J. Phys. Chem. Solids 4, 241 (1958).

[9] T. Moriya, Phys. Rev. Lett. 4, 228 (1960).

[10] T. Moriya, Phys. Rev. 120, 91 (1960).

[11] T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940).

[12] A.L. Chernyshev Phys. Rev. B. 72.174414 (2005)

[13] James Patterson, Bernard Bailey, Solid-State Physics: Introduction to the Theory, 2nd Edition, Springer-Verlag (2010).

[14] Daping Chu and Jue-lian Shen, Phys. Rev. B 44 4689 (1991).

[15] F. J. Dyson, Phys. Rev. 102, 1217 (1956) 102, 1230 (1956)

[16] S. V. Maleev, Zh. Eksp. Teor. Fiz. 30, 1010 (1957)

[17] D. J. Griffiths, Introduction to Quantum Mechanics, 2nd Edition, Pearson.

[18] M. Takahashi, Phys. Rev. B 40 2494 (1989).

[19] Jean-Paul Blaizot, Georges Ripka, Quantum Theory of Finite Systems. The MIT Press (1985)