

A STUDY OF THE J_1 - J_2 Quantum Heisenberg Antiferromagnets

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Abstract

In this thesis, we formulated the J_1 - J_2 Heisenberg Hamiltonian in terms of the pesudofermion, in which a exact constraint of single occupancy for each site is imposed through the Popov-Fedotov procedure [1]. We have also introduced a more generalized approach to apply the Hubbard-Stratonovich transformation, which enables the decoupling of the Hamiltonian with an interaction matrix that is not positive definite. The investigation of the ground state magnetic properties and low-energy excitations has been conducted within the framework of the path integral formalism. Additionally, an effective field theory is proposed for determining the critical temperature of the nematic phase of J_1 - J_2 Heisenberg model.

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Chapter 1 Introduction

The general aim of our research in the following thesis could be described as the understanding of the magnetism of insulators (or semiconductors). The microscopic physical picture that we refer to is portrayed by the Heisenberg Hamiltonian. Heisenberg model (HM) was first proposed by Werner Heisenberg in order to give a theoretical explanation for the observation of the curie temperature. The paper was published in 1928, 8 years after Wilhelm Lenz had invented the later called Ising model. As pointed out by Dirac in 1929 [2], the isotropic two-body exchange interaction in the HM is originated from taking both of the effects of the Coulomb repulsion and the Pauli exclusion principle into consideration. A more detailed illustration of this will be given in the next chapter. The limitations of such model are mentioned clearly by P.W.Anderson in his paper [3]: Due to the strong locality of the magnetic moments in HM, the exchange interaction of the Heisenberg type has its own problems in explaining the experimental results that are caused by metallic (anti-)ferromagnetism, which requires another theory that can stress the itinerant properties of these magnetic materials. And that is the reason why in the beginning of this paragraph we stressed that the type of magnetic materials that we focus on investigating in are insulators, in which the alignment of the local spins gives rise to most of the magnetic effects.

The specific one that we studied in this thesis is called antiferromagnetic spin-1/2 J_1 - J_2 quantum Heisenberg model. Since we have used the word "quantum" to describe our model, we have to first make a distinction between the classic HM and the quantum HM. Like Ising model(N=1), the classic HM(N=3) should both be classified as a O(N) model, which is formulated by the spin operators that obey the certain SU(N) Lie algebra. In our case, all the magnetic moments are being localized on the sites of a two dimensional square lattice and the occupation number of the spin on each site is constrained to be one. Only the exchange interactions between two spins that are nearest neighbors(NN) or the next nearest neighbors(NNN) are taken into consideration, and the coupling strengths are characterized by J_1 and J_2 respectively. One quite interesting scenario that could happen in such model is that a large degeneracy of ground states is found when tuning these coupling constants to fulfill $J_1 = 2J_2 > 0$. In order to describe such phenomenon, we have to introduce the concept of frustration, which can be roughly characterized by the large ground state degeneracy that we just mentioned. In our case, frustration is introduced to our system due to the competing interactions described by

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 J_1 and J_2 . Frustration can also be included by the geometry construction: for example, when only consider the NN interaction, by placing local spins on a triangular lattice instead.

In low dimensional materials, effects of both the frustration and fluctuation are relatively strong, especially in the low temperature limit. Hence, how to understand the nature of them turn out to be very crucial in order to reveal some mysteries in such materials.



Figure 1.1: Schematic phase diagram of cuprate superconductors as a function of hole doping p. [4]

One straightforward example is the puzzling narvre of the the cuprates unconventional superconductors, for example the $La_{2-x}Sr_xCuO_4$ compound. The key properties of these materials are believed to be characterized by the CuO₂ layer. In a certain low temperature range shown in Fig.1.1, as the holes are being doped into the cuprates parent compound, the system will enter a non-magnetic pseudo gap state first, and only later become superconducting as the hole concentration is further increased. In the undoped regime, the insulating antiferromagnetic state can be qualitatively explained by spin- $\frac{1}{2}$ HM. In order to give a possible explanation for such a strange phase diagram, P.W.Anderson proposed the resonating valence bond (RVB) theory in 1987 [5]. A novel non-magnetic ground state named "quantum spin liquid state" is used to capture the formation mechanism of magnetic singlet pairs. The existence of the connection between these magnetic singlet pairs and the charged Cooper pairs was also pointed out in the paper, and so that the doping of the holes might be treated as the "trigger" of transition

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processes between them. His proposal was formulated in the frame of the spin-1/2 two dimensional antiferromagnetic HM, and as we mentioned before, the quantum fluctuations in lower dimensions and the effect of frustration were considered as two essential effects to suppress the long range magnetic order, which can create the "space" for the emergence of non-magnetic (RVB) state.



Figure 1.2: A ground state phase diagram of spin-1/2 J_1 - J_2 square lattice magnets as tuning the strength of J_1 and J_2 . The NAF, FM, and CAF refer to the Néel antiferromagnetic, the ferromagnetic, and the columnar antiferromagnetic states, respectively. [6]

After we above mentioned theoretical impact of studying the J_1 - J_2 HM, we shall shortly discuss the experimental realization of it. As we can see from the Fig.1.2, multiple chemical compounds were reported that could be viewed as the J_1 - J_2 HM in different J_1/J_2 ratio. In order to get a more vivid impression of such materials, we shall briefly discuss two typical examples among them: Li₂VOSiO₄ and VOMoO₄.

The crystal structure of both Li₂VOSiO₄ and VOMoO₄Fig.1.3 are reported as the realization of the frustrated two-dimensional J_1 - J_2 HM. These two chemical compounds share several common features of their crystal structure: both have a layered structure which contains V⁴⁺ ions, located at the center of VO₅ pyramids that can be treated as local spins(S=1/2) in the quantum Heisenberg representation. Such pyramids either point upward or downward in the direction that is roughly perpendicular to the pseudo two dimensional square lattice plane formed by the V⁴⁺ ions. It is shown more clearly in the Fig.1.3(b), J_1 and J_2 can be used to describe the effective coupling strength between the V-V bonds along the side and the diagonal of the square, respectively.

However, while the in-plane alignments of V^{4+} ions in Li₂VOSiO₄ crystals is found to be in a Collinear antiferromagnetic state, in VOMoO₄ it exhibits antiferromagnetic

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order, which can be explained by the different J_1/J_2 ratio in these two compounds. This difference can be also seen from the relative angle between the pyramid and the MO₄ or SiO₄ tetrahedra. In Li₂VOSiO₄, these tetrahedras are not rotated, but they are in the VOMoO₄ case. Whether these two chemical compounds are in a weak or strong frustration regime is still not conclusive.



Figure 1.3: The crystal structure of $\text{Li}_2\text{VOSiO}_4(a)$ and $\text{VOMoO}_4(b)$. [7], where VO_5 pyramids are marked red. SiO₄ and MO₄ tetrahedras are marked grey and yellow, respectively.

We will discuss the motivation for the methodology that have been chosen for this thesis. As we mentioned above, the spin operators obey SU(N) Lie algebra, which means that these operators have their own commutation relation. Analytical method like Feynman diagram expansion is not directly adaptable to the Hamiltonian formed by spin operators, due to the "painful" fact that they do not satisfy Wick's theorem. In our work, we represent spin operators in terms of the pseudofermion. By using such method, we are able to rephrase the Hamiltonian into fermionic creation and annihilation operators, allowing us to tackle the problem with the help of the Feynman diagram expansion in the path integral formalism. In order to get the corresponding physical picture for the local spin as described in the HM, we use the Popov and Fedotov procedure (PFP) to impose such constraint, only allow the spin occupation number of each site to be exactly one.

1.1 Outline of thesis

This thesis is organized in the following way:

- 1. In chapter 2, some basics of the magnetic interaction are reviewed. After that, the origin of the magnetic exchange interaction of the Heisenberg type is discussed. The concept of superexchange interaction is introduced in the end in order to build a connection between the microscopic Heisenberg Hamiltonian and effective interactions in magnetic materials.
- 2. In **chapter** 3, we give a derivation of the path integral formalism in the fermionic case and illustrate the spirit of the Hubbard-Stratonovich transformation. In the end a of this chapter we show a way of imposing the local constraint on the site occupancy known as the Popov-Fedatov procedure.
- 3. In chapter 4, we introduce the basic properties of the J_1 - J_2 HM in order to give readers some feeling of the model.
- 4. In chapter 5 we begin with writing down the path integral formulation for the J_1 - J_2 HM. Then we perform a study of this model by using the saddle point approximation. A critical temperature for Néel and Collinear phases are found at the mean field level.
- 5. In **chapter 6** the effects of the fluctuations around the saddle point are taken into the consideration. The spin-wave dispersion relation for both Néel state and Collinear state are found. In the end the chapter, we shortly prove the Mermin–Wagner–Hohenberg Theorem.
- 6. In chapter 7 We first illustrated the key features of the nematic phase transition by a toy model. Then we perform the Feynman diagram expansion to fourth order, and an attempt for computing the T_c of nematic transition is made, but the results of which is not correct so far and a further modification towards it is needed.

Chapter 2

Exchange interaction

The concept of exchange interaction is always linked with a commonly known effect, which is the ordering phenomenon of magnetic moments in certain materials below the critical temperature. People may ask the following question: is this ordering necessary to bring in this type of exchange interaction, or can we just use magnetic dipole-dipole interactions to explain the Curie temperature instead? Unfortunately, the answer is no, and the reason is that the magnitude of magnetic dipole-dipole interactions is too small to account for the mechanism of the ordering phenomenon. The energy of the interaction of this type for two magnetic dipoles μ_1 and μ_2 , whose magnitude are described by the Bohr magneton (μ_B), takes the form:

$$E = \frac{\mu_0}{r^3} \Big[\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_1 - \frac{3}{r^2} (\boldsymbol{\mu}_1 \cdot \boldsymbol{r}) (\boldsymbol{\mu}_2 \cdot \boldsymbol{r}) \Big], \qquad (2.1)$$

where μ_0 is the magnetic constant, \mathbf{r} is a unit vector parallel to the line joining the centers of the two dipoles. r is the distance between the centers of μ_1 and μ_2 , and the magnitude of it is comparable to the lattice spacing, which is around 1 Å. Therefore, we can make an estimation by using Eq.2.1 with all the parameters we just mentioned, and if we convert this energy scale into the scale of temperature, we find that the corresponding temperature of magnetic dipolar interaction is roughly 1K, which is way smaller than the Curie temperature of most magnetic materials. For example, the Curie temperature of iron is around 1043K.

2.1 The origin of exchange interaction

To begin with, we shall consider a model with two electrons, which are located in the spatial coordinates r_1 and r_2 . Due to the fact that the electrons are ferminons and their overall wave-functions must be antisymmetric, a singlet pair acquires a symmetric spatial wave-function and a triplet pair acquires an antisymmetric spatial wave-function, as given by:

$$\Psi_S = \frac{1}{\sqrt{2}} \Big[\psi_a(\boldsymbol{r_1}) \psi_b(\boldsymbol{r_2}) + \psi_a(\boldsymbol{r_2}) \psi_b(\boldsymbol{r_1}) \Big], \qquad (2.2a)$$

$$\Psi_T = \frac{1}{\sqrt{2}} \Big[\psi_a(\boldsymbol{r_1}) \psi_b(\boldsymbol{r_2}) - \psi_a(\boldsymbol{r_2}) \psi_b(\boldsymbol{r_1}) \Big].$$
(2.2b)

We use \hat{H} to represent the Hamiltonian for our model and we can write the energy for both cases as:

$$E_S = \int \Psi_S^* \hat{H} \Psi_S d\boldsymbol{r_1} d\boldsymbol{r_2}, \qquad (2.3a)$$

$$E_T = \int \Psi_T^* \hat{H} \Psi_T d\boldsymbol{r_1} d\boldsymbol{r_2}, \qquad (2.3b)$$

$$E_S - E_T = 2 \underbrace{\int \psi_a^*(\boldsymbol{r_1}) \psi_b^*(\boldsymbol{r_2}) \hat{H} \psi_a(\boldsymbol{r_2}) \psi_b(\boldsymbol{r_1}) d\boldsymbol{r_1} d\boldsymbol{r_2}}_{I}.$$
(2.3c)

Now we have to recall some knowledge of the first quantization of the spin, in order to link the energy difference shown in Eq.2.3 with the model of two coupled spins. For a model of two coupled spins $(\frac{1}{2})$. We can use the total spin representation to get the following relations:

$$\hat{\boldsymbol{S}}_{tot} = \hat{\boldsymbol{S}}_a + \hat{\boldsymbol{S}}_b, \tag{2.4a}$$

$$\hat{S}_{a/b}^{2}|S\rangle = \frac{3}{4}|S\rangle$$
 (S = $\frac{1}{2}$), (2.4b)

$$\hat{S}_{tot}^2 |S\rangle = S(S+1) |S\rangle$$
 (S = 0, 1). (2.4c)

From Eq.2.4 it is not difficult to show that the operator of $\hat{S}_a \cdot \hat{S}_b$ takes the following eigenvalues:

$$\hat{\boldsymbol{S}}_{a} \cdot \hat{\boldsymbol{S}}_{b} = \begin{cases} -\frac{3}{4} & (S = 0, \text{ Singlet pair}) \\ +\frac{1}{4} & (S = 1, \text{ Triplet pair}). \end{cases}$$
(2.5)

Using the J that has been defined in Eq.2.3c, we can further write:

$$2J(\frac{1}{4} - \hat{\boldsymbol{S}}_a \cdot \hat{\boldsymbol{S}}_b) = \begin{cases} 2J & (S = 0, \text{ Singlet pair}) \\ 0J & (S = 1, \text{ Triplet pair}). \end{cases}$$
(2.6)

By putting together Eq.2.3c and Eq.2.6 we have:

$$E_{S/T} = E_0 + 2J(\frac{1}{4} - \hat{S}_a \cdot \hat{S}_b) = \underbrace{(E_0 + \frac{J}{2})}_{\text{const.}} - 2J\hat{S}_a \cdot \hat{S}_b.$$
(2.7)

As the final step, we can simply absorb the constant part in Eq.2.7 into chemical potential and arrive at our effective Heisenberg Hamiltonian:

.

$$\hat{H}_{\text{eff}} = -2J\hat{S}_a \cdot \hat{S}_b \tag{2.8}$$

2.2 The basic of superexchange

First we should examine the sign of the formulation of J that is defined by Eq.2.3c. This term can be described as the self energy of the charge distribution $\psi_a^*(\mathbf{r_1})\psi_b(\mathbf{r_2})$ and it is valid only for truly orthogonal orbitals. Hence, it is expected to acquire a small positive value, and this mean a weak ferromagnetism is always favoured in order to lower the energy. On the other hand, the universal existence of the chemical bonds that characterized by the electron pairs with opposite spin suggest that we are still missing a term that accounts for the mechanism of antiferromagnetism.

In order to come up with a mechanism for antiferromagnetism, we should first think about in what sense the spin singlet pair can lower the energy compared to the triplet pairs. Following this idea, we notice that what we are missing should be the tunneling effect of electrons between the neighbouring lattice sites. This effect is only allowed for anti-parallel spin pairs due to the Pauli exclusive principle, and it is really this delocalization of electron pairs with opposite spin that actually lower the kinetic energy of each electron.



Figure 2.1: A picture of the connection between the delocalization of electron pair and the kinetic energy sketched by the idea of particle in the box.

In Fig.2.1 we borrow the idea of "particle in the box" to examine the kinetic energy of each electron on each lattice site. Since we have the electron pairs with opposite spin, they are allowed to move between neighbouring lattice sites which can be qualitatively imagined as moving in a "box" which has a length comparable to the atomic spacing. The electrons are more localized around the ion if they acquire the same spin, and this shrinks the size of the box and cause a significant increase of the kinetic energy of each electron. As discussed in Chapter 2.2 of [8], with the help of applying the second quantization of spin to the Hubbard model, we can show the tunneling effect can result in antiferromagnetism analytically. To begin with, we shall first introduce the auxiliary-fermion formulation for later convenience:

$$\boldsymbol{S_i} = f_{i\alpha}^{\dagger} (\frac{\boldsymbol{\sigma}}{2})_{\alpha\beta} f_{i\beta}, \qquad (2.9)$$

where we note:

$$\boldsymbol{\sigma} = (\underline{\sigma_1}, \underline{\sigma_2}, \underline{\sigma_3}) = \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right)$$
(2.10)

In the Hubbard model, the tunneling intensity between the neighbouring sites is characterized by t, and the Coulomb interaction is described by the factor U. So the Hamiltonian takes the following form:

$$\hat{H} = \underbrace{-t \sum_{\langle ij \rangle} f_{i\sigma}^{\dagger} f_{j\sigma}}_{\hat{H}_t} + \underbrace{U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}_{\hat{H}_U}.$$
(2.11)

Table 2.1: A table for different occupation scenarios of two sites model

Site A	Site B	\hat{H}
$\uparrow\downarrow$	0	$\hat{H}_t + \hat{H}_U$
0	$\uparrow\downarrow$	$\hat{H}_t + \hat{H}_U$
\uparrow	\downarrow	\hat{H}_t
\downarrow	\uparrow	\hat{H}_t
\uparrow	\uparrow	0
\downarrow	\downarrow	0

From Table 2.1 we can learn that in the limit of $\frac{U}{t} \gg 1$, the term of \hat{H}_U is significantly larger than \hat{H}_t , which results in a ground state that prefers a single occupancy on each lattice site. For the sake of probing more properties of the spin alignment of the ground state, we shall impose a perturbation theory in the following way: the general idea is by treating the term \hat{H}_t as a week perturbation of \hat{H}_U , we can get the expression of the effective Hamiltonian \hat{H}_{eff} . To begin with, we are always allowed to perform a unitary transformation (change of basis) to our Hamiltonian:

.

$$U\hat{H}U^{\dagger} = \hat{\mathcal{H}}.$$
 (2.12)

Here we have to restrict the form of our unitary transformation as follows, which preserves the Lie structure of the problem:

$$U = e^{-t\hat{G}}, \quad \text{with:} \ \hat{G} = -\hat{G}^{\dagger}.$$
 (2.13)

Inserting Eq.2.13 into Eq.2.12 and apply the **Baker–Campbell–Hausdorff** formula we can get:

$$\hat{\mathcal{H}} = e^{-t\hat{G}}\hat{H}e^{t\hat{G}} = \hat{H} - \frac{t}{1!}[\hat{G},\hat{H}] + \frac{t^2}{2!}[\hat{G},[\hat{G},\hat{H}]] + \cdots$$
(2.14)

Because we are interest in the limit $\frac{U}{t} \gg 1$, we can neglect the higher order correction terms of t to get the following effective Hamiltonian:

$$\hat{\mathcal{H}}_{\text{eff}} = \hat{H} - t[\hat{G}, \hat{H}] + O(t^3) = \hat{H}_U + t[\hat{H}_t, \hat{G}] + \underbrace{\hat{H}_t + t[\hat{H}_U, \hat{G}]}_{\text{Term 1}}.$$
(2.15)

Now we can apply the ansatz $\hat{G} = \frac{1}{tU}(\hat{P}_s\hat{H}_t\hat{P}_d - \hat{P}_d\hat{H}_t\hat{P}_s)$ in order to get rid of the Term 1 shown in Eq.2.15 and fulfill the restriction of \hat{G} described in Eq.2.13 at the same time. By inserting this ansatz into Eq.2.15 we have:

$$\hat{\mathcal{H}}_{\text{eff}} = \hat{H}_U + t[\hat{H}_t, \frac{1}{tU}(\hat{P}_s\hat{H}_t\hat{P}_d - \hat{P}_d\hat{H}_t\hat{P}_s)].$$
(2.16)

Where \hat{P}_s and \hat{P}_d represent the projection operator to the single and double occupied subspace, respectively. We can further project the effective Hamiltonian to the single occupation subspace to get:

$$\hat{P}_{s}\hat{\mathcal{H}}_{\text{eff}}\hat{P}_{s} = -2\frac{t^{2}}{U}\hat{P}_{s}\Big(1 + f_{i\sigma}^{\dagger}f_{j\sigma'}^{\dagger}f_{i\sigma'}f_{j\sigma}\Big)\hat{P}_{s} = J\hat{P}_{s}\Big(-\frac{1}{2}f_{i\sigma}^{\dagger}f_{j\sigma'}^{\dagger}f_{i\sigma'}f_{j\sigma} - \frac{1}{2}\Big)\hat{P}_{s}, \quad (2.17)$$
where $J = \frac{4t^{2}}{U}$.

Then we shall link the expression in Eq.2.17 with the spin operators by using the second quantization of the spin shown in Eq.2.9:

$$\hat{\boldsymbol{S}}_{i} \cdot \hat{\boldsymbol{S}}_{j} = \frac{1}{4} \sum_{\alpha,\beta,\gamma,\eta} f_{i\alpha}^{\dagger}(\boldsymbol{\sigma})_{\alpha\beta} f_{i\beta} \cdot f_{j\eta}^{\dagger}(\boldsymbol{\sigma})_{\eta\gamma} f_{j\gamma}.$$
(2.18)

We shall carry out the sum over Pauli-matrixes first by using following identity:

$$(\boldsymbol{\sigma})_{\alpha\beta} \cdot (\boldsymbol{\sigma})_{\eta\gamma} = 2\delta_{\alpha\gamma}\delta_{\beta\eta} - \delta_{\alpha\beta}\delta_{\gamma\eta}.$$
(2.19)

Applying Eq.2.19 to Eq.2.18 and carries out the sum over spins, we will ended up with:

$$\hat{\boldsymbol{S}}_{i} \cdot \hat{\boldsymbol{S}}_{j} = \frac{1}{2} f_{i\alpha}^{\dagger} f_{i\beta} f_{j\beta}^{\dagger} f_{j\alpha} - \frac{1}{4} f_{i\alpha}^{\dagger} f_{i\alpha} f_{j\beta}^{\dagger} f_{j\beta}.$$
(2.20)

Recalling the anti-commutation relation of fermions

$$\{f_{i\alpha}^{\dagger}, f_{j\beta}\} = \delta_{ij}\delta_{\alpha\beta} \qquad \{f_{i\alpha}^{\dagger}, f_{j\beta}^{\dagger}\} = \{f_{i\alpha}, f_{j\beta}\} = 0, \tag{2.21}$$

we can swap the first term of Eq.2.20 to get:

$$\hat{\boldsymbol{S}}_{i} \cdot \hat{\boldsymbol{S}}_{j} = -\frac{1}{2} f_{i\alpha}^{\dagger} f_{j\beta}^{\dagger} f_{i\beta} f_{j\alpha} - \frac{1}{4} \hat{n}_{i} \hat{n}_{j}.$$

$$(2.22)$$

By inserting Eq.2.22 into Eq.2.17 we can get the final description of the effective Hamiltonian that is achieved by perturbation theory:

$$\hat{P}_s \hat{\mathcal{H}}_{\text{eff}} \hat{P}_s = J \Big(\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j - \frac{1}{4} \Big).$$
(2.23)

From Eq.2.23 it is clear to see that since $J = \frac{t^2}{U} > 0$, the antiferromagnetic spin configuration is more favourable now with the consideration of the tunneling effect as the perturbation of the strong Coulomb onsite repulsion. The projection operators appear in Eq.2.23 tell us that the electron system that is related to the Heisenberg Hamiltonian should be considered as the scenario of single occupancy of each site, namely the system is in the insulating phase. And in order to fulfill this constrain, we can use a specific method involves a kind of single occupancy projector and it is known as the Popov-Fedotov procedure. This method will be discussed in the following chapter. In this way, we managed to show that by considering hybridization effects between two orbitals of the electrons on neighbouring sites, anti-parallel spins can take advantage of the tunneling effect to lower their kinetic energy.



Figure 2.2: The crystal structure of manganese (II) oxide. Purple: Mn, red: O

Then, we shall briefly discuss about what mechanism is possible to account for this kind of neighbouring magnetic orbitals hybridization in real materials, namely the **superechange**. First of all, the direct overlap between neighbouring magnetic orbitals is usually very small and insufficient to determine the magnetic properties of the material. This is mainly because in rare earths or even transition metals, the electrons are localized closely around the nucleus, hence the overlap between the probability density of two neighbouring electrons is very small. In order to find a more realistic picture for

such mechanism, we have to consider the **indirect exchange interaction** in the ionic solids. Let us now look at the example of one antiferromagnet: Manganese (II) Oxide (MnO). The crystal structure of MnO is shown in Fig.2.2, in which the dashed box marks an important structure that connected with the mechanism of the superexchange. The superexchange can be imagined as an indirect exchange interaction between two non-neighbouring magnetic ions (Mn²⁺) that is mediated by a non-magnetic ion (O²⁻) in the middle, or so to speak, the co-tunneling effect. With the help of valence electrons in the oxygen orbitals, the hybridization intensity is significantly increased. In general, the above superexchange mechanism results in anti-ferromagnetism, and only in few cases can lead to ferromagnetism, which is due to the existence of Hund's coupling when more than one orbitals need to be taken into consideration.

In conclusion, we first discussed about the origins of the Heisenberg Hamiltonian, which can be attributed to the interplay between the Coulomb interaction and the Pauli exclusion principle. Afterwards, the tunneling effect is considered in order to provide an explanation for the common occurrence of antiferromagnetism in real materials. Furthermore, we also stressed the significant role played by the indirect mechanism of superexchange in this context.

Chapter 3

Theoretical background

3.1 Path Integral formalism

The Feynman path integral is a vivid way of formulating and illustrating the relation between quantum mechanics and classical mechanics. The probability amplitude for a particle propagating from state $|i\rangle$ to state $|f\rangle$ has the following formulation:

$$\langle f | e^{\frac{-i\hat{H}t}{\hbar}} | i \rangle = \sum_{\text{Path: } i \to f} \exp\left[i\frac{S_{Path}}{\hbar}\right]$$
 (3.1)

As we can see from above, if we go to the classical limit $(\hbar \to 0)$, those paths that do not fulfill the condition $\delta S[x] = 0$, but acquire a strong oscillating phase ($\varphi = \frac{S_{Path}}{\hbar} \to \pm \infty$), which means that the contribution of these paths average to zero after carrying out the sum, hence the only one remains is the classical path that minimizes the action. We can use the **stationary phase approximation** to include quantum effects into the frame of the classic limit. We shall not discuss the details about this method here, but the similar method is used in **Chapter 6** in order to consider effects of the quantum fluctuations. In the context of the path integral formalism, one may imagine these quantum fluctuations as a smearing effect to the boundary of the classical path.

By using the same strategy of summing over all the possible trajectories of a moving particle that described by the time evolution operator, we can sum over all the possible configurations of the quantum field that described by the Boltzmann density matrix, since these two operators have a similar structure $\left(e^{\frac{-i\hat{H}t}{\hbar}}\right)$ and $e^{-\beta\hat{H}}$. In order to do so, like we find the eigenstate of coordinate and momentum operators for the single-particle quantum mechanics, naturally we want to find the expression for the eigenstate of the creation and annihilation operators, which are widely used for the many body system. Mathematically, coherent states are possible to be defined as the **eigenstates of the annihilation operators**:

$$|\phi\rangle = e^{\xi \sum_{i} \phi_{i} \hat{a}_{i}^{\dagger}} |0\rangle, \qquad (3.2)$$

where $\xi = 1(-1)$ for Bosons(Fermions). From Eq.3.2 we can use the commutation relations of the bosonic and fermionic operators to have:

$$[\hat{a}_{\eta}, \hat{a}_{\lambda}]_{\pm} |\phi\rangle = [a_{\eta}, a_{\lambda}]_{\pm} |\phi\rangle = 0.$$
(3.3)

Chapter 3 Theoretical background

From Eq.3.3 we notice that the eigenvalues of the bosonic annihilation operators (+) obey the commutation relations and thus can be represented by complex numbers, while for fermionic annihilation operators (-), they obey anti-commutation relation, which requires a new definition. This kind of numbers are actually classified as the **Grassman numbers**. We will use the notation: \bar{a}_{λ} to represent the conjugate of a_{λ} in the following discussions.

Here we give a prove of the following identity:

$$\mathcal{Z} = \operatorname{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] = \int D[\overline{\psi},\psi]e^{-S[\overline{\psi},\psi]},\qquad(3.4a)$$

$$S[\overline{\psi},\psi] = \int_0^\beta d\tau \Big(\overline{\psi}\partial_\tau \psi + H[\overline{\psi},\psi] - \mu N[\overline{\psi},\psi]\Big), \qquad (3.4b)$$

which constitutes the central expression of the Path integral formalism. Due to the limitation of the length of this thesis, we shall show this derivation for fermions, which can be easily extended to the case of bosons.

First, one can define a complete set of Fock space states $(|n\rangle)$, then we can further write the left hand side of the Eq.3.4a as:

$$\mathcal{Z} = \sum_{n} \langle n | e^{-\beta(\hat{H} - \mu \hat{N})} | n \rangle .$$
(3.5)

Here we first introduce the expression for the **resolution of the identity**:

$$\int d[\overline{\psi}_0, \psi_0] e^{-\overline{\psi}_0 \psi_0} |\psi_0\rangle \left\langle \overline{\psi}_0 \right| = \mathbb{I}.$$
(3.6)

Now we are allowed to insert this identity into Eq.3.5,

$$\mathcal{Z} = \int d[\overline{\psi}_0, \psi_0] e^{-\overline{\psi}_0 \psi_0} \sum_n \langle n | \psi_0 \rangle \left\langle \overline{\psi}_0 \right| e^{-\beta (\hat{H} - \mu \hat{N})} | n \rangle .$$
(3.7)

The fermionic coherent states fulfill $\langle n|\psi_0\rangle \left\langle \overline{\psi}_0 \right| n \right\rangle = \left\langle -\overline{\psi}_0 \left| n \right\rangle \langle n|\psi_0\rangle$, so that we can carry out the sum over states $|n\rangle$ and get:

$$\mathcal{Z} = \int d[\overline{\psi}_0, \psi_0] e^{-\overline{\psi}_0 \psi_0} \left\langle -\overline{\psi}_0 \right| e^{-\beta(\hat{H} - \mu \hat{N})} \left| \psi_0 \right\rangle.$$
(3.8)

First of all, we have to apply the **antiperodic (perodic) boundary condition**, for fermion (bosons) which forces $\overline{\psi}_N = -\overline{\psi}_0$ ($\overline{\psi}_N = \overline{\psi}_0$). Then we can reformulate $e^{-\beta(\hat{H}-\mu\hat{N})}$ into $(e^{-\Delta\tau(\hat{H}-\mu\hat{N})})^N$, where $\Delta\tau = \frac{\beta}{N}$. In the end we insert the **resolution** of identity N-1 times into Eq.3.8 and get:

$$\mathcal{Z} = \int \underbrace{\left[\prod_{i=1}^{N} d[\overline{\psi}_{i}, \psi_{i}]\right]}_{D[\overline{\psi}, \psi]} e^{-\sum_{i=1}^{N} \overline{\psi}_{i} \psi_{i}} \prod_{i=1}^{N} \left\langle \overline{\psi}_{i} \right| \underbrace{e^{-\Delta \tau (\hat{H} - \mu \hat{N})}}_{\approx 1 - \Delta \tau (\hat{H} - \mu \hat{N})} |\psi_{i-1}\rangle.$$
(3.9)

Using the properties of the coherent states: $\langle \overline{\psi_i} | \psi_j \rangle = e^{\overline{\psi_i} \psi_j}$ and expanding the exponential to first order we can get:

$$\mathcal{Z} = \int D[\overline{\psi}, \psi] e^{-\sum_{i=0}^{N} \Delta \tau \left[\overline{\psi}_i(\frac{\psi_i - \psi_{i-1}}{\Delta \tau}) + H[\overline{\psi}, \psi] - \mu N[\overline{\psi}, \psi]\right]},$$
(3.10)

which in the limit of $N \to \infty$ gives:

$$\mathcal{Z} = \int D[\overline{\psi}, \psi] e^{-\int_0^\beta d\tau \left(\overline{\psi}\partial_\tau \psi + H[\overline{\psi}, \psi] - \mu N[\overline{\psi}, \psi]\right)}.$$
(3.11)

In practice, we usually perform the Fourier transformation so that we can diagonalize our derivative operators. This is done in a similar way in the case of real time. Here we have to use the expressions of the matsubara frequencies for bosons and fermions in order to fulfill the **periodic and antiperiodic** boundary conditions, respectively:

$$\psi(\tau_B) = \frac{1}{\sqrt{\beta}} \sum_{i\nu_m} e^{-i\nu_m \tau} \psi(i\nu_m) \qquad i\nu_m = \frac{2n\pi}{\beta}$$
(Boson) (3.12a)

$$\psi(\tau_F) = \frac{1}{\sqrt{\beta}} \sum_{i\omega_n} e^{-i\omega_n \tau} \psi(i\omega_n) \qquad i\omega_n = \frac{(2n+1)\pi}{\beta} \qquad (\text{Fermion}). \tag{3.12b}$$

The path integral is exactly solvable when it take the form of the Gaussian integral, for a single real variable is

$$\int_{\infty}^{\infty} dx e^{-\frac{1}{2}ax^2 + bx} = e^{\frac{b^2}{2a}} \sqrt{\frac{2\pi}{a}} \qquad (a > 0).$$
(3.13)

The Gaussian integral can be readily extended to the case of bosonic operators which is the complex matrix version of it:

$$\int \left[\prod_{\alpha} \frac{d\overline{Z}_{\alpha} dZ_{\alpha}}{2\pi i}\right] e^{-\overline{\underline{Z}}\left[\underline{\underline{M}}\right]\underline{Z} + \overline{\underline{J}} \underline{Z} + \overline{\underline{Z}} \underline{J}} = (\det \underline{\underline{M}})^{-1} e^{\overline{\underline{J}}\left[\underline{\underline{M}}^{-1}\right]\underline{J}}.$$
(3.14)

The single underline and double underline stress that the variable should be viewed as a vector and a matrix, respectively.

Similarly one can show that in the fermionic case this Gaussian integral takes the following form instead:

$$\int \left[\prod_{j} d\bar{c}_{j} dc_{j}\right] e^{-\underline{\bar{c}}\left[\underline{\underline{M}}\right]\underline{c} + \underline{\overline{J}} \underline{c} + \underline{\overline{c}} \underline{J}} = (\det \underline{\underline{M}}) e^{\underline{\overline{J}}\left[\underline{\underline{M}}^{-1}\right]\underline{J}}.$$
(3.15)

By generalizing Gaussian integral we are able to deal with an action that contains with quadratic terms, and one point that needs to be stress is that the matrix \underline{M} above has to be a **positive definite** matrix in order to make the integration converge.

Chapter 3 Theoretical background

However, when dealing with interactions (for example Coulomb interaction), one normally has to consider a non-Gaussian integral which contains a quartic term inside the action. Therefore we need a method to decouple the fermionic quartics, and that can be done by **Hubbard-stratonovich transformation**. As we can see from Fig.3.1, after carrying out the whole procedure of the Hubbard-stratonovich transformation, the quartics are decoupled into bilinears that are coupled to a fluctuating Weiss field, which is actually a combination of the white noise field and the physical field. Then, we can absorb this Weiss field term into the prefactors of the bilinears, so that we managed to reduce the partition function as the Gaussian integral. We shall not show the prove of the Hubbard-stratonivich transformation here, for we will show a derivation of it in section 4.1.



Figure 3.1: The procedure of the Hubbard-stratonovich transformation, where the grey and orange diamond represent the white noise field and the Weiss field respectively.

In a short conclusion, so far we managed to show the process of adapting the Feynman path integral method into the quantum many body system, which is in our great interest. In the later chapters we will show how to perform a study of J_1 - J_2 Heisenberg model in the path integral formalism.

3.2 The Popov-Fedotov procedure(PFP)

The Popov-Fedatov method [1] manages to impose a local constrain of exact single occupancy per site in a ingenious way such that it allows the Feynman diagram expansion for spin operators within only a small modification to the matsubara frequencies of the fermionic propagator. Once again, in the auxiliary-fermion formulation, spin- $\frac{1}{2}$ can be represented by fermionic field operators and the corresponding elements in Pauli matrices:

$$\boldsymbol{S_i} = f_{i\alpha}^{\dagger} (\frac{\vec{\sigma}}{2})_{\alpha\beta} f_{i\beta}. \tag{3.16}$$

However, the auxiliary-fermion formulation of spin brings in two nonphysical states which are zero occupation and double occupation of a single site on the lattice. As we have shown in section 2.2, the Heisenberg Hamiltonian is an effective Hamiltonian for the half filled Hubbard model and therefore a local constrain in each site i is needed in order to project all possible states to the physical states for the lattice model only.

$$\sum_{\alpha} f_{i\alpha}^{\dagger} f_{i\alpha} = n_f^{(i)} = 1 \qquad (\alpha = \uparrow, \downarrow).$$
(3.17)

For example if we have N lattice sites on a square lattice, and m is some set of physical quantum numbers and in the Fock space of the pesudofermion, a state can be written as:

 $|m, n_1, n_2, n_3 \cdots n_i \cdots n_N\rangle$ $(n_i = 0, 1, 2).$ (3.18)

The only physical state that we care about can be written as:

$$|\mathbf{Physical}\rangle = |m, 1, 1, 1, \cdots, 1, \cdots, 1\rangle.$$
(3.19)

Then, we know that any nonphysical state should contains at least one zero or double occupation site, and the nonphysical states must appear in pairs of a given site n_i , for example we can have such two states that only have occupation number different on site i:

$$|\mathbf{Nonphysical-i0}\rangle = |m, 2, 0, 1, \cdots, n_i = 2, \cdots, 1\rangle,$$
 (3.20a)

$$|\mathbf{Nonphysical-i2}\rangle = |m, 2, 0, 1, \cdots, n_i = 0, \cdots, 1\rangle.$$
 (3.20b)

Notice that the spin operators has following properties:

$$\hat{\boldsymbol{S}}_i |\mathbf{Nonphysical-i0}\rangle = 0,$$
 (3.21a)

$$\hat{\boldsymbol{S}}_i | \mathbf{Nonphysical-i2} \rangle = 0.$$
 (3.21b)

Which will leads to the same eigenenergy for both states:

$$\hat{H} | \mathbf{Nonphysical-i0} \rangle = E_{i0} | \mathbf{Nonphysical-i0} \rangle, \qquad (3.22a)$$

$$\hat{H} | \mathbf{Nonphysical-i2} \rangle = E_{i2} | \mathbf{Nonphysical-i2} \rangle.$$
 (3.22b)

$$E_{i0} = E_{i2}$$
 (3.23)

The beauty of this method is that an imaginary chemical potential for pesudo-fermions is introduced to project out these pairs of nonphysical states with each other:

$$\lambda_f = i\pi \frac{T}{2} \tag{3.24}$$

Then, the partition function of the Hamiltonian is written as follows:

$$Z_{ppv} = \text{Tr}[e^{-\beta[H+\sum_{i} i\pi \frac{T}{2}(n_f^{(i)}-1)]}] = (-i)^N \text{Tr}[e^{-\beta H^{(ppv)}}].$$
 (3.25)

If we write out the explicit form of the trace we will find:

$$(-i)^{N} \operatorname{Tr}[e^{-\beta H^{(ppv)}}] = (-i)^{N} \sum_{m} \sum_{n_{1}, \cdots, n_{N}} \langle m, n_{1}, \cdots n_{i} \cdots n_{N} | e^{-\beta H^{(ppv)}} | m, n_{1}, \cdots n_{i} \cdots n_{N} \rangle$$

$$(3.26)$$

Now with this complex chemical potential in our Hamiltonian, we will find the following fact:

$$\langle \mathbf{Nonphysical-i0} | e^{-\beta H^{(ppv)}} | \mathbf{Nonphysical-i0} \rangle = e^{-i\frac{\pi}{2}} E_{i0},$$
 (3.27a)

$$\langle \mathbf{Nonphysical-i2} | e^{-\beta H^{(ppv)}} | \mathbf{Nonphysical-i2} \rangle = e^{i\frac{\pi}{2}} E_{i2}.$$
 (3.27b)

It is obvious now that these two elements will sum to zero after applying the complex chemical potential, and if we keep computing in pairs like this we can first find that we ended up projecting only onto the physical states with respect to site i, and then repeating this process site by site we can eventually show that:

$$(-i)^{N} \operatorname{Tr}[e^{-\beta H^{(ppv)}}] = (-i)^{N} \sum_{m} \langle m, 1, \dots 1 \dots 1 | e^{-\beta H^{(ppv)}} | m, 1, \dots 1 \dots 1 \rangle$$
$$= (-i)^{N} \sum_{m} \langle m, 1, \dots 1 \dots 1 | e^{-\beta H} | m, 1, \dots 1 \dots 1 \rangle$$
$$= (-i)^{N} \mathbf{Z}.$$
(3.28)

After that we can introduce a physical operator $\hat{\mathcal{O}}$ that is consisted with linear combination of spin operators, and it's expectation value in the Popov-Fedatov method is computed as:

$$\langle \hat{\mathcal{O}}^{(ppv)} \rangle = \frac{(-i)^N \operatorname{Tr}[e^{-\beta H^{(ppv)}} \hat{\mathcal{O}}]}{(-i)^N \operatorname{Tr}[e^{-\beta H^{(ppv)}}]}.$$
(3.29)

Since we already know the expression for the numerator of Eq.3.29 we only need to compute the denominator:

$$(-i)^{N} \operatorname{Tr}[e^{-\beta H^{(ppv)}} \hat{\mathcal{O}}] = (-i)^{N} \sum_{m} \sum_{n_{1}, \cdots, n_{N}} \langle m, n_{1}, \cdots n_{i} \cdots n_{N} | e^{-\beta H^{(ppv)}} \hat{\mathcal{O}} | m, n_{1}, \cdots n_{i} \cdots n_{N} \rangle$$

$$(3.30)$$

Then we need to introduce an identity commonly used in quantum mechanics:

$$1 = \sum_{m'} \sum_{n'_1, \cdots, n'_N} |m', n'_1, \cdots n'_i \cdots n'_N\rangle \langle m, n'_1, \cdots n'_i \cdots n'_N|.$$

$$(3.31)$$

Inserting this identity into Eq.3.30 we will find that:

$$(-i)^{N} \operatorname{Tr}[e^{-\beta H^{(ppv)}} \hat{\mathcal{O}}] = (-i)^{N} \sum_{m} \sum_{n_{1}, \cdots, n_{N}} \langle m, n_{1}, \cdots n_{i} \cdots n_{N} | e^{-\beta H^{(ppv)}} \hat{\mathcal{O}} | m, n_{1}, \cdots n_{i} \cdots n_{N} \rangle$$
$$= (-i)^{N} \sum_{m} \sum_{n_{1}, \cdots, n_{N}} \langle m, n_{1}, \cdots n_{N} | e^{-\beta H^{(ppv)}} | m, n_{1}, \cdots n_{N} \rangle$$
$$\times \langle m, n_{1}, \cdots n_{N} | \hat{\mathcal{O}} | m, n_{1}, \cdots n_{N} \rangle.$$
$$(3.32)$$

The expectation value of the operator \mathcal{O} has the same eigenenergy for a pair of states that only have difference on the occupancy on single site (zero and double). Therefore, the total sum of the expectation value of the operator \mathcal{O} becomes identical to the state that only allow single occupancy:

$$(-i)^{N} \operatorname{Tr}[e^{-\beta H^{(ppv)}} \hat{\mathcal{O}}] = (-i)^{N} \sum_{m} \langle m, 1, \cdots 1 \cdots 1 | e^{-\beta H^{(ppv)}} \hat{\mathcal{O}} | m, 1, \cdots 1 \cdots 1 \rangle$$

$$= (-i)^{N} \sum_{m} \langle m, 1, \cdots 1 \cdots 1 | e^{-\beta H} \hat{\mathcal{O}} | m, 1, \cdots 1 \cdots 1 \rangle \qquad (3.33)$$

$$= (-i)^{N} \operatorname{Tr}[e^{-\beta H} \hat{\mathcal{O}}].$$

Finally by combining Eq.3.28, Eq.3.29 and Eq.3.33 we can get:

$$\langle \hat{\mathcal{O}}^{(ppv)} \rangle = \frac{(-i)^N \operatorname{Tr}[e^{-\beta H^{(ppv)}} \hat{\mathcal{O}}]}{(-i)^N \operatorname{Tr}[e^{-\beta H^{(ppv)}}]} = \frac{\operatorname{Tr}[e^{-\beta H} \hat{\mathcal{O}}]}{\operatorname{Tr}[e^{-\beta H}]}.$$
(3.34)

Then we have shown the following identity:

$$\langle \hat{\mathcal{O}}^{(ppv)} \rangle = \langle \hat{\mathcal{O}} \rangle_{\text{Physical.}}$$
 (3.35)

In conclusion, we proved that by introducing the imaginary chemical potential into the Hamiltonian, the contribution to the partition function of the nonphysical states are all canceled out by pairs, which eventually leaves an identical expectation value to the physical expectation value of the observable. Later we will apply this method to our square lattice J_1 - J_2 Heisenberg model. Practically, if we want to apply this method to Feynman diagram expansion for spin- $\frac{1}{2}$ system, we can use a propagator with a shifted matsubara frequency $\tilde{\omega}_n = 2\pi T (n + \frac{1}{4})$. For example a bare propagator looks like:

$$\mathcal{G}(i\tilde{\omega_n}) = \frac{1}{i\omega_n - \lambda_f} = \frac{1}{i2\pi T(n + \frac{1}{4})} = \frac{1}{i\tilde{\omega_n}}.$$
(3.36)

Chapter 4

The J_1 - J_2 Heisenberg model

In the J_1 - J_2 Heisenberg model, all spins are considered to be located on the sites of a square lattice, and the occupation number of the electron on each site should be exactly one. For our convenience, the lattice spacing a is set to one in the following discussion. The interaction strength between the nearest and the next nearest neighbours are characterized by the factor of J_1 and J_2 , respectively. Therefore we can represent the J_1 - J_2 Heisenberg model by the following Hamiltonian:

$$H = \frac{J_1}{2} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{J_2}{2} \sum_{\langle \langle ij \rangle \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

= $\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j,$ (4.1)

where in above, $\langle ij \rangle$ and $\langle \langle ij \rangle \rangle$ denote the nearest and the next nearest neighbours, respectively. J_{ij} represent the matrix elements of the interaction matrix.



Figure 4.1: The plot of the structure of J_1 - J_2 Heisenberg model in two penetrating Néel lattices, which are stressed in the color of black and blue respectively.

As we have shown in Fig.4.1, we can define two sub-lattices which are known as the Néel lattices. In this way, we can view J_1 (J_2) as the coupling intensity between (within) two Néel lattices respectively.

In order to find the ground state of the J_1 - J_2 Heisenberg model for a give value of J_1 and J_2 in the classical limit, we can use Fourier transformation to diagonalize our Hamiltonian and find the lowest eigenvalue and the corresponding eigenvector. This is done by using the Fourier conventions:

$$\boldsymbol{S_i} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\boldsymbol{r_i}} \boldsymbol{S_q}$$
(4.2)

$$\boldsymbol{S}_{\boldsymbol{q}} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{i}} e^{-i\boldsymbol{q}\boldsymbol{r}_{\boldsymbol{i}}} \boldsymbol{S}_{\boldsymbol{i}}$$
(4.3)

Due to the fact that J_{ij} only depends on the relative distance between sites *i* and *j*, we can use the following Fourier convention for it:

$$J_{ij} = \frac{1}{N} \sum_{\boldsymbol{q}} e^{i\boldsymbol{q}(\boldsymbol{r_i} - \boldsymbol{r_j})} J_{\boldsymbol{q}}$$

$$\tag{4.4}$$

$$J_{\boldsymbol{q}} = \sum_{\boldsymbol{i}} e^{-i\boldsymbol{q}(\boldsymbol{r}_{\boldsymbol{i}} - \boldsymbol{r}_{\boldsymbol{j}})} J_{ij} \tag{4.5}$$

Then we can perform the Fourier transformation of Eq.4.1 to get:

$$H = \frac{1}{2} \sum_{\boldsymbol{q}} J_{\boldsymbol{q}} \boldsymbol{S}_{\boldsymbol{q}} \cdot \boldsymbol{S}_{-\boldsymbol{q}}$$
(4.6)

with

$$J_{q} = 2J_{1}(\cos q_{x} + \cos q_{y}) + 4J_{2}\cos q_{x}\cos q_{y}.$$
(4.7)

From Eq.4.7, for a given $J_1 > 0$ and $J_2 > 0$, we can find the magnetic wave vector $\boldsymbol{q} = (q_x, q_y)$ that minimizes $J_{\boldsymbol{q}}$, which corresponds to the classical ground state configuration of our spin system. As shown in Fig.4.2, in the limit $\frac{J_2}{J_1} < 0.5$, we obtain $\boldsymbol{q} = (\pi, \pi)$ and the ground state is found to be in the Néel state, in which all the spins are aligned anti parallel to all their nearest neighbours. Nevertheless, in the limit $\frac{J_2}{J_1} > 0.5$, we have $\boldsymbol{q} = (0, \pi)$ or $\boldsymbol{q} = (\pi, 0)$ and the ground state is found to be in the Collinear state, in which all the spins (1) aligned anti parallel to all their nearest neighbours along either the X or Y direction, and (2) aligned parallel to all their nearest neighbours a different direction. One special case that needs to be stressed is when the system is finely tuned to be in the limit $\frac{J_2}{J_1} = 0.5$. In this case a infinite number of \boldsymbol{q} are found on the edge of the first Brillouin zone, which implies that there is a massive ground state degeneracy and it is in this regime that the frustration of each spin is maximized.

Here we want to give a more detailed discussion of the meaning of **frustration**, and let us start with following equation:

$$[S_i^x, \boldsymbol{S_i} \cdot \boldsymbol{S_j}] = i\hbar(S_i^z S_j^y - S_i^y S_j^z).$$
(4.8)



Figure 4.2: The upper figures are the contour plot of J_q in the regime:(a) $\frac{J_2}{J_1} = 0.2$, (b) $\frac{J_2}{J_1} = 0.5$,(c) $\frac{J_2}{J_1} = 5$. The lower figures are examples of the corresponding classical ground state configurations within a unit cell.

From Eq.4.7 we can first conclude that $[H, S_i] \neq 0$, unless we go to the classical limit $(\hbar \rightarrow 0)$, where we can treat the spin operators as vectors, which corresponds to the classical Heisenberg model. In classical limit, the energy per bond of a spin- $\frac{1}{2}$ system can be represented as:

$$\frac{E_{\text{Classical}}}{N_{\text{Bonds}}} = \langle \boldsymbol{S}_{\boldsymbol{i}} \rangle \cdot \langle \boldsymbol{S}_{\boldsymbol{j}} \rangle = \frac{\cos\theta}{4}, \qquad (4.9)$$

where θ represent the average angle between all spin pairs due to existence of frustration. Then we are manage to construct a configuration that fulfill $\cos\theta = -1$ when there is no frustration, where each spin is anti-aligned with all it's neighbours. However, in the scenario shown in the Fig.4.2(b), notice that the energy per bond is significantly suppressed due to the existence of frustration.

Alternatively, we can start our consideration from the quantum entanglement between two spins. We can use the total spin representation to write:

$$\frac{E_{\text{Singlet}}}{N_{\text{Bonds}}} = \langle \mathbf{S}_{i} \cdot \mathbf{S}_{j} \rangle = \frac{1}{N_{c}} \langle \frac{1}{2} (\underbrace{\mathbf{S}_{i} + \mathbf{S}_{j}}_{\text{Stot}=0})^{2} - \frac{3}{4} \rangle = -\frac{3}{4N_{c}}.$$
(4.10)

Now, if we compare Eq.4.9 and Eq.4.10, we find that if the quantum entanglement between spins is allowed, we have to pay a "price" for the coordinate number: N_c , for we

can not optimising all bonds at the same time. On the other hand the system constructed in this way is "robust" against frustrations.



Figure 4.3: An illustration of the possible singlet paring ways when the frustration of the system is maximized.

As a result, when the system is maximally frustrated, it may favour more being constructed with the spin singlets, and we can further lower the total energy of the system by allowing these pairs resonate, namely, by constructing the ground states as the superposition of all these possible ways of paring. In Fig.4.3, we illustrate the ways of paring of four spins in total. The proper theory for describing this crossover $(\frac{J_2}{J_1} \simeq 0.5)$ is called the resonating valence bond theory first proposed by the P.W.Anderson et al. [9]. The system is believed to enter the spin-liquid phase, which means that spins are not well described by the vector model, for they should not be viewed as a rigid body anymore, and instead a vanishing spin stiffness is found [10].



Figure 4.4: The extrapolated value of the spin stiffness in the ref. [10]

The above discussion can also be viewed as different ways of mean field decoupling the Hamiltonian. In order to see this more clearly, first we shall use the auxiliary-fermion formulation to rewrite our Hamiltonian as:

$$H = \frac{1}{4} \sum_{\langle \langle i,j \rangle \rangle} \sum_{\alpha,\beta,\gamma,\eta} \mathcal{J}_{ij} f^{\dagger}_{i\alpha}(\boldsymbol{\sigma})_{\alpha\beta} f_{i\beta} \cdot f^{\dagger}_{j\eta}(\boldsymbol{\sigma})_{\eta\gamma} f_{j\gamma}.$$
(4.11)

From Eq.4.11, by using the PFP we can decouple the Hamiltonian directly, with the local order parameters that represent the magnetic moment being $\frac{1}{2} \sum_{\alpha\beta} \langle f_{i\alpha}^{\dagger}(\boldsymbol{\sigma})_{\alpha\beta} f_{i\beta} \rangle$. This is the way we choose to decouple the Hamiltonian in the following chapters, for we are more interested in the magnetic ordering properties, especially regarding the Nematic order of the J_1 - J_2 Heisenberg model.

For the resonating valence bond theory, we need to further carry out the sum over the Pauli matrices in Eq.4.11 obtaining:

$$H = -\frac{1}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha,\beta} \mathcal{J}_{ij} f_{i\alpha}^{\dagger} f_{j\alpha} f_{j\beta}^{\dagger} f_{i\beta} + \underbrace{\frac{1}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha,\beta} \mathcal{J}_{ij} (n_i - \frac{1}{2} n_i n_j)}_{\text{Constant}}.$$
 (4.12)

If we impose the constrain of single occupancy by a Lagrangian multiplier instead of using the (PFP) ($\langle f_{i\alpha}^{\dagger} f_{i\alpha} \rangle = 1$) the fermion are allowed to hop between neighbouring sites. The second term of Eq.4.11 is still a constant, while the first term now can be expressed in terms of the non-local order parameter $\langle f_{i\alpha}^{\dagger} f_{j\alpha} \rangle$, a non zero value of which reflects a broken gauge invariance of the system.

On the other hand, as reported before by [11], we can also decouple the Hamiltonian directly into the local order parameters that represent the magnetic moment: $\frac{1}{2}\sum_{\alpha\beta}\langle f_{i\alpha}^{\dagger}(\boldsymbol{\sigma})_{\alpha\beta}f_{i\beta}\rangle$. And this is the way we choose to decouple the Hamiltonian in the following chapters, for we are more interested in the magnetic ordering properties of the system.

In summary, the J_1 - J_2 Heisenberg model exhibits distinctive magnetic properties, depending on the ratio between J_2 and J_1 , except when the ratio approaches the maximal frustration point of $\frac{J_2}{J_1} = 0.5$. When $\frac{J_2}{J_1} < 0.5$, the system assumes a Néel state, whereas for $\frac{J_2}{J_1} > 0.5$, a Collinear state is observed. These states are valid when the effects of thermal and quantum fluctuations are not considered. Additionally, there exists a non-magnetic state in the intermediate range between these two states. The detailed analysis of this state is beyond the scope of our discussion, as it requires applying mean field decoupling to non-local parameters.

Chapter 5

Mean field theory

5.1 The Hubbard-Stratonovich transformation

In this section, mainly by following similar procedures that are discussed in Chapter 13 of [12], we provide a study of the properties of magnetic ground state of J_1 - J_2 model obtained at the mean-field level. The introduction of the bosonic Weiss field results in the emergence of non-diagonal elements in momentum space, posing challenges when attempting to invert the corresponding matrix to derive the expression for the Green function. Consequently, we will proceed with the mean-field theory in real space in the subsequent analysis. Our objective is to address the problem using the path integral formalism, so that

$$Z = \int \mathcal{D}[\bar{\psi}, \psi] e^{-S[\bar{\psi}, \psi]}, \qquad (5.1)$$

with

$$S[\bar{\psi},\psi] = \int_0^\beta d\tau \sum_i \bar{\psi}_i (\partial_\tau \underline{\underline{\sigma}_0}) \psi_i + \frac{1}{2} \sum_{i,j} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j.$$
(5.2)

Here, we introduced $\underline{\sigma_0}$ as the 2 × 2 identity matrix and the spinor operators

$$\bar{\psi}_i = \begin{pmatrix} \bar{f}_{\uparrow i} & \bar{f}_{\downarrow i} \end{pmatrix}, \psi_i = \begin{pmatrix} f_{\uparrow i} \\ f_{\downarrow i} \end{pmatrix}.$$
(5.3)

As we can see from Eq.4.7, the eigenvalue J_q of the exchange matrix can range from negative to positive values. In order to apply the Hubbard Stratonovich decoupling to this special case, we use following procedures that is motivated by [13]. Firstly, we include a term that introduce a the white-noise vector field $\varphi_q = (\varphi_q^x, \varphi_q^y, \varphi_q^z)$ into the partition function:

$$Z_H = \int \mathcal{D}[\boldsymbol{\varphi}] e^{-s[\boldsymbol{\varphi}]},\tag{5.4}$$

with

$$S[\boldsymbol{\varphi}] = \sum_{\boldsymbol{q}} \int_0^\beta d\tau \frac{\boldsymbol{\varphi}_{\boldsymbol{q}} \cdot \boldsymbol{\varphi}_{-\boldsymbol{q}}}{2|J_{\boldsymbol{q}}|}.$$
 (5.5)

Because $|J_q|$ is now a positive definite matrix, we can demonstrate that the product of 5.1 and 5.4 is equivalent to rescale the original partition function by a constant rate. This ensures that the physical properties of the system remain unchanged. Therefore we can write our the new partition function as:

$$Z \times Z_H = \int \mathcal{D}[\bar{\psi}, \psi] \int \mathcal{D}[\varphi] e^{-s[\bar{\psi}, \psi, \varphi]}, \qquad (5.6)$$

with

$$S[\bar{\psi},\psi,\varphi] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}} (\partial_{\tau} \underline{\underline{\sigma}_{0}}) \psi_{-\boldsymbol{q}} + \frac{1}{2} J_{\boldsymbol{q}} \boldsymbol{S}_{\boldsymbol{q}} \cdot \boldsymbol{S}_{-\boldsymbol{q}} + \frac{\varphi_{\boldsymbol{q}} \cdot \varphi_{-\boldsymbol{q}}}{2|J_{\boldsymbol{q}}|}.$$
 (5.7)

Noticing that J_q can be both positive and negative, we can make good use of this property by shifting our auxiliary bosonic fields as follows:

$$\varphi_{q} \rightarrow m_{q} - P(q) J_{q} S_{q}$$
 (5.8a)

$$\varphi_{-q} \to m_{-q} - P(q) J_q S_{-q},$$
 (5.8b)

where P(q) is a function that only depends on whether the specific q makes J_q positive or negative.

$$P(q) = \begin{cases} -i & (J_q > 0), \\ 1 & (J_q < 0). \end{cases}$$
(5.9)

Then, by inserting Eq.5.8 into Eq.5.7 we will get:

$$S[\bar{\psi},\psi,\boldsymbol{m}] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}} (\partial_{\tau} \underline{\underline{\sigma}_{0}}) \psi_{-\boldsymbol{q}} + \frac{1}{2} J_{\boldsymbol{q}} \boldsymbol{S}_{\boldsymbol{q}} \cdot \boldsymbol{S}_{-\boldsymbol{q}} + \frac{\left[\boldsymbol{m}_{\boldsymbol{q}} - P(\boldsymbol{q}) J_{\boldsymbol{q}} \boldsymbol{S}_{\boldsymbol{q}}\right] \cdot \left[\boldsymbol{m}_{-\boldsymbol{q}} - P(\boldsymbol{q}) J_{\boldsymbol{q}} \boldsymbol{S}_{-\boldsymbol{q}}\right]}{2|J_{\boldsymbol{q}}|}$$
(5.10)

which can be further grouped as:

$$S[\bar{\psi},\psi,\boldsymbol{m}] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}} (\partial_{\tau} \underline{\underline{\sigma}_{0}}) \psi_{-\boldsymbol{q}} + \frac{1}{2} J_{\boldsymbol{q}} (1 + \frac{|J_{\boldsymbol{q}}|}{J_{\boldsymbol{q}}} P(\boldsymbol{q})^{2}) \boldsymbol{S}_{\boldsymbol{q}} \cdot \boldsymbol{S}_{-\boldsymbol{q}} + \frac{\boldsymbol{m}_{\boldsymbol{q}} \cdot \boldsymbol{m}_{-\boldsymbol{q}}}{2|J_{\boldsymbol{q}}|} - \frac{|J_{\boldsymbol{q}}|}{J_{\boldsymbol{q}}} P(\boldsymbol{q}) \boldsymbol{S}_{\boldsymbol{q}} \cdot \boldsymbol{m}_{-\boldsymbol{q}}$$

$$(5.11)$$

Notice that the second term in Eq.5.11 is zero for all \boldsymbol{q} since

$$\frac{|J_{\boldsymbol{q}}|}{J_{\boldsymbol{q}}}P(\boldsymbol{q})^2 = \begin{cases} -1 & (J_{\boldsymbol{q}} > 0), \\ -1 & (J_{\boldsymbol{q}} < 0). \end{cases}$$
(5.12)

By renaming $\frac{|J_{\boldsymbol{q}}|}{J_{\boldsymbol{q}}}P(\boldsymbol{q})$ as $-\mathcal{P}(\boldsymbol{q})$, we can rewrite Eq.5.11 as:

$$S[\bar{\psi},\psi,\boldsymbol{m}] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}} (\partial_{\tau} \underline{\underline{\sigma}_{0}}) \psi_{-\boldsymbol{q}} + \frac{\boldsymbol{m}_{\boldsymbol{q}} \cdot \boldsymbol{m}_{-\boldsymbol{q}}}{2|J_{\boldsymbol{q}}|} + \mathcal{P}(\boldsymbol{q}) \boldsymbol{S}_{\boldsymbol{q}} \cdot \boldsymbol{m}_{-\boldsymbol{q}},$$
(5.13)

where $\mathcal{P}(\boldsymbol{q})$ is defined as:

$$\mathcal{P}(\boldsymbol{q}) = \begin{cases} i & (J_{\boldsymbol{q}} > 0), \\ 1 & (J_{\boldsymbol{q}} < 0). \end{cases}$$
(5.14)

We also have to rename two auxiliary fields: $m_q = \frac{M_q}{P(q)}$ and $m_{-q} = \frac{M_{-q}}{P(-q)}$, so that we get:

$$S[\bar{\psi},\psi,\mathcal{M}] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}} (\partial_{\tau} \underline{\underline{\sigma}_{0}}) \psi_{-\boldsymbol{q}} + \frac{\mathcal{M}_{\boldsymbol{q}} \cdot \mathcal{M}_{-\boldsymbol{q}}}{2|J_{\boldsymbol{q}}|\mathcal{P}(\boldsymbol{q})^{2}} + S_{\boldsymbol{q}} \cdot \mathcal{M}_{-\boldsymbol{q}},$$
(5.15)

after noticing the fact that:

$$|J_{q}|\mathcal{P}(q)^{2} = \begin{cases} -J_{q} & (J_{q} > 0), \\ -J_{q} & (J_{q} < 0). \end{cases}$$
(5.16)

Using Eq.5.15 in Eq.5.16 we get a decoupled Hamiltonian in momentum space:

$$S[\bar{\psi},\psi,\mathcal{M}] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}} (\partial_{\tau} \underline{\underline{\sigma}_{0}}) \psi_{-\boldsymbol{q}} + S_{\boldsymbol{q}} \cdot \mathcal{M}_{-\boldsymbol{q}} - \frac{\mathcal{M}_{\boldsymbol{q}} \cdot \mathcal{M}_{-\boldsymbol{q}}}{2J_{\boldsymbol{q}}}, \qquad (5.17)$$

and due to the reason we mentioned in the very beginning we want to perform meanfield theory in real space so we have to Fourier transform to Eq.5.17 obtaining:

$$S[\bar{\psi},\psi,\mathcal{M}] = \int_0^\beta d\tau \Big(\sum_i \bar{\psi}_i(\partial_\tau \sigma_0)\psi_i + S_i \cdot \mathcal{M}_i\Big) - \frac{1}{2}\sum_{i,j}\mathcal{M}_i(J^{-1})_{ij} \cdot \mathcal{M}_j, \quad (5.18)$$

By replacing the spin operator by the auxiliary-fermion formulation in Eq.5.18, we get the action:

$$S[\bar{\psi},\psi,\mathcal{M}] = \int_0^\beta d\tau \sum_i \bar{\psi}_i (\partial_\tau \sigma_0 + \frac{1}{2}\mathcal{M}_i \cdot \vec{\sigma})\psi_i - \frac{1}{2}\sum_{i,j}\mathcal{M}_i (J^{-1})_{ij} \cdot \mathcal{M}_j.$$
(5.19)

5.2 Saddle point approximation

In order to explore how the fluctuating Weiss field \mathcal{M}_i is related to the spin polarization S_i we have to make a saddle-point approximation, hence, let us start by writing down the partition function:

$$Z = \int D[\bar{\psi}, \psi, \mathcal{M}] e^{-S[\bar{\psi}, \psi, \mathcal{M}]} = \int D[\mathcal{M}] e^{-S_E[\mathcal{M}]}, \qquad (5.20)$$

with

$$e^{-S_E[\mathcal{M}]} = \int D[\bar{\psi}, \psi] e^{-S[\mathcal{M}, \bar{\psi}, \psi]}.$$
(5.21)

In the mean field theory, we assume all spins polarized along the z-axis $\mathcal{M}_i = \begin{pmatrix} 0 & 0 & \mathcal{M}_i \end{pmatrix}$ and we approximate the partition function by its value at the saddle point:

$$Z = \int D[\mathcal{M}] e^{-S_E[\mathcal{M}]} \approx e^{-S_E[\mathcal{M}^{(0)}]}, \qquad (5.22)$$

where:

$$\frac{\delta S_E[\mathcal{M}]}{\delta \mathcal{M}}|_{\mathcal{M}=\mathcal{M}^{(0)}} = 0, \qquad (5.23)$$

which means that if we differentiate on the both side in Eq.5.22, the saddle point condition implies:

$$\frac{\delta S_E[\mathcal{M}]}{\delta \mathcal{M}} = \frac{1}{e^{-S_E[\mathcal{M}]}} \int D[\bar{\psi}, \psi] [\sum_j (J^{-1})_{ij} \mathcal{M}_j - \frac{1}{2} \bar{\psi}_i \vec{\sigma} \psi_i] e^{-S[\mathcal{M}, \bar{\psi}, \psi]}.$$
 (5.24)

Applying the saddle point approximation (Eq.5.23) to Eq.5.24:

$$\sum_{j} (J^{-1})_{ij} \mathcal{M}_{j}^{(0)} = \frac{1}{2} \langle \bar{\psi}_{i} \sigma_{z} \psi_{i} \rangle |_{h_{E}[\mathcal{M}^{(0)}]} = \langle \mathbf{S}_{i}^{z} \rangle |_{h_{E}[\mathcal{M}^{(0)}]}, \qquad (5.25)$$

and inserting a term $\sum_i J_{\alpha i}$ on both side of Eq.5.25 so that we can get,

$$\sum_{i} J_{\alpha i} \langle \boldsymbol{S}_{i}^{z} \rangle |_{h_{E}[\boldsymbol{\mathcal{M}}^{(0)}]} = \sum_{j} \sum_{i} J_{\alpha i} (J^{-1})_{ij} \boldsymbol{\mathcal{M}}_{j}^{(0)} = \sum_{j} \boldsymbol{\mathcal{M}}_{j}^{(0)} \delta_{\alpha j} = \boldsymbol{\mathcal{M}}_{\alpha}^{(0)}.$$
(5.26)

Here we have to introduce a useful identity for later convenience:

$$\sum_{j} (J^{-1})_{ij} J_{j\alpha} = \delta_{i\alpha}.$$
(5.27)

By using the above identity we have:

$$\mathcal{M}_{i}^{(0)} = \sum_{j} J_{ij} \langle \boldsymbol{S}_{j}^{z} \rangle |_{h_{E}[\boldsymbol{\mathcal{M}}^{(0)}]}.$$
(5.28)

In the mean-field descriptions of both the Néel and Collinear orders, all spins are polarized along the same axis, and for our convenience we can choose this direction as the z-axis. Nevertheless, we are also allowed to define an ordering factor $\mathbf{Q} = (Q_x, Q_y) =$ $(0,0), (\pi,\pi), (0,\pi), (\pi,0)$ for each phase, so that we can track the spatial dependence of the spins in different orders shown as follows:

$$\langle \boldsymbol{S}_i \rangle |_{h_E[\boldsymbol{\mathcal{M}}^{(0)}]} = \langle \boldsymbol{S}_j \rangle |_{h_E[\boldsymbol{\mathcal{M}}^{(0)}]} e^{i \boldsymbol{Q}(\vec{R}_j - \vec{R}_i)}, \qquad (5.29)$$

By using Eq.5.28 together with Eq.5.29 allows us to construct the relation between the fluctuating Weiss field \mathcal{M}_i and the spin polarization S_i as:

$$\mathcal{M}_{i}^{(0)} = J_{\boldsymbol{Q}} \langle \boldsymbol{S}_{i}^{z} \rangle |_{h_{E}[\boldsymbol{\mathcal{M}}^{(0)}]}, \qquad (5.30)$$

where,

$$J_{\boldsymbol{Q}} = 2J_1(\cos Q_x + \cos Q_y) + 4J_2 \cos Q_x \cos Q_y \tag{5.31}$$

5.3 Mean-field theory as a saddle point of the path integral

The next step is to obtain the self-consistent equation for the J_1 - J_2 model. In order to do this we start with writing down the constrained action using the Popov-Fedatov method on our lattice model :

$$S^{ppv}[\bar{\psi},\psi,\mathcal{M}] = \int_0^\beta d\tau \sum_i \bar{\psi}_i [(\partial_\tau + \lambda_f) \cdot \underline{\sigma_0} + \frac{1}{2}\mathcal{M}_i \cdot \vec{\sigma}]\psi_i - \frac{1}{2}\sum_{i,j}\mathcal{M}_i (J^{-1})_{ij}\mathcal{M}_j.$$
(5.32)

Then we can apply the saddle point approximation described by Eq.5.23, which simply replaces the fluctuating Weiss field by its value at static saddle point:

$$S^{ppv}[\bar{\psi},\psi,\mathcal{M}^{(0)}] = \int_0^\beta d\tau \sum_i \bar{\psi}_i [(\partial_\tau + \lambda_f)\underline{\sigma_0} + \frac{1}{2}\mathcal{M}_i^{(0)} \cdot \vec{\sigma}]\psi_i - \frac{1}{2}\sum_{i,j}\mathcal{M}_i^{(0)}(J^{-1})_{ij}\mathcal{M}_j^{(0)}.$$
(5.33)

We can apply the fourier transform to Replace ∂_{τ} by matsubara frequency $-i\omega_n$ and carrying out the Gaussian integral over $\bar{\psi}$ and ψ . Then, we obtain the expression for the constrained effective action:

$$S_E^{ppv}[\mathcal{M}^{(0)}] = -\mathrm{Trln}[-(i\omega_n - \lambda_f)\underline{\underline{\sigma}_0} + \frac{1}{2}\mathcal{M}_i^{(0)} \cdot \vec{\sigma}] - \frac{\beta}{2}\sum_{i,j}\mathcal{M}_i^{(0)}(J^{-1})_{ij}\mathcal{M}_j^{(0)}.$$
 (5.34)

Now, we can denote the matrix $-(i\omega_n - \lambda_f)\underline{\sigma_0} + \frac{1}{2}\mathcal{M}_i^{(0)} \cdot \vec{\sigma}$ as $-\underline{\underline{G_i}}(i\omega_n)^{-1}$, where $\underline{G_i}(i\omega_n)$ is given by:

$$\underline{\underline{G}}_{\underline{i}}(i\omega_n) = \frac{(i\omega_n - \lambda_f)\underline{\underline{\sigma}}_{\underline{0}} + \frac{1}{2}\mathcal{M}_i^{(0)} \cdot \vec{\sigma}}{(i\omega_n - \lambda_f)^2 - \left|\frac{1}{2}\mathcal{M}_i^{(0)}\right|^2}$$
(5.35)

In order to identify a local equilibrium magnetization $\mathcal{M}_i^{(0)}$, we shall minimize the action $S_E^{ppv}[\mathcal{M}^{(0)}]$, which will lead to a self consistent equation:

$$\beta \sum_{j} (J^{-1})_{ij} \mathcal{M}_{j}^{(0)} = \operatorname{Tr}\left[-\frac{1}{2} \underline{\underline{G}_{i}}(i\omega_{n}) \cdot \vec{\sigma}\right].$$
(5.36)

Now, inserting Eq.5.35, we get:

$$\beta \sum_{j} (J^{-1})_{ij} \mathcal{M}_{j}^{(0)} = \operatorname{Tr} \left[-\frac{1}{2} \frac{(i\omega_{n} - \lambda_{f}) \cdot \vec{\sigma} + \frac{1}{2} \mathcal{M}_{i}^{(0)} \cdot \vec{\sigma} \cdot \vec{\sigma}}{(i\omega_{n} - \lambda_{f})^{2} - \left| \frac{1}{2} \mathcal{M}_{i}^{(0)} \right|^{2}} \right].$$
(5.37)

Noticing the fact that σ is traceless, so that we can carry out the trace over the spins and Eq.5.37 can be simplified as:

$$\sum_{j} (J^{-1})_{ij} \mathcal{M}_{j}^{(0)} = T \frac{\mathcal{M}_{i}^{(0)}}{2 \left| \mathcal{M}_{i}^{(0)} \right|} \sum_{i\omega_{n}} \left[\frac{1}{(i\omega_{n} - \lambda_{f}) + \left| \frac{1}{2} \mathcal{M}_{i}^{(0)} \right|} - \frac{1}{(i\omega_{n} - \lambda_{f}) - \left| \frac{1}{2} \mathcal{M}_{i}^{(0)} \right|} \right].$$
(5.38)

Using the results from Eq.5.30, this equation can be rewritten as:

$$\frac{\mathcal{M}_{i}^{(0)}}{J_{\boldsymbol{Q}}} = T \frac{\mathcal{M}_{i}^{(0)}}{2\left|\mathcal{M}_{i}^{(0)}\right|} \sum_{i\omega_{n}} \left[\frac{1}{(i\omega_{n}-\lambda_{f})+\left|\frac{1}{2}\mathcal{M}_{i}^{(0)}\right|} - \frac{1}{(i\omega_{n}-\lambda_{f})-\left|\frac{1}{2}\mathcal{M}_{i}^{(0)}\right|}\right], \quad (5.39)$$

which can be further simplified as:

$$\frac{2\left|\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|}{J_{\boldsymbol{Q}}} = T \sum_{i\omega_{n}} \left[\frac{1}{(i\omega_{n} - \lambda_{f}) + \left|\frac{1}{2}\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|} - \frac{1}{(i\omega_{n} - \lambda_{f}) - \left|\frac{1}{2}\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|} \right].$$
 (5.40)

By carrying out the matsubara sum we get:

$$\frac{2\left|\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|}{J_{\boldsymbol{Q}}} = \oint \frac{dz}{2\pi i} f(z) \left[\frac{1}{(i\omega_{n} - \lambda_{f}) + \left|\frac{1}{2}\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|} - \frac{1}{(i\omega_{n} - \lambda_{f}) - \left|\frac{1}{2}\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|} \right] = -\operatorname{tanh}\left(\frac{\beta}{2}\left|\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|\right),$$
(5.41)

so our constrained self-consistent equation for the J_1 - J_2 model read as:

$$2\frac{\left|\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|}{J_{\boldsymbol{Q}}} = \tanh\left(-\frac{\beta}{2}\left|\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|\right).$$
(5.42)

Now let us explore what happens if we go to the $T \to 0$ limit. Recalling that $\lambda_f = i\pi \frac{T}{2}$, so the $\lambda_f \to 0$ in the zero temperature limit and we end up with the equation:

$$\frac{2\left|\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|}{J_{\boldsymbol{Q}}} = \oint \frac{dz}{2\pi i} f(z) \left[\frac{1}{i\omega_{n} + \left|\frac{1}{2}\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|} - \frac{1}{i\omega_{n} - \left|\frac{1}{2}\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|}\right]$$
$$= -\operatorname{tanh}\left(\frac{\beta}{4}\left|\boldsymbol{\mathcal{M}}_{i}^{(0)}\right|\right)$$
(5.43)

Within mean field theory, in both the Néel and Collinear phases the spins on all sites are polarized along the same direction, but can point align or anti-align with this axis, leading however to the same norm of the magnetization $\left|\frac{1}{2}\mathcal{M}_{i}^{(0)}\right| = \mathcal{M}^{(0)}$ for all sites. We can use this $\frac{1}{2}\mathcal{M}^{(0)}$ as an order parameter and evaluate the critical temperatures for both phases at $Q_{\rm N} = (\pi, \pi)$ and $Q_{\rm C} = (0, \pi)$, respectively.

$$2\mathcal{M}_{(N\acute{e}el)}^{(0)} = -J_{\boldsymbol{Q}=\boldsymbol{Q}_{N}} \tanh(\frac{\beta}{2}\mathcal{M}_{(N\acute{e}el)}^{(0)})$$
(5.44a)

$$2\mathcal{M}_{(Col.)}^{(0)} = -J_{\boldsymbol{Q}=\boldsymbol{Q}_{C}} \tanh(\frac{\beta}{2}\mathcal{M}_{(Col.)}^{(0)}), \qquad (5.44b)$$

where we use the short hand notation of J_Q that is defined in Eq.5.31. From Eq.5.44 we can write down critical temperatures for both phases:

$$T_c^{(\text{N\acute{e}el})} = J_1 - J_2 \tag{5.45a}$$

$$T_c^{(\text{Coll.})} = J_2, \tag{5.45b}$$

which are shown visually in the Fig.5.1 below.



Figure 5.1: Results of the critical temperature of the Nematic phase transition

In conclusion, we find the critical temperature of two magnetic states by mean field theory, and the transition point of two states is predicted to be located at: $g_c = 0.5$, which is consistent with the results suggested from the previous chapter. One point need to stressed is that the critical temperatures for both phases computed without the constraint are reduced to one half of those with the constraint. The exact mechanism account for this difference is not very clear to us. Qualitatively, when there is no constraint imposed, more non-magnetic states are introduced into the system, which may impede magnetic ordering and lead to the decreasing of the transition temperature.
Chapter 6

Fluctuations in the magnetization

6.1 Beyond Mean field theory

Within the mean field theory, we neglects the effects that are brought in by fluctuations in the order parameter, which can be viewed as a key element that could compete and potential wash away the long range magnetic orders. Nevertheless, according to the Mermin-Wigner theorem: There is no phase with spontaneous breaking of a continuous symmetry for T > 0, in $d \le 2$ dimensions. Therefore we need to go beyond the mean-field theory to examine the fluctuations in the order parameter. We use mean field theory as our starting point, in which we assume the polarization of spin on all sites is along the z-axis, so that

$$\mathcal{M}_{i}^{(0)} = J_{\boldsymbol{Q}} \langle \boldsymbol{S}_{i} \rangle \big|_{h_{E}[\mathcal{M}^{(0)}]} = J_{\boldsymbol{Q}} \mathcal{S}_{i} \underline{\underline{\sigma}_{\underline{z}}}.$$
(6.1)

In both the Néel and Collinear phases, S_i is a real number which has same norm on all sites but can have different signs in front. If we expand the action in Eq.5.34 in the fluctuations by replacing $\mathcal{M}_i = J_Q S_i \underline{\sigma_z} + \delta \mathcal{M}_i$ and carrying out the path integral over $\overline{\psi}$ and ψ , we will get the leading-order corrections to the effective action, which are quadratic in the fluctuations, and the following expression for the effective action:

$$S_{E}^{ppv}[\mathcal{M}] = -\operatorname{Trln}\left[-\underline{\underline{G}_{i}}(i\omega_{n})^{-1} + \frac{1}{2}\delta\mathcal{M}_{i}\cdot\boldsymbol{\sigma}\right] \\ - \frac{\beta}{2}\sum_{i,j}\left(J_{\boldsymbol{Q}}\mathcal{S}_{i}\underline{\underline{\sigma}_{z}} + \delta\mathcal{M}_{i}\right)(J^{-1})_{ij}\left(J_{\boldsymbol{Q}}\mathcal{S}_{j}\underline{\underline{\sigma}_{z}} + \delta\mathcal{M}_{j}\right) + O(\delta\mathcal{M}^{3}),$$

$$(6.2)$$

with the expression of our renormalized propagator:

$$\underline{\underline{G}}_{\underline{i}}(i\omega_n) = \left[(i\omega_n - \lambda_f)\boldsymbol{\sigma}_0 - \frac{1}{2}J_{\boldsymbol{Q}}\mathcal{S}_{\underline{i}}\underline{\underline{\sigma}}_{\underline{z}} \right]^{-1}.$$
(6.3)

Now we need to examine the difference between the action that includes the fluctuations and the one that does not:

$$\Delta S_E^{ppv}[\mathcal{M}] = S_E^{ppv}[\mathcal{M}] - S_E^{ppv}[\mathcal{M}^{(0)}].$$
(6.4)

Due to the fact that the action is stationary with respect to fluctuations, the linear terms in $\delta \mathcal{M}$ should sum to zero, which leaves us the following description of $\Delta S_E^{ppv}[\mathcal{M}]$ up to 2nd order:

$$\Delta S_E^{ppv}[\mathcal{M}] = -\text{Trln}[1 - \frac{1}{2}\underline{\underline{G}}_i(i\omega_n)\delta\mathcal{M}_i \cdot \boldsymbol{\sigma}] - \frac{\beta}{2}\sum_{i,j}\delta\mathcal{M}_i(J^{-1})_{ij}\delta\mathcal{M}_j.$$
(6.5)

Then we can do the expansion of the first term above like this:

$$\operatorname{Trln}(1 - G_0 V) = \operatorname{Tr}\left(-G_0 V - \frac{1}{2}(G_0 V)^2 - \frac{1}{3}(G_0 V)^3 - \frac{1}{4}(G_0 V)^4 + \cdots\right).$$
(6.6)

Here we expand to second order like we did above, and due to the same reason the linear term drops off. After the expansion we get:

$$\Delta \mathcal{F}_{E}^{ppv}[\mathcal{M}] = -\frac{1}{2N_{s}} \sum_{i,j,\alpha,\beta} \delta \mathcal{M}_{i}^{\alpha} \left(\underbrace{-\frac{\delta_{ij}}{4\beta} \operatorname{Tr}[\underline{\sigma}^{\alpha} \underline{\underline{G}_{i}}(i\omega_{n} + i\nu_{m})\underline{\sigma}^{\beta} \underline{\underline{G}_{i}}(i\omega_{n})]}_{\Pi_{i}^{\alpha\beta}(i\nu_{m})\delta_{ij}} + (J^{-1})_{ij}\delta_{\alpha\beta} \right) \delta \mathcal{M}_{j}^{\beta}$$

$$(6.7)$$

Now with these expression of bare susceptibility, we can write Eq.6.7 as:

$$\Delta \mathcal{F}_{E}^{ppv}[\mathcal{M}] = -\frac{1}{2N_{s}} \sum_{i,j,\alpha,\beta} \delta \mathcal{M}_{i}^{\alpha} \underbrace{\left(\prod_{i}^{\alpha\beta} (i\nu_{m})\delta_{ij} + (J^{-1})_{ij}\delta_{\alpha\beta} \right)}_{(\underline{\mathfrak{I}}^{-1})_{ij}^{\alpha\beta}} \delta \mathcal{M}_{j}^{\beta}. \tag{6.8}$$

In order to compute the spin correlation function, we need to introduce a source term h into the expression of Eq.6.5:

$$\Delta S_E^{ppv}[\mathcal{M}] = -\operatorname{Trln}[1 - \frac{1}{2}\underline{\underline{G}}_i(i\omega_n)(\delta\mathcal{M}_i + h_i) \cdot \boldsymbol{\sigma}] - \frac{\beta}{2}\sum_{i,j}\delta\mathcal{M}_i(J^{-1})_{ij}\delta\mathcal{M}_j.$$
(6.9)

With the source term included we can carry out the same procedure to get a new expression for Eq.6.9:

$$\Delta \mathcal{F}_{E}^{ppv}[\mathcal{M}] = -\frac{1}{2N_{s}} \sum_{i,j,\alpha,\beta} \delta \mathcal{M}_{i}^{\alpha} \left((\underline{\mathfrak{I}}^{-1})_{ij}^{\alpha\beta} \right) \delta \mathcal{M}_{j}^{\beta} + \delta \mathcal{M}_{i}^{\alpha} \left(\Pi_{i}^{\alpha\beta}(i\nu_{m})\delta_{ij} \right) h_{j}^{\beta} + h_{i}^{\alpha} \left(\Pi_{i}^{\alpha\beta}(i\nu_{m})\delta_{ij} \right) h_{j}^{\beta} + h_{i}^{\alpha} \left(\Pi_{i}^{\alpha\beta}(i\nu_{m})\delta_{ij} \right) h_{j}^{\beta}.$$

$$(6.10)$$

Completing the square:

$$\Delta \mathcal{F}_{E}^{ppv}[\mathcal{M}] = -\frac{1}{2N_{s}} \sum_{i,j,k,l,\alpha,\beta,\eta,\xi,\varphi,\gamma} \left(\delta \mathcal{M}_{i}^{\alpha} + h_{k}^{\eta} \Pi_{k}^{\eta\xi} (i\nu_{m}) (\underline{\mathfrak{J}})_{ki}^{\xi\alpha} \right) \left((\underline{\mathfrak{J}}^{-1})_{ij}^{\alpha\beta} \right) \left(\delta \mathcal{M}_{j}^{\beta} + (\underline{\mathfrak{J}})_{jl}^{\beta\varphi} \Pi_{l}^{\varphi\gamma} (i\nu_{m}) h_{l}^{\gamma} + h_{i}^{\alpha} \left(\underbrace{\Pi_{i}^{\alpha\beta} (i\nu_{m}) \delta_{ij} - \Pi_{i}^{\alpha\gamma} (i\nu_{m}) (\underline{\mathfrak{J}})_{ij}^{\gamma\varphi} \Pi_{j}^{\varphi\beta} (i\nu_{m})}_{\chi_{ij}^{\alpha\beta}} \right) h_{j}^{\beta},$$

$$(6.11)$$

Explicitly, the spin correlation term can be acquired by the following way:

$$\langle TS_i^{\alpha}S_j^{\beta}\rangle = \frac{1}{Z[h]} \frac{\delta^2 Z[h]}{\delta h_j^{\beta} \delta h_i^{\alpha}},\tag{6.12}$$

and in the generating functional we can integrate out the fluctuations leaving a effective free energy for the source fields:

$$Z[\boldsymbol{h}] = \text{const.} \times e^{\frac{1}{2}\sum_{i,j,\alpha,\beta} h_i^{\alpha} \chi_{ij}^{\alpha\beta} h_j^{\beta}}.$$
(6.13)

Together with Eq.6.11, Eq.6.12 and Eq.6.13 we obtain:

$$\langle TS_{i}^{\alpha}S_{j}^{\beta}\rangle = \frac{1}{Z[\boldsymbol{h}]}\frac{\delta^{2}Z[\boldsymbol{h}]}{\delta h_{j}^{\beta}\delta h_{i}^{\alpha}} = \chi_{ij}^{\alpha\beta}(i\nu_{m}) = \Pi_{i}^{\alpha\beta}(i\nu_{m})\delta_{ij} - \sum_{\gamma,\varphi}\Pi_{i}^{\alpha\gamma}(i\nu_{m})(\underline{\mathfrak{J}})_{ij}^{\gamma\varphi}\Pi_{j}^{\varphi\beta}(i\nu_{m})$$

$$\tag{6.14}$$

where,

$$(\underline{\mathfrak{Y}})_{ij}^{\gamma\varphi} = \left(\Pi_i^{\gamma\varphi}(i\nu_m)\delta_{ij} + (J^{-1})_{ij}\delta_{\gamma\varphi}\right)^{-1}$$
(6.15)

Combining Eq.6.15 with Eq.6.16, and reformulating, we obtain:

$$\chi_{ij}^{\alpha\beta}(i\nu_m) = \Pi_i^{\alpha\beta}(i\nu_m)\delta_{ij} - \sum_{j',\eta}\Pi_i^{\alpha\eta}(i\nu_m)J_{ij'}\chi_{j'j}^{\eta\beta}(i\nu_m).$$
(6.16)

The detailed derivation from Eq.6.14 to Eq.6.16 can be found in Appendix.A.

Now we begin evaluating the non-zero components of the bare susceptibility $\Pi_{ij}^{(\alpha\beta)}(i\nu_m)$ by first noticing the fact that our propagator is purely localized on the site which leads to our bare susceptibility:

$$\Pi_{ij}^{\alpha\beta}(i\nu_m) = \Pi_i^{\alpha\beta}(i\nu_m)\delta_{ij},\tag{6.17}$$

$$\Pi_{i}^{(xx)}(i\nu_{m}) = -\frac{1}{4\beta} \sum_{i\omega_{n}} \operatorname{Tr}[\underline{\sigma}^{x} \underline{\underline{G}}_{i}(i\omega_{n} + i\nu_{m})\underline{\sigma}^{x} \underline{\underline{G}}_{i}(i\omega_{n})], \qquad (6.18)$$

$$\Pi_{i}^{(xx)}(i\nu_{m}) = -\frac{1}{4\beta} \sum_{i\omega_{n}} \operatorname{Tr}[\underline{\underline{G}_{i}^{\uparrow}}(i\omega_{n}+i\nu_{m})\underline{\underline{G}_{i}^{\downarrow}}(i\omega_{n}) + \underline{\underline{G}_{i}^{\downarrow}}(i\omega_{n}+i\nu_{m})\underline{\underline{G}_{i}^{\uparrow}}(i\omega_{n})]. \quad (6.19)$$

By inserting Eq.6.3 into Eq.6.18 and carrying out the trace we get:

$$\Pi_{i}^{(xx)}(i\nu_{m}) = -\frac{1}{4\beta} \sum_{i\omega_{n}} \frac{1}{(i\omega_{n} - \lambda_{f} - \frac{1}{2}J_{Q}\mathcal{S}_{i} + i\nu_{m})(i\omega_{n} - \lambda_{f} + \frac{1}{2}J_{Q}\mathcal{S}_{i})} + \frac{1}{(i\omega_{n} - \lambda_{f} + \frac{1}{2}J_{Q}\mathcal{S}_{i} + i\nu_{m})(i\omega_{n} - \lambda_{f} - \frac{1}{2}J_{Q}\mathcal{S}_{i})}.$$
(6.20)

By further carrying out the contour integration we get:

$$\Pi_i^{(xx)}(i\nu_m) = \frac{\frac{1}{2}J_{\boldsymbol{Q}}\mathcal{S}_i}{(J_{\boldsymbol{Q}}\mathcal{S}_i)^2 - (i\nu_m)^2} \tanh(\frac{1}{2}\beta J_{\boldsymbol{Q}}\mathcal{S}_i).$$
(6.21)

By using the same procedure, the rest of the components can be evaluated:

$$\Pi_{i}^{(xx)}(i\nu_{m}) = \Pi_{i}^{(yy)}(i\nu_{m}) = \frac{\frac{1}{2}J_{Q}S_{i}}{(J_{Q}S_{i})^{2} - (i\nu_{m})^{2}} \tanh(\frac{1}{2}\beta J_{Q}S_{i}), \qquad (6.22)$$

$$\Pi_{i}^{(xy)}(i\nu_{m}) = -\Pi_{i}^{(yx)}(i\nu_{m}) = \frac{1}{2i} \frac{i\nu_{m}}{(J_{Q}S_{i})^{2} - (i\nu_{m})^{2}} \tanh(\frac{1}{2}\beta J_{Q}S_{i}), \qquad (6.23)$$

$$\Pi_i^{(zz)}(i\nu_m) = \frac{\beta}{4\cosh^2(\frac{1}{2}\beta J_Q \mathcal{S}_i)} \delta_{i\nu_m,0}.$$
(6.24)

Combining Eq.6.22-6.24, we have the bare susceptibility in matrix form:

$$\underline{\underline{\Pi}}_{i} = \begin{pmatrix} \Pi_{i}^{(xx)}(i\nu_{m}) & \Pi_{i}^{(xy)}(i\nu_{m}) & 0\\ -\Pi_{i}^{(xy)}(i\nu_{m}) & \Pi_{i}^{(xx)}(i\nu_{m}) & 0\\ 0 & 0 & \Pi_{i}^{(zz)}(i\nu_{m}). \end{pmatrix}$$
(6.25)

Here by using the concept of the ordering factor $e^{\pm i \mathbf{Q} \cdot \mathbf{R}_i}$, which can pose the local magnetic moment into the alignments of the corresponding Néel and Collinear phases. Then we can rewrite Eq.6.25 as:

$$\underline{\underline{\Pi}}_{\underline{i}} = \begin{pmatrix} \Pi_{0}^{(xx)}(i\nu_{m}) & \Pi_{0}^{(xy)}(i\nu_{m})e^{\pm i\boldsymbol{Q}\cdot\boldsymbol{R}_{i}} & 0\\ -\Pi_{0}^{(xy)}(i\nu_{m})e^{\pm i\boldsymbol{Q}\cdot\boldsymbol{R}_{i}} & \Pi_{0}^{(xx)}(i\nu_{m}) & 0\\ 0 & 0 & \Pi_{0}^{(zz)}(i\nu_{m}) \end{pmatrix}$$
(6.26)

Recalling that our spin correlation function in real space reads:

$$\chi_{ij}^{\alpha\beta}(i\nu_m) = \Pi_i^{\alpha\beta}(i\nu_m)\delta_{ij} - \sum_{j',\eta} \Pi_i^{\alpha\eta}(i\nu_m)J_{ij'}\chi_{j'j}^{\eta\beta}(i\nu_m), \qquad (6.27)$$

We can write it in a matrix form in spin space as follows:

$$\underline{\underline{\chi}_{ij}}(i\nu_m) = \underline{\underline{\Pi}_i}(i\nu_m)\delta_{ij} - \underline{\underline{\Pi}_i}(i\nu_m)\sum_{j'}J_{ij'}\underline{\underline{\chi}_{j'j}}(i\nu_m)$$
(6.28)

The Fourier transform forms of both χ^{ab}_{ij} and J^{ab}_{ij} are define as follow:

$$\chi_{ij}^{ab} = \frac{1}{N^2} \sum_{k,k'} e^{i(\boldsymbol{k}\cdot\boldsymbol{R_i} - \boldsymbol{k'}\cdot\boldsymbol{R_j})} \chi_{kk'}^{ab}$$
(6.29a)

$$\mathcal{J}_{ij}^{ab} = \frac{1}{N} \sum_{k} e^{i \mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} J_k^{ab}$$
(6.29b)

So substituting in Eq.6.28, one obtains:

$$\sum_{i,j} e^{-i(\boldsymbol{k}\cdot\boldsymbol{R_i}-\boldsymbol{k'}\cdot\boldsymbol{R_j})} \underline{\underline{\chi_{ij}}}(i\nu_m) = \sum_{i,j,j'} e^{-i(\boldsymbol{k}\cdot\boldsymbol{R_i}-\boldsymbol{k'}\cdot\boldsymbol{R_j})} \Big(\underline{\underline{\Pi_i}}(i\nu_m)\delta_{ij} - \underline{\underline{\Pi_i}}(i\nu_m)J_{ij'}\underline{\underline{\chi_{j'j}}}(i\nu_m)\Big)$$
(6.30)

Noticed that from Eq.6.24, the longitudinal susceptibility $(\Pi_0^{(zz)}(i\nu_m))$ is exponentially decreasing while lowing the temperature as shown in the Fig.6.1 below.



Figure 6.1: Plot of bare longitudinal susceptibility $\Pi_0^{(zz)}(T)$

Therefore if we only consider the low temperature physics of the system, we can reduce the matrix in Eq.6.26 as a 2×2 matrix only containing the X and Y components and in this low temperature limit we also have $\tanh(\frac{1}{2}\beta J_Q S) \rightarrow -1$, we can write Eq.6.22-24 explicitly as:

$$\Pi_0^{(xx)}(i\nu_m) = \Pi_0^{(yy)}(i\nu_m) \approx -\frac{\frac{1}{4}J_Q}{(\frac{1}{2}J_Q)^2 - (i\nu_m)^2}$$
(6.31a)

$$\Pi_0^{(xy)}(i\nu_m) = -\Pi_0^{(yx)}(i\nu_m) \approx -\frac{1}{2i} \frac{i\nu_m}{(\frac{1}{2}J_Q)^2 - (i\nu_m)^2}$$
(6.31b)

$$\Pi_0^{(zz)}(i\nu_m) \approx 0, \tag{6.31c}$$

which means that the expression of the bare susceptibility in matrix form can be reduced to:

$$\underline{\underline{\Pi}}_{i} = \begin{pmatrix} \Pi_{0}^{(xx)}(i\nu_{m}) & \Pi_{0}^{(xy)}(i\nu_{m})e^{\pm i\boldsymbol{Q}\cdot\boldsymbol{R}_{i}} \\ -\Pi_{0}^{(xy)}(i\nu_{m})e^{\pm i\boldsymbol{Q}\cdot\boldsymbol{R}_{i}} & \Pi_{0}^{(xx)}(i\nu_{m}) \end{pmatrix}$$
(6.32)

Inserting Eq.6.32 into Eq.6.30 we obtain:

$$\underline{\underline{\chi}_{kk'}} = N_s \begin{pmatrix} \Pi_0^{(xx)} \delta_{\boldsymbol{k},\boldsymbol{k'}} & \Pi_0^{(xy)} \delta_{\boldsymbol{k},\boldsymbol{k'}\pm Q} \\ -\Pi_0^{(xy)} \delta_{\boldsymbol{k},\boldsymbol{k'}\pm Q} & \Pi_0^{(xx)} \delta_{\boldsymbol{k},\boldsymbol{k'}} \end{pmatrix} - \sum_{\boldsymbol{q}} \begin{pmatrix} \Pi_0^{(xx)} \delta_{\boldsymbol{k},\boldsymbol{q}} & \Pi_0^{(xy)} \delta_{\boldsymbol{k},\boldsymbol{q}\pm Q} \\ -\Pi_0^{(xy)} \delta_{\boldsymbol{k},\boldsymbol{q}\pm Q} & \Pi_0^{(xx)} \delta_{\boldsymbol{k},\boldsymbol{q}} \end{pmatrix} J_{\boldsymbol{q}} \underline{\underline{\chi}_{qk'}}$$
(6.33)

In order to solve Eq.6.33 we also need to acquire the expression for $\underline{\chi_{kk'}}$ by checking the following power series:

$$N_{s} \sum_{q} \begin{pmatrix} \Pi_{0}^{(xx)} \delta_{k,q} & \Pi_{0}^{(xy)} \delta_{k,q\pm Q} \\ -\Pi_{0}^{(xy)} \delta_{k,q\pm Q} & \Pi_{0}^{(xx)} \delta_{k,q} \end{pmatrix} J_{q} \begin{pmatrix} \Pi_{0}^{(xx)} \delta_{q,k'} & \Pi_{0}^{(xy)} \delta_{q,k'\pm Q} \\ -\Pi_{0}^{(xy)} \delta_{q,k'\pm Q} & \Pi_{0}^{(xx)} \delta_{q,k'} \end{pmatrix}$$

$$= N_{s} \begin{pmatrix} \left(\Pi_{0}^{(xx)^{2}} - \Pi_{0}^{(xy)^{2}} \right) \delta_{k,k'} & 2\Pi_{0}^{(xx)} \Pi_{0}^{(xy)} \delta_{k,k'\pm Q} \\ -2\Pi_{0}^{(xx)} \Pi_{0}^{(xy)} \delta_{k,k'\pm Q} & \left(\Pi_{0}^{(xx)^{2}} - \Pi_{0}^{(xy)^{2}} \right) \delta_{k,k'} \end{pmatrix}$$

$$(6.34)$$

From Eq.6.34 we can infer that the same matrix structure will hold for the expression of $\chi_{kk'}$:

$$\underline{\chi_{kk'}} = N_s \begin{pmatrix} \chi^{(xx)}(\mathbf{k'})\delta_{\mathbf{k,k'}} & \chi^{(xy)}(\mathbf{k'} \pm Q)\delta_{\mathbf{k,k'}\pm Q} \\ -\chi^{(xy)}(\mathbf{k'} \pm Q)\delta_{\mathbf{k,k'}\pm Q} & \chi^{(xx)}(\mathbf{k'})\delta_{\mathbf{k,k'}} \end{pmatrix}$$
(6.35)

By inserting Eq.6.35 into Eq.6.33 we can find an expression for the renormalized susceptibility:

$$\frac{1}{N_s} \underline{\chi_{kk'}} = \begin{pmatrix} \Pi_0^{(xx)} \delta_{\mathbf{k},\mathbf{k'}} & \Pi_0^{(xy)} \delta_{\mathbf{k},\mathbf{k'}\pm Q} \\ -\Pi_0^{(xy)} \delta_{\mathbf{k},\mathbf{k'}\pm Q} & \Pi_0^{(xx)} \delta_{\mathbf{k},\mathbf{k'}} \end{pmatrix} - \underline{\underline{A}_{k,k'}}, \tag{6.36}$$

where the matrix elements of $\underline{A_{k,k'}}$ is a 2 × 2 takes the following form:

$$A_{11}(\boldsymbol{k},\boldsymbol{k'}) = A_{22}(\boldsymbol{k},\boldsymbol{k'}) = \left[\Pi_0^{(xx)}\mathcal{J}(\boldsymbol{k'})\chi^{(xx)}(\boldsymbol{k'}) - \Pi_0^{(xy)}\mathcal{J}(\boldsymbol{k'}\pm\boldsymbol{Q})\chi^{(xy)}(\boldsymbol{k'}\pm\boldsymbol{Q})\right]\delta_{\boldsymbol{k},\boldsymbol{k'}}$$
$$-A_{21}(\boldsymbol{k},\boldsymbol{k'}) = A_{12}(\boldsymbol{k},\boldsymbol{k'}) = \left[\Pi_0^{(xx)}\mathcal{J}(\boldsymbol{k'}\pm\boldsymbol{Q})\chi^{(xy)}(\boldsymbol{k'}\pm\boldsymbol{Q}) + \Pi_0^{(xy)}\mathcal{J}(\boldsymbol{k'})\chi^{(xx)}(\boldsymbol{k'})\right]\delta_{\boldsymbol{k},\boldsymbol{k'}\pm\boldsymbol{Q}},$$
$$(6.37)$$

Combing Eq.6.36 and Eq.6.37 we have:

$$\begin{pmatrix} 1 + \mathcal{J}(\boldsymbol{k})\Pi_{0}^{(xx)} & -\mathcal{J}(\boldsymbol{k} \pm \boldsymbol{Q})\Pi_{0}^{(xy)} \\ \mathcal{J}(\boldsymbol{k})\Pi_{0}^{(xy)} & 1 + \mathcal{J}(\boldsymbol{k} \pm \boldsymbol{Q})\Pi_{0}^{(xx)} \end{pmatrix} \begin{pmatrix} \chi^{(xx)}(\boldsymbol{k}) \\ \chi^{(xy)}(\boldsymbol{k} \pm \boldsymbol{Q}) \end{pmatrix} = \begin{pmatrix} \Pi_{0}^{(xx)} \\ \Pi_{0}^{(xy)} \end{pmatrix}$$
(6.38)

By solving Eq.6.38 we end up with:

$$\chi^{(xx)}(\boldsymbol{k}, i\nu_m) = \frac{\Pi_0^{(xx)} + [(\Pi_0^{(xx)})^2 + (\Pi_0^{(xy)})^2]J(\boldsymbol{k} \pm Q)}{[1 + \Pi_0^{(xx)}J(\boldsymbol{k})][1 + \Pi_0^{(xx)}J(\boldsymbol{k} \pm Q)] + (\Pi_0^{(xy)})^2J(\boldsymbol{k})J(\boldsymbol{k} \pm Q)}, \quad (6.39a)$$

$$\chi^{(xy)}(\boldsymbol{k}, i\nu_m) = \frac{\Pi_0^{(xy)}}{[1 + \Pi_0^{(xx)}J(\boldsymbol{k})][1 + \Pi_0^{(xx)}J(\boldsymbol{k} \pm Q)] + (\Pi_0^{(xy)})^2 J(\boldsymbol{k})J(\boldsymbol{k} \pm Q)}.$$
 (6.39b)

Then by using Eq.6.31a and 6.31b we can carry out the exact form of our renormalized susceptibility:

$$\chi^{(xx)}(\mathbf{k}, i\nu_m) = \chi^{(yy)}(\mathbf{k}, i\nu_m) = \frac{J(\mathbf{k} \pm \mathbf{Q}) - J(\mathbf{Q})}{E(\mathbf{k})^2 - (i\nu_m)^2}$$
(6.40a)

$$\chi^{(xy)}(\mathbf{k}, i\nu_m) = -\chi^{(yx)}(\mathbf{k}, i\nu_m) = \frac{(2i)i\nu_m}{E(\mathbf{k})^2 - (i\nu_m)^2},$$
(6.40b)

where,

$$E(\boldsymbol{k}) = \frac{1}{2} \sqrt{\left[(J(\boldsymbol{k}) - J(\boldsymbol{Q})) \right] \left[J(\boldsymbol{k} \pm \boldsymbol{Q}) - J(\boldsymbol{Q}) \right]}$$
(6.41)

$$J(\boldsymbol{k}) = 2J_1(\cos \boldsymbol{k_x} + \cos \boldsymbol{k_y}) + 4J_2 \cos \boldsymbol{k_x} \cos \boldsymbol{k_y}$$
(6.42)

6.2 Spin wave dispersion relation

The spectral function of magnon takes the following form:

$$\mathcal{A}(\boldsymbol{q},\omega) = \frac{1}{\pi} \mathrm{Im}\chi^{(xx)}(\boldsymbol{q},\omega+i\delta)$$

= $\left[\frac{J(\boldsymbol{q}\pm\boldsymbol{Q}) - J(\boldsymbol{Q})}{2\pi E(\boldsymbol{q})}\right] \mathrm{Im}\left[\frac{1}{E(\boldsymbol{q}) + (\omega+i\delta)} + \frac{1}{E(\boldsymbol{q}) - (\omega+i\delta)}\right]$ (6.43)

The Cauchy-Dirac relation:

$$\frac{1}{\omega' - \omega \mp i\delta} = \mathbf{P} \frac{1}{\omega' - \omega} \pm i\pi\delta(\omega' - \omega)$$
(6.44)

By using the Cauchy-Dirac relation we are allowed to further reduce the form of Eq.6.43 to get:

$$\mathcal{A}(\boldsymbol{q},\omega) = \left[\frac{J(\boldsymbol{q} \pm \boldsymbol{Q}) - J(\boldsymbol{Q})}{2E(\boldsymbol{q})}\right] \left[\delta(\omega - E(\boldsymbol{q})) - \delta(\omega + E(\boldsymbol{q}))\right]$$
(6.45)

Then we get the dispersion relations of spin wave in both magnetic ordered states:

$$\omega_{\text{N\acute{e}el}} = \frac{1}{2} \sqrt{\left[(J(\boldsymbol{q}) - J(\boldsymbol{Q}_{\text{N}}) \right] \left[J(\boldsymbol{q} \pm \boldsymbol{Q}_{\text{N}}) - J(\boldsymbol{Q}_{\text{N}}) \right]}$$
(6.46a)

$$\omega_{\text{Coll.}} = \frac{1}{2} \sqrt{\left[(J(\boldsymbol{q}) - J(\boldsymbol{Q}_{\text{C}})) \right] \left[J(\boldsymbol{q} \pm \boldsymbol{Q}_{\text{C}}) - J(\boldsymbol{Q}_{\text{C}}) \right]}$$
(6.46b)

$$J(\boldsymbol{q}) = 2J_1(\cos \boldsymbol{q_x} + \cos \boldsymbol{q_y}) + 4J_2 \cos \boldsymbol{q_x} \cos \boldsymbol{q_y}$$
(6.46c)

Where we use the notations: $Q_{\rm N} = (\pi, \pi)$ and $Q_{\rm C} = (0, \pi), (\pi, 0)$.



Figure 6.2: Dispersion relations of the spin wave in the Néel state(Q_N) with different ratios between J_1 and $J_2:(a)\frac{J_2}{J_1} = 0$, $(b)\frac{J_2}{J_1} = 0.25$, $(c)\frac{J_2}{J_1} = 0.5$



Figure 6.3: Dispersion relations of the spin wave in the Collinear state($Q_{\rm C}$) with different ratios between J_1 and $J_2:(a)\frac{J_2}{J_1} = 0.5$, $(b)\frac{J_2}{J_1} = 1$, $(c)\frac{J_2}{J_1} = 5$

From above Fig.6.2, two zero excitation energy modes are found at : $q_1 = (\pi, \pi)$ and $q_2 = (0,0)$ when the system ordered in Néel state. While the point $q_2 = (0,0)$ is not a Goldstone mode, for its spectral weight is evaluated to zero which can be seen from Eq.6.45. Similar argument applied to Collinear state too, and the corresponding two zero excitation energy modes are found at: $q_1 = (\pi, 0)$ and $q_2 = (0,0)$. The spin wave velocity is found being suppressed to zero at the maximum frustration point $\frac{J_2}{J_1} = 0.5$ in both magnetic ordered state. This may partial expresses that the magnetic ordering effect is greatly suppressed by the existence of the frustration. From above Fig.6.2 and Fig.6.3 one may conclude that the long range magnetic order found when $\frac{J_2}{J_1} \neq 0.5$ is still true. Then we should compute from the second order corrections to the mean field magnetization to check whether this term will total destroy the long range magnetic order, or namely, we want to prove the Mermin-Wagner theorem for our 2D spin system.

6.3 Check of Mermin–Wagner–Hohenberg Theorem

Now we can shortly prove the Mermin–Wagner–Hohenberg Theorem by following:

$$\langle S_i^z \rangle = \frac{1}{2} - \left(\langle S_i^x S_i^x \rangle + \langle S_i^y S_i^y \rangle \right) = \frac{1}{2} - 2 \langle S_i^x S_i^x \rangle \tag{6.47}$$

Here we have to use fluctuation dissipation Theorem:

$$\langle S_i^x S_i^x \rangle = \frac{1}{N_s} \sum_q \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{1 - e^{-\beta\omega}} \chi^{(xx)''}(\boldsymbol{q}, \omega) d\omega$$
(6.48a)

$$\chi^{(xx)''}(\boldsymbol{q},\omega) = \operatorname{Im}\left[\chi^{(xx)}(\boldsymbol{q},\omega)\right]$$
(6.48b)

Using the results from above section we have:

$$\chi^{(xx)''}(\boldsymbol{q},\omega) = \pi \left(\frac{J(\boldsymbol{q} \pm \boldsymbol{Q}) - J(\boldsymbol{Q})}{2E(\boldsymbol{q})}\right) \left[\delta(\omega - E(\boldsymbol{q})) - \delta(\omega + E(\boldsymbol{q}))\right]$$
(6.49)

Inserting Eq.6.49 into Eq.6.48 we can get:

$$\langle S_i^x S_i^x \rangle = \frac{1}{N_s} \sum_q \int_{-\infty}^{+\infty} \frac{1}{1 - e^{-\beta\omega}} \left(\frac{J(\boldsymbol{q} \pm \boldsymbol{Q}) - J(\boldsymbol{Q})}{2E(\boldsymbol{q})} \right) \left[\delta(\omega - E(\boldsymbol{q})) - \delta(\omega + E(\boldsymbol{q})) \right] d\omega$$
(6.50)

Carry out the integral over ω in Eq.6.50 we get:

$$\langle S_i^x S_i^x \rangle = \frac{1}{N_s} \sum_q \left(\frac{J(\boldsymbol{q} \pm \boldsymbol{Q}) - J(\boldsymbol{Q})}{2E(\boldsymbol{q})} \right) \operatorname{coth}(\frac{E(\boldsymbol{q})}{2T})$$
(6.51)

In the low temperature limit, the fluctuations becomes long range compare the the lattice spacing, so it is reasonable we going to the continuum limit to get:

$$\langle S_i^x S_i^x \rangle = \frac{1}{N_s} \int_{\frac{1}{L}}^{\pi} \frac{dq_x dq_y}{(2\pi)^2} \left(\frac{J(\boldsymbol{q} \pm \boldsymbol{Q}) - J(\boldsymbol{Q})}{2E(\boldsymbol{q})} \right) \coth(\frac{E(\boldsymbol{q})}{2T})$$
(6.52)

When $q = Q + \delta q$, from Eq.6.55 we know that E(q) now becomes a small parameter which allows us to expand the $\operatorname{coth}(x)$ as $\frac{1}{x}$:

$$\langle S_i^x S_i^x \rangle = \frac{T}{4N_s \pi^2} \int_{\frac{1}{L}}^{\pi} \left(\frac{J(q \pm Q) - J(Q)}{E(q)^2} \right) d^2 q$$
 (6.53)

Where,

$$E(\boldsymbol{q})^{2} = \frac{1}{4} \Big[(J(\boldsymbol{q}) - J(\boldsymbol{Q})) \Big] \Big[J(\boldsymbol{q} \pm \boldsymbol{Q}) - J(\boldsymbol{Q}) \Big]$$
(6.54)

$$J(\boldsymbol{q}) = 2J_1(\cos \boldsymbol{q_x} + \cos \boldsymbol{q_y}) + 4J_2 \cos \boldsymbol{q_x} \cos \boldsymbol{q_y}$$
(6.55)

When $\boldsymbol{q} = \boldsymbol{Q} + \delta \boldsymbol{q}$, we can choose $\boldsymbol{Q} = (0, \pi)$ and write $E(\boldsymbol{q})^2$ as:

$$E(\boldsymbol{Q} + \delta \boldsymbol{q})^2 = \frac{1}{4} \Big[(J(\boldsymbol{Q} + \delta \boldsymbol{q}) - J(\boldsymbol{Q}) \Big] \Big[J(\delta \boldsymbol{q}) - J(\boldsymbol{Q}) \Big]$$

= $2J_2 \Big[J(\delta \boldsymbol{q}) - J(\boldsymbol{Q}) \Big] \delta \boldsymbol{q}^2$ (6.56)

By change the origin point of our integration shown in Eq.6.53 from (0,0) to $(0,\pi)$, we have:

$$\langle S_i^x S_i^x \rangle = \frac{T}{4N_s \pi^2} \int_{\frac{1}{L}}^{\pi} \left(\frac{1}{2J_2 \delta \boldsymbol{q}^2}\right) d^2 \delta \boldsymbol{q}$$
(6.57)

Then we can carry out the integration in 6.57 to find:

$$\langle S_i^x S_i^x \rangle \propto \ln(1/L)$$
 (6.58)

This implies that the correlation function of the spin exhibits a logarithmic divergence as we approach the thermodynamic limit, indicating that the long-range magnetic order does not emerge in our 2D system at any finite temperature.

In a short summary: we managed to find the dispersion relation of the spin wave for both the Néel and Collinear states, and the corresponding Goldstone modes is obtained. The relation between the frustration and the low-energy excitations is partially revealed by the fact that both the intensity and velocity of the spin wave is decreasing when it reaches the higher frustration limit. Moreover, we proved the Mermin-Wagner theorem by showing the long range magnetic orders can be totally washed away by fluctuations in the thermodynamic limit.

Chapter 7

Nematic order of J_1 - J_2 Heisenberg model

From last chapter, we found that the long range magnetic orders are washed away by the quantum fluctuation in the thermodynamic limit, which prohibits the spontaneous breaking of a continue symmetry in any two dimensional system. The nematic phase, characterized by discrete symmetry breaking, was initially predicted to occur in the J_1 - J_2 Heisenberg model by P. Chandra et al. [14]. Our particular interest lies in understanding the relationship between the critical temperature (T_c) for the nematic phase and the degree of frustration within the system, as quantified by the ratio of J_1 and J_2 .



Figure 7.1: The critical temperature (T_c) as a function of different frustrating ratios between J_1 and J_2 : (a) Predicted by Monte Carlo simulation [15], (b) Predicted by Nematic Bond Theory [16].

The critical temperature (T_c) prediction, as a function of various frustrating ratios between J_1 and J_2 , is illustrated in Fig. 7.1 through computational methods. However, the outcomes obtained from the analytical method proposed by [14] do not exhibit strong agreement with those from [15] and [16], especially in the regime of strong frustration. Consequently, it is essential to explore alternative analytical approaches that can may effectively resolve this conflict, which serves as the primary motivation for the research conducted in this chapter.

7.1 A toy model for illustrating the nematic phase transition

Here we shall first consider about a naive toy model that may describe some characteristics of the nematic phase transition.



Figure 7.2: An illustration of a little ball passing the energy barrier with respect of different J_1 and J_2 ratios. (a) $\frac{J_2}{J_1} = 1$, (b) $\frac{J_2}{J_1} = 10$

As we can see for Fig. 7.2, the height of yellow configurations in the 3D plot corresponds to the eigenenergy (J_q) of the J_1 - J_2 Heisenberg Hamiltonian (see Eq.4.7) as the function of q_x and q_y . The order parameter for the nematic phase is imagined as a red ball shown above. A finite temperature is considered as some disturbances to kick the ball away from the saddle points: $\mathbf{Q} = (0, \pm \pi), (\pm \pi, 0)$. When the intensity of the disturbance is strong enough to move the ball from one saddle point to another one, the critical temperature for the nematic phase transition is believed to be reached. As pointed out in [14], the nematic T_c is proportional to the size of the magnetic domain, which is estimated by the square of the correlation length: $N \propto \xi^2 \approx e^{\frac{aJ_2}{T}}$. Here we assume that the transition temperature for nematic phase should also be proportional to the lowest barrier value of (J_q) that lies in between two saddle points. In Fig.4.2(b), one notices that this lowest barrier height should be found along the lines: $(q_x = q_y)$ or $q_x = -q_y$, for the J_q has a fourfold symmetry along these two lines. We may choose $q_x = q_y$ and get the following description for the barrier value of (J_q) along this line:

$$J_q = 4J_1 \cos(q) + 4J_2 \cos^2(q). \tag{7.1}$$

The saddle point of the value of J_q along this line is find by using: $\frac{\partial J_q}{\partial q} = 0$, from which we found: $q = \arccos(\frac{-J_1}{2J_2})$. Hence, the lowest value of J_q along this line is found to be:

$$J_{\min} = -\frac{J_1^2}{J_2}.$$
 (7.2)

The true lowest barrier value of (J_q) is the difference between J_{\min} and $J_{q=(0,\pi)}$:

$$B_0 = J_{\min} - J_{\boldsymbol{q}=(0,\pi)} = J_2 \left(4 - \frac{J_1^2}{J_2^2}\right),\tag{7.3}$$

where B_0 stands for the lowest barrier value, and we find the it becomes zero at the maximal frustration point $(\frac{J_2}{J_1} = 0.5)$. As we mentioned above, the critical temperature of nematic phase is proportional to both N and B_0 . Hence, we obtain:

$$T_c \propto a J_2 (4 - \frac{J_1^2}{J_2^2}) e^{\frac{b J_2}{T_c}},$$
(7.4)

where a and b are the undecided coefficients, and for our convenient, here we set $J_1 = 1$ and solve the approximation solution for the T_c and we find:

$$T_c \propto \frac{bJ_2}{W_0\left[\frac{2bJ_2^2}{a(4J_2^2-1)}\right]},$$
(7.5)

where $W_0(x)$ stands for the main branch of the Lambert W function. From Eq.7.5 we get the Fig.7.3 below:



Figure 7.3: The transition temperature for the nematic phase is estimated by fixing b = 1and varying a at values of 0.1, 0.2, 0.5, and 1.0 for tuning purposes.

In this study, we did not extensively delve into the precise determination of these coefficients, as the model employed is considered a simplified representation. Nevertheless, the observed behavior of the function in proximity to the critical point $(\frac{J_2}{J_1} = 0.5)$ remains consistent, suggesting that this model may captures certain characteristics relates to the critical behavior of the nematic T_c .

7.2 An effective Heisenberg Hamiltonian

In the subsequent chapters, our objective is to establish a formulation for the nematic T_c utilizing the path integral formalism and the methodologies developed in the preceding chapters. Apart from the procedure that are used to perform the Hubbard-stratonovich transformation in Chapter 5, here alternatively, one may choose to use a effective Heisenberg Hamiltonian with a positive definite interaction matrix to replace the original one. And this can be done in the following way:

First we subtract the maximum eigenvalue $J_{\text{max}} = 2J_1 + 2J_2$ for the Hamiltonian to get:

$$H = NS^{2}J_{\max} + \sum_{q} (\frac{1}{2}J_{q} - J_{\max})S_{q} \cdot S_{-q}$$

$$= E_{\max} - \sum_{q} (J_{\max} - \frac{1}{2}J_{q})S_{q} \cdot S_{-q}.$$
(7.6)

We have $S^2 = \frac{3}{4}$ for our spin- $\frac{1}{2}$ system, ensuring that the term E_{max} can be regarded as a constant shift to the eigenenergy, without altering the physical properties of the system. Hence we can neglect the contribution of the this term to obtain a effective Hamiltonian for our model:

$$H_{\text{eff}} = \sum_{q} -J_{q}^{>} \boldsymbol{S}_{q} \cdot \boldsymbol{S}_{-q}$$
$$= \sum_{ij} -J_{ij}^{>} \boldsymbol{S}_{i} \cdot \boldsymbol{S}_{j}$$
(7.7)

where we note $J_{\boldsymbol{q}}^{>} = J_{\max} - \frac{1}{2}J_{\boldsymbol{q}}$ and $J_{ij}^{>} = J_{\max}\delta_{ij} - \frac{1}{2}J_{ij}$, which are both positive definite matrices. By using the path integral formalism we have:

$$Z = e^{-\beta E_{\max}} \int \mathcal{D}[\bar{\psi}, \psi] e^{-s[\bar{\psi}, \psi]}$$
(7.8a)

$$S[\bar{\psi},\psi] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}} (\partial_{\tau} \underline{\underline{\sigma}_{0}}) \psi_{-\boldsymbol{q}} - J_{ij}^{\geq} \boldsymbol{S}_{\boldsymbol{i}} \cdot \boldsymbol{S}_{\boldsymbol{j}}, \qquad (7.8b)$$

where in above ψ_i is related to spin operators by: $S_i = \psi_i^{\dagger}(\frac{\sigma}{2})\psi_i$ Again we introduce a white-noise vector field $\varphi_i = (\varphi_i^x, \varphi_i^y, \varphi_i^z)$ into the partition function and entangle it with the original partition function to get:

$$Z \times Z_H = \int \mathcal{D}[\bar{\psi}, \psi] \int \mathcal{D}[\varphi] e^{-s[\bar{\psi}, \psi, \varphi]}$$
(7.9a)

$$S[\bar{\psi},\psi,\varphi] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}}(\partial_{\tau}\underline{\underline{\sigma}_{0}})\psi_{-\boldsymbol{q}} + \sum_{ij} \left[-J_{ij}^{>}\boldsymbol{S}_{\boldsymbol{i}} \cdot \boldsymbol{S}_{\boldsymbol{j}} + \frac{\varphi_{\boldsymbol{i}} \cdot \varphi_{\boldsymbol{j}}}{J_{ij}^{>}} \right].$$
(7.9b)

Then we shift the white-noise field as follow:

$$\boldsymbol{\varphi}_{i} \rightarrow \boldsymbol{m}_{i} - \sum_{k} J_{ki}^{>} \boldsymbol{S}_{k}$$
 (7.10a)

$$\varphi_{j} \rightarrow m_{j} - \sum_{h} J_{jh}^{>} S_{h}.$$
 (7.10b)

Then by inserting the Eq.7.10 into Eq.7.9b we get:

$$S[\bar{\psi},\psi,\boldsymbol{m}] = \sum_{\boldsymbol{q}} \int_{0}^{\beta} d\tau \bar{\psi}_{\boldsymbol{q}} (\partial_{\tau} \underline{\underline{\sigma}_{0}}) \psi_{-\boldsymbol{q}} - \sum_{i} 2\boldsymbol{S}_{\boldsymbol{i}} \cdot \boldsymbol{m}_{\boldsymbol{i}} + \sum_{ij} \frac{\boldsymbol{m}_{\boldsymbol{i}} \cdot \boldsymbol{m}_{\boldsymbol{j}}}{J_{\boldsymbol{i}\boldsymbol{j}}^{>}}.$$
 (7.11)

We apply Fourier transformation to Eq.7.11 with the following conventions:

$$\boldsymbol{S}_{\boldsymbol{i}} = N^{-1/2} \sum_{\mathbf{q}} S_{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}_{\boldsymbol{i}}}, \qquad (7.12a)$$

$$\boldsymbol{m_i} = N^{-1} \sum_{\mathbf{q}} m_{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}_i}, \qquad (7.12b)$$

$$\psi_i = N^{-1/2} \sum_{\mathbf{q}} \psi_{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}_i}, \qquad (7.12c)$$

$$J_{ij} = N^{-1} \sum_{\boldsymbol{q}} e^{i\boldsymbol{q}(\boldsymbol{r_i} - \boldsymbol{r_j})} J_{\boldsymbol{q}}, \qquad (7.12d)$$

to get:

$$S[\bar{\psi},\psi,\mathbf{\Delta}] = \int_0^\beta d\tau \sum_{\boldsymbol{k},\boldsymbol{k'}} \psi^{\dagger}_{\boldsymbol{k'}} (\partial_\tau \delta_{\boldsymbol{k},\boldsymbol{k'}} \underline{\sigma_0} - \frac{1}{N} \boldsymbol{m}_{\tau,\boldsymbol{k'}-\boldsymbol{k}} \cdot \boldsymbol{\sigma}) \psi_{\boldsymbol{k}} + \frac{1}{N} \sum_{\boldsymbol{q}} \frac{\mathbf{\Delta}_{\boldsymbol{q}} \cdot \mathbf{\Delta}_{-\boldsymbol{q}}}{J_{\boldsymbol{q}}^{\geq}}.$$
 (7.13)

we can rescale the Hubbard field as follow:

$$\boldsymbol{\Delta}_{\boldsymbol{q}} = \frac{1}{J_{\boldsymbol{q}}^{>}} \boldsymbol{m}_{\boldsymbol{q}},\tag{7.14}$$

Then from above we can write down the action:

$$S[\bar{\psi},\psi,\mathbf{\Delta}] = \int_{0}^{\beta} d\tau \sum_{\boldsymbol{k},\boldsymbol{k'}} \psi^{\dagger}_{\boldsymbol{k'}} (\partial_{\tau} \delta_{\boldsymbol{k},\boldsymbol{k'}} \underline{\underline{\sigma}_{0}} - \frac{1}{N} J_{\boldsymbol{k'}-\boldsymbol{k}}^{>} \mathbf{\Delta}_{\tau,\boldsymbol{k'}-\boldsymbol{k}} \cdot \boldsymbol{\sigma}) \psi_{\boldsymbol{k}} + \frac{1}{N} \sum_{\boldsymbol{q}} J_{\boldsymbol{q}}^{>} \mathbf{\Delta}_{\boldsymbol{q}} \cdot \mathbf{\Delta}_{-\boldsymbol{q}}.$$
(7.15)

Then we carry out the Gaussian integral of the quadratic term we can get:

$$S_E[\mathbf{\Delta}] = -\mathrm{Trln}\left((-i\omega_n \delta_{k,k'}\underline{\sigma_0}) \left[1 + (i\omega_n \delta_{k,k'}\underline{\sigma_0})^{-1} (\frac{1}{N}J_{k'-k}^{>}\mathbf{\Delta}_{m,k'-k}\cdot\boldsymbol{\sigma})\right]\right) + \frac{\beta}{N}\sum_q J_q^{>}\mathbf{\Delta}_q\cdot\mathbf{\Delta}_{-q}$$
(7.16)

Then we note $(i\omega_n \delta_{k,k'} \underline{\sigma_0})^{-1}$ as $G_0(n,k)$ and $\frac{1}{N} J_{k'-k}^{>} \Delta_{m,k'-k} \cdot \boldsymbol{\sigma}$ as $-V_{m,k,k'}$ and we can get:

$$S_E[\mathbf{\Delta}] = -\operatorname{Trln}(-G_0^{-1}) - \operatorname{Trln}(1 - G_0 V_{m,k,k'}) + \frac{\beta}{N} \sum_q J_q^{\geq} \mathbf{\Delta}_q \cdot \mathbf{\Delta}_{-q}.$$
 (7.17)

7.3 Feynman diagram expansion up to fourth order

In this section, we perform the Feynman diagram expansion in momentum space up to the fourth order. This is necessary because the nematic order is connected to the fluctuations ($\langle \Delta^2 \rangle$) of the Weiss field, and the susceptibility of nematic phase is then suggested by the quadratic form of fluctuations, which is a fourth order correction.

Eq.7.17 is obtained by using the formula for the Taylor expansion of a logarithmic function, together with the fact that the term G_0V is a small parameter and can be treated as a perturbation:

$$\operatorname{Trln}(1 - G_0 V_{m,k,k'}) = \operatorname{Tr}\left[-G_0 V_{m,k,k'} - \frac{1}{2}(G_0 V_{m,k,k'})^2 - \frac{1}{3}(G_0 V_{m,k,k'})^3 - \frac{1}{4}(G_0 V_{m,k,k'})^4 + \cdots\right]$$
(7.18)

Here we compute it to fourth order. Firstly due to Pauli-matrix are trace-less so the odd order term is zero and for the second order we find:

$$-\frac{1}{2}\sum_{i\cdots l} (G_{0ij}V_{jk}G_{0kl}V_{li}\delta_{ij}\delta_{kl}).$$
(7.19)

Here "ij" stands for kk', nn' and $\sigma\sigma'$ and for the momentum and matsubara frequency dependence we found:

$$-\frac{1}{2}\sum_{n,n',k,k'}G_0(n,k)V_{n-n',k'-k}G_0(k',n')V_{n'-n,k-k'},$$
(7.20)

which is:

$$-\frac{1}{2}\sum_{n,n',k,k',i,j,a,b}\frac{(J_{k'-k}^{\geq})^2}{N^2}G_0(n,k)\Delta_{n-n',k-k'}^{(i)}\sigma_{ab}^{(i)}G_0(n',k')\Delta_{n'-n,k-k'}^{(j)}\sigma_{ba}^{(j)}.$$
 (7.21)

By using the properties of the Pauli matrices: $\text{Tr}(\sigma^{(i)}\sigma^{(j)}) = \sum_{a,b} \sigma^{(i)}_{ab} \sigma^{(j)}_{ba} = 2\delta_{ij}$ we can further get:

$$-\sum_{n,n',\boldsymbol{k},\boldsymbol{k'},i} \frac{(J_{\boldsymbol{k'}-\boldsymbol{k}}^{>})^2}{N^2} G_0(n,\boldsymbol{k}) \Delta_{n-n',\boldsymbol{k'}-\boldsymbol{k}}^{(i)} G_0(n',\boldsymbol{k'}) \Delta_{n'-n,\boldsymbol{k'}-\boldsymbol{k}}^{(i)}.$$
 (7.22)

We can rewrite it as:

$$-\sum_{n,m,k,q,i} \frac{(J_q^{>})^2}{N^2} G_0(n,k) \Delta_{m,q}^{(i)} G_0(n-m,k-q) \Delta_{-m,-q}^{(i)},$$
(7.23)

where i stands for x,y,z.

Notice that there is no actual momentum dependence of the propagator G_0 . Hence we can further simplified above equation as:

$$-\sum_{n,m,\boldsymbol{q}} \frac{J_{\boldsymbol{q}}^{>2}}{N(i\omega_n)(i\omega_n - i\nu_m)} \boldsymbol{\Delta}_{m,\boldsymbol{q}} \cdot \boldsymbol{\Delta}_{-m,-\boldsymbol{q}}$$
(7.24)

In above ω_n stands for the fermionic matsubara frequency $\left(2\pi(n+\frac{1}{2})k_BT\right)$, and ν_m stands for the bosonic matsubara frequency $(2\pi nk_BT)$. So far we have not put any constraint on the occupation number for each site.

If $i\nu_m$ is non-zero than we carry out the matsubara sum we will get:

$$-\sum_{m,\boldsymbol{q}} \frac{1}{N} J_{\boldsymbol{q}}^{>2} \left[\frac{f(0)}{-i\nu_m} + \frac{f(i\nu_m)}{i\nu_m} \right] \boldsymbol{\Delta}_{m,\boldsymbol{q}} \cdot \boldsymbol{\Delta}_{-m,-\boldsymbol{q}}.$$
(7.25)

And if we apply the periodicity of the Fermi-Dirac function: we can have $f(i\nu_m) = f(0)$ so that this gives zero, by considering the case for $i\nu_m$ is zero we should get:

$$-\sum_{n,\boldsymbol{q}} \frac{J_{\boldsymbol{q}}^{>2}}{N(i\omega_n)(i\omega_n)} \boldsymbol{\Delta}_{0,\boldsymbol{q}} \cdot \boldsymbol{\Delta}_{0,-\boldsymbol{q}}.$$
(7.26)

And we can carry out the matsubara sum to get:

$$\frac{\beta^2}{4N} \sum_{\boldsymbol{q}} J_{\boldsymbol{q}}^{>2} \boldsymbol{\Delta}_{0,\boldsymbol{q}} \cdot \boldsymbol{\Delta}_{0,-\boldsymbol{q}}.$$
(7.27)

For the third order term we have:

$$-\frac{1}{3}\sum_{i\cdots q} (G_{0ij}V_{jk}G_{0kl}V_{lp}G_{0pq}V_{qi}\delta_{ij}\delta_{kl}\delta_{pq}).$$

$$(7.28)$$

This can be simplified as:

$$-\frac{1}{3}\sum_{i,k,p} (G_{0i}V_{ik}G_{0k}V_{kp}G_{0p}V_{pi}).$$
(7.29)

By using the same procedure that we just used in computing the second order terms, we found the results for the static configuration of the white-noise field $(i\nu_{m_1} = i\nu_{m_2} = 0)$ is zero, and the detailed calculations of this can be found in Appendix.B.

For the fourth order term we find:

$$-\frac{1}{4}\sum_{i\cdots r} (G_{0ij}V_{jk}G_{0kl}V_{lp}G_{0pq}V_{qh}G_{0hr}V_{ri}\delta_{ij}\delta_{kl}\delta_{pq}\delta_{hr}), \qquad (7.30)$$

which can be simplified as:

$$-\frac{1}{4}\sum_{i,l,p,h} (G_{0i}V_{il}G_{0l}V_{lp}G_{0p}V_{ph}G_{0h}V_{hi}).$$
(7.31)

Final result for the static fourth order correction reads:

$$-\frac{\beta^4}{96N^3} \sum_{\boldsymbol{q_1}, \boldsymbol{q_2}, \boldsymbol{q_3}, i, j} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^> \Delta_{0, \boldsymbol{q_1}}^{(i)} \Delta_{0, \boldsymbol{q_2}}^{(j)} \Delta_{0, \boldsymbol{q_3}}^{(j)} \Delta_{0, -\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^{(i)}.$$
(7.32)

We also include detailed calculations of this in Appendix.C. One may notice that there are also third and fourth order non-static corrections to the action, which is beyond the scope of this thesis, but we do include these terms in Appendix.D just in case it may be needed in the future.

Now if we only consider the static part of the action up to fourth order we will get:

$$S_{E}[\mathbf{\Delta}] = S_{0} + \frac{\beta}{N} \sum_{q} J_{q}^{>} \mathbf{\Delta}_{q} \cdot \mathbf{\Delta}_{-q} - \frac{\beta^{2}}{4N} \sum_{q} J_{q}^{>2} \mathbf{\Delta}_{q} \cdot \mathbf{\Delta}_{-q} + \frac{\beta^{4}}{96N^{3}} \sum_{q_{1},q_{2},q_{3}} J_{q_{1}}^{>} J_{q_{2}}^{>} J_{q_{3}}^{>} J_{-q_{1}-q_{2}-q_{3}}^{>} (\mathbf{\Delta}_{q_{1}} \cdot \mathbf{\Delta}_{q_{2}}) (\mathbf{\Delta}_{q_{3}} \cdot \mathbf{\Delta}_{-q_{1}-q_{2}-q_{3}}).$$

$$(7.33)$$

Then let us write what happen if we go out from $T \to 0$ limit, which means we have to apply the projection to the physical state and here we done this by using the Popov-Fedatov method: instead using $G_0(n, \mathbf{k}) = (i\omega_n \delta_{\mathbf{k},\mathbf{k}'} \underline{\sigma_0})^{-1}$, we have to add a so-called imaginary chemical potential to map out the unphysical state, which leads to: $G_0(n, \mathbf{k}) = \frac{\delta_{\mathbf{k},\mathbf{k}'}}{(i\omega_n - \lambda_f)\underline{\sigma_0}}$, where $\lambda_f = \frac{i\pi T}{2}$. By using this trick we get a new expression for the action:

$$S_{E}[\boldsymbol{\Delta}] = S_{0} + \frac{\beta}{N} \sum_{q} J_{q}^{\geq} \boldsymbol{\Delta}_{q} \cdot \boldsymbol{\Delta}_{-q} - \frac{\beta^{2}}{2N} \sum_{q} J_{q}^{\geq 2} \boldsymbol{\Delta}_{q} \cdot \boldsymbol{\Delta}_{-q} + \frac{\beta^{4}}{12N^{3}} \sum_{q_{1},q_{2},q_{3}} J_{q_{1}}^{\geq} J_{q_{2}}^{\geq} J_{q_{3}}^{\geq} J_{-q_{1}-q_{2}-q_{3}}^{\geq} (\boldsymbol{\Delta}_{q_{1}} \cdot \boldsymbol{\Delta}_{q_{2}}) (\boldsymbol{\Delta}_{q_{3}} \cdot \boldsymbol{\Delta}_{-q_{1}-q_{2}-q_{3}}).$$

$$(7.34)$$

7.4 An effective theory for computing the nematic T_c

In this section, our goal is to use the form of action that is described in Eq.7.33 to derive a expression for the nematic T_c as a function of the ratio between J_1 and J_2 . To begin with, we make following approximations in order to capture the feature of the nematic order. In the Collinear phase $(J_2 \gg J_1)$, the $J_q^>$ is peaked at points in the momentum space as shown in Fig.7.4 $Q_1 = (\pm \pi, 0)$, $Q_2 = (0, \pm \pi)$. Nevertheless, from Eq.7.33, we observe that $J_q^>$ acts as a prefactor for the Weiss field, representing contributions from fields with same momentum dependence. In a simplified scenario, we impose an energy cutoff near the peak intensity, allowing us to focus solely on the small region around Q_1 and Q_2 . Within this energy cutoff, we may also disregard the q-dependence of the order parameter, introducing two new notations $\Delta_{X/Y}$ and $J_{Q_1}^>(\delta q)$ to replace $\Delta(Q_1/Q_2)$ and $J^>(Q_1 + \delta q)$, respectively. By employing this approximation, we can express our new action up to second order as follows:

$$S^{(2)}[\boldsymbol{\Delta}_X, \boldsymbol{\Delta}_Y] = S_0 + \frac{\beta^2}{2N} \sum_{\boldsymbol{\delta}\boldsymbol{q}} J_{\boldsymbol{Q}_1}^{\geq}(\boldsymbol{\delta}\boldsymbol{q}) \bigg[2T - J_{\boldsymbol{Q}_1}^{\geq}(\boldsymbol{\delta}\boldsymbol{q}) \bigg] (|\boldsymbol{\Delta}_X|^2 + |\boldsymbol{\Delta}_Y|^2), \quad (7.35)$$

where we used the fact that the $J^{>}_{Q_1}(\delta q)$ and $J^{>}_{Q_2}(\delta q)$ can transform into each other by the $\frac{\pi}{2}$ rotation around the point (0,0) in the momentum space to further reduced its form.

And the fourth order term reads as the following:

$$S^{(4)}[\boldsymbol{\Delta}] = \frac{\beta^4}{12N^3} \sum_{\boldsymbol{\delta q_1, \delta q_2, \delta q_3}} \left[J_{\boldsymbol{Q_1}}^{>}(\boldsymbol{\delta q_1}) J_{\boldsymbol{Q_1}}^{>}(\boldsymbol{\delta q_2}) J_{\boldsymbol{Q_1}}^{>}(\boldsymbol{\delta q_3}) J_{\boldsymbol{Q_1}}^{>}(-\boldsymbol{\delta q_1} - \boldsymbol{\delta q_2} - \boldsymbol{\delta q_3}) (|\boldsymbol{\Delta}_X|^4 + |\boldsymbol{\Delta}_Y|^4) \right. \\ \left. + 2J_{\boldsymbol{Q_1}}^{>}(\boldsymbol{\delta q_1}) J_{\boldsymbol{Q_1}}^{>}(\boldsymbol{\delta q_2}) J_{\boldsymbol{Q_2}}^{>}(\boldsymbol{\delta q_3}) J_{\boldsymbol{Q_2}}^{>}(-\boldsymbol{\delta q_1} - \boldsymbol{\delta q_2} - \boldsymbol{\delta q_3}) |\boldsymbol{\Delta}_X|^2 |\boldsymbol{\Delta}_Y|^2 \right. \\ \left. + 4J_{\boldsymbol{Q_1}}^{>}(\boldsymbol{\delta q_1}) J_{\boldsymbol{Q_1}}^{>}(\boldsymbol{\delta q_2}) J_{\boldsymbol{Q_2}}^{>}(\boldsymbol{\delta q_3}) J_{\boldsymbol{Q_2}}^{>}(-\boldsymbol{\delta q_1} - \boldsymbol{\delta q_2} - \boldsymbol{\delta q_3}) |\boldsymbol{\Delta}_X \cdot \boldsymbol{\Delta}_Y|^2 \right]$$

$$(7.36)$$



Figure 7.4: Contour plot of $J_{\bm{q}}^>$ in the regime J2 \gg J1 , the value of $J_{\bm{q}}^>$ is reflected by the color, namely warm and cold colors each corresponds the high and low value of $J_{\bm{q}}^>$ respectively.

In order to stress the core of the problem and get rid off the lengthy mathematical

expressions in Eq.7.35, we shall define following new parameters:

$$\mathcal{K}_1 = \sum_{\delta q} J_{Q_1}^{>}(\delta q) \tag{7.37a}$$

$$\mathcal{K}_2 = \sum_{\delta q} J_{Q_1}^{>} (\delta q)^2 \tag{7.37b}$$

$$\mathcal{K}_{aa} = \sum_{\delta q_1, \delta q_2, \delta q_3} J^{>}_{Q_1}(\delta q_1) J^{>}_{Q_1}(\delta q_2) J^{>}_{Q_1}(\delta q_3) J^{>}_{Q_1}(-\delta q_1 - \delta q_2 - \delta q_3)$$
(7.37c)

$$\mathcal{K}_{ab} = \sum_{\delta q_1, \delta q_2, \delta q_3} J^{>}_{Q_1}(\delta q_1) J^{>}_{Q_1}(\delta q_2) J^{>}_{Q_2}(\delta q_3) J^{>}_{Q_2}(-\delta q_1 - \delta q_2 - \delta q_3).$$
(7.37d)

If we note the angle between the two parameters $(\Delta_X \text{ and } \Delta_Y)$ as φ , we can rewrite the above action as the norms of Δ_X and $\Delta_Y(\Delta_X \text{ and } \Delta_Y)$ together with the angle φ .

$$S_E[\Delta_X, \Delta_Y] = S_0 + \frac{\beta^2}{2N} \left(2\mathcal{K}_1 T - \mathcal{K}_2 \right) (\Delta_X^2 + \Delta_Y^2) + \frac{\beta^4}{12N^3} \left[\mathcal{K}_{aa} \left(\Delta_X^4 + \Delta_Y^4 \right) + \left(4 + 2\cos(2\varphi) \right) \mathcal{K}_{ab} \Delta_X^2 \Delta_Y^2 \right].$$
(7.38)

We can further carry out the path integral over the variable φ to get a effective action that only contains Δ_X and Δ_Y :

$$e^{-S_E[\Delta_X, \Delta_Y]} = \int D[\varphi] e^{-S[\Delta_X, \Delta_Y, \varphi]}.$$
(7.39)

The only relevant term of this integral over φ will be the following:

$$\int_{0}^{\pi} \exp\left(-S[\varphi]\right) d\varphi = \frac{1}{2} \int_{0}^{\frac{\pi}{2}} \exp\left[-2\mathcal{K}_{ab}\Delta_{X}^{2}\Delta_{Y}^{2}\cos(2\varphi)\right] d(2\varphi)$$

$$= \frac{\pi}{4} \left[I_{0}\left(2\mathcal{K}_{ab}\Delta_{X}^{2}\Delta_{Y}^{2}\right) - L_{0}\left(2\mathcal{K}_{ab}\Delta_{X}^{2}\Delta_{Y}^{2}\right)\right],$$
(7.40)

where I_0 stands for zeroth modified Bessel function of the first kind and L_0 stands for zeroth modified Struve function.

Now we can write down the new form of the effective action after integrated over φ and we also absorb the constant $-\ln(\frac{\pi}{4})$ into the S_0 :

$$S_{E}[\Delta_{X}, \Delta_{Y}] = S_{0} + \frac{\beta^{2}}{2N} \Big(2\mathcal{K}_{1}T - \mathcal{K}_{2} \Big) (\Delta_{X}^{2} + \Delta_{Y}^{2}) - \frac{\beta^{4}}{12N^{3}} \ln \bigg[I_{0} \Big(2\mathcal{K}_{ab} \Delta_{X}^{2} \Delta_{Y}^{2} \Big) - L_{0} \Big(2\mathcal{K}_{ab} \Delta_{X}^{2} \Delta_{Y}^{2} \Big) \Big] + \frac{\beta^{4}}{12N^{3}} \bigg[\frac{\mathcal{K}_{aa} + 2\mathcal{K}_{ab}}{2} \Big(\Delta_{X}^{2} + \Delta_{Y}^{2} \Big)^{2} + \frac{\mathcal{K}_{aa} - 2\mathcal{K}_{ab}}{2} \Big(\Delta_{X}^{2} - \Delta_{Y}^{2} \Big)^{2} \bigg].$$

$$(7.41)$$

The later two terms in above equation are crucial for inducing the Nematic phase transition. If the sign of $\frac{\kappa_{aa}-2\kappa_{ab}}{2}$ is negative, then the last term will definitely favours Collinear phase in the sense of minimizing the free energy. Moreover the third term may also promote the emergency of Collinear phase. In order to illustrated this idea, we shall take a look at the series expansion of this term:

$$\ln\left(I_0[A(\Delta_X, \Delta_Y)] - L_0[A(\Delta_X, \Delta_Y)]\right) = -\frac{2}{\pi}A(\Delta_X, \Delta_Y) + \left(\frac{1}{4} - \frac{2}{\pi^2}\right)A(\Delta_X, \Delta_Y)^2 + \cdots$$
(7.42)



Figure 7.5: Plot of the series expansion up to 1st and 2nd order compare to the full description

Here we have to make an approximation which means we only keep the linear term in the series expansion. As we can clearly tell from the Fig.7.5, this approximation is valid only when $A(\Delta_X, \Delta_Y)$ can be considered as a small parameter. So that in the small Δ_X and Δ_Y limit, this term can be approximated as a term also favours nematic:

$$-\ln\left[I_0(2\mathcal{K}_{ab}\Delta_X^2\Delta_Y^2) - L_0(2\mathcal{K}_{ab}\Delta_X^2\Delta_Y^2)\right] \approx +\frac{4}{\pi}\left(\mathcal{K}_{ab}\Delta_X^2\Delta_Y^2\right)$$
(7.43)

Which means by using the approximation shown in Eq.7.42 and drop out the term

 S_0 we can rewrite Eq.7.40 as:

$$S_E[\Delta_X, \Delta_Y] = r_0(\Delta_X^2 + \Delta_Y^2) + \frac{u}{2} \left(\Delta_X^2 + \Delta_Y^2\right)^2 - \frac{g}{2} \left(\Delta_X^2 - \Delta_Y^2\right)^2$$
(7.44a)

$$r_0 = \frac{\beta^2}{2N} \left(2\mathcal{K}_1 T - \mathcal{K}_2 \right) \tag{7.44b}$$

$$u = \frac{\beta^4}{12N^3} \left[\mathcal{K}_{aa} + (2 + \frac{2}{\pi}) \mathcal{K}_{ab} \right]$$
(7.44c)

$$g = \frac{\beta^4}{12N^3} \left[(2 + \frac{2}{\pi})\mathcal{K}_{ab} - \mathcal{K}_{aa} \right]$$
(7.44d)

Where the r_0 , \mathcal{K}_{aa} and \mathcal{K}_{ab} are defined in the Eq.7.36.

By using the notation $(|\Delta_X|, |\Delta_Y|) = \Delta(\sin(\theta), \cos(\theta))$, we can rewrite Eq.7.43a as:

$$S_E[\Delta,\theta] = r_0 \Delta^2 + \frac{u}{2} \Delta^4 - \frac{g}{2} \Delta^4 \cos^2(2\theta)$$
(7.45)

Then we apply the saddle point approximations to Δ and θ to get:

$$\frac{\partial S_E}{\partial \Delta} = \Delta \left(2r_0 \Delta + 2u\Delta^2 - 2g\Delta^2 \cos^2(2\theta) \right) = 0$$
(7.46a)

$$\frac{\partial S_E}{\partial \theta} = g \Delta^4 \sin(4\theta) = 0 \tag{7.46b}$$

From Eq.7.45 we find:

$$\Delta_{1,2,3} = 0, \pm \sqrt{\frac{r_0}{g \cos^2(2\theta) - u}}$$
(7.47a)

$$\theta_{1,2,3} = n\pi, \frac{(2n+1)\pi}{2}, \frac{(2n+1)\pi}{4}$$
 (7.47b)

In our case, as shown in Eq.7.43c,d, u > g and u > 0 are always fulfilled, therefore a finite value for the magnetic order parameter is developed only when $r_0 < 0$.

When $\theta = n\pi$, $\frac{(2n+1)\pi}{2}$, the order parameters have the corresponding form: $(\Delta_X, 0)$ and $(0, \Delta_Y)$, which characterizes the **Collinear phase** and we have the following action:

$$S_{E[\text{Coll.}]} = \frac{-r_0^2}{2(u-g)}$$
(7.48)

When $\theta = \frac{(2n+1)\pi}{4}$, the order parameter have the corresponding form: $(|\Delta|, |\Delta|)$, which characterizes the **Spin density wave phase** and we have the following action:

$$S_{E[\text{SDW}]} = \frac{-r_0^2}{2u}$$
 (7.49)

By comparing Eq.7.47 and 7.48, $g_c = 0$ is found for the critical value for the transition between Collinear phase and charge-spin density wave phase.

Then we shall further simplified our case by neglecting all fluctuations. Recall the expressions of $J_{\boldsymbol{q}}^{>} = J_{\max} - \frac{1}{2}J_{\boldsymbol{q}}$ and $J_{\boldsymbol{q}} = 2J_1(\cos \boldsymbol{q}_{\boldsymbol{x}} + \cos \boldsymbol{q}_{\boldsymbol{y}}) + 4J_2 \cos \boldsymbol{q}_{\boldsymbol{x}} \cos \boldsymbol{q}_{\boldsymbol{y}}$. Since we are not considering the whole q range anymore and also regarding the fact that $J_2 > 0$, we could simply remove the J_{\max} . N = 2, for \boldsymbol{Q}_1 and \boldsymbol{Q}_2 are the only two points we pick in the momentum space, which means in this case we could use this expression: $J_{\boldsymbol{Q}_1}^{>} = J_{\boldsymbol{Q}_2}^{>} = J_2 > 0$ in Eq.7.43 and get:

$$r_0 = \frac{\beta^2 J_2}{2} \left(T - J_2 \right) \tag{7.50a}$$

$$u = \frac{(J_2\beta)^4}{12} \left(3 + \frac{2}{\pi}\right)$$
(7.50b)

$$g = \frac{(J_2\beta)^4}{12} \left(1 + \frac{2}{\pi} \right)$$
(7.50c)

From Eq.7.49, when $T_c < J_2$, we have $r_0 < 0$, and together with the fact u > g > 0, the transition temperature for the Collinear phase is found equals to J_2 , which is consist with the result found in chapter5.



Figure 7.6: The contour plot of $S_E[\Delta_X^2, \Delta_Y^2]$ when (a)T = 8 and (b)T = 12. $(J_2 = 10, J_1 = 1)$

Alternatively we can check whether we can find a Collinear phase transition when lowing the temperature by doing a contour plot of the action as the function of Δ_X^2 and Δ_Y^2 . From Fig.7.6 we observe what we have expected above. We found that when T=12, there is only one minima corresponds to $|\Delta_X| = |\Delta_Y| = 0$, but when the temperature cool down to 8, two minima are found on either X-axis or Y-axis ($|\Delta_X| = 0, |\Delta_Y| \neq 0$ or vice versa), which corresponds to the Collinear phase. While we adjust the value J_2 , we always found $T_c \approx J_2$, which confirm that our approximation is valid to some extent.

As we have shown before in the section 6.3 about Mermin-Wagner theorem, the order parameter Δ_X or Δ_Y which characterizes the Collinear phase, obtains zero expectation value $(\langle \Delta_X \rangle = \langle \Delta_Y \rangle = 0)$ in any finite temperature. But this shall not be the case for the fluctuations in these two degenerate Collinear orders $(\langle \Delta_X^2 \rangle = \langle \Delta_Y^2 \rangle \neq 0)$, which means what we should check is whether the fluctuations along either X or Y direction can be stronger than the other direction $(\langle \Delta_X^2 \rangle \neq \langle \Delta_Y^2 \rangle)$ and that is the feature of the nematic order. Hence we can decouple the quadratic terms in the Eq.7.43a by Hubbardstratonivich transformation again to get:

$$S[\Delta_X, \Delta_Y, \psi, \phi] = r_0 (\Delta_X^2 + \Delta_Y^2) - \frac{\psi^2}{2u} + \frac{\phi^2}{2g} + \psi \left(\Delta_X^2 + \Delta_Y^2 \right) - \phi \left(\Delta_X^2 - \Delta_Y^2 \right)$$
(7.51)

The saddle point approximations to ψ and ϕ implies:

$$\langle \psi \rangle = u \Big(\langle \Delta_X^2 \rangle + \langle \Delta_Y^2 \rangle \Big)$$
 (7.52a)

$$\langle \phi \rangle = g \Big(\langle \Delta_X^2 \rangle - \langle \Delta_Y^2 \rangle \Big)$$
 (7.52b)

From Eq.7.51a, it is evident that the quantity $\langle \psi \rangle$ always possesses a finite expectation value. Therefore, it cannot serve as an order parameter. On the other hand, the value of $\langle \phi \rangle$ is zero when the fluctuations along the X and Y directions are equal. However, when these fluctuations differ, $\langle \phi \rangle$ can assume a finite value. This characteristic enables $\langle \phi \rangle$ to be used as an order parameter for characterizing the nematic phase.

Rewriting Eq.7.50 as:

$$S[\Delta_X, \Delta_Y, \psi, \phi] = \begin{pmatrix} \Delta_X & \Delta_Y \end{pmatrix} \begin{pmatrix} r_0 + \psi - \phi & 0 \\ 0 & r_0 + \psi + \phi \end{pmatrix} \begin{pmatrix} \Delta_X \\ \Delta_Y \end{pmatrix} - \frac{\psi^2}{2u} + \frac{\phi^2}{2g} \quad (7.53)$$

Integrate out the quadratic terms using Gaussian integral to get an effective action for ψ and ϕ :

$$S_E[\psi,\phi] = \frac{1}{2} \ln\left[(r_0+\psi)^2 - \phi^2\right] - \frac{\psi^2}{2u} + \frac{\phi^2}{2g}$$
(7.54)

For later convenient, here we choose to rename $r_0 + \psi$ as r so that we have:

$$S_E[r,\phi] = \frac{1}{2} \ln\left(r^2 - \phi^2\right) - \frac{(r-r_0)^2}{2u} + \frac{\phi^2}{2g}$$
(7.55)

We can apply saddle point approximation once again to ψ and ϕ :

$$\frac{\partial S_E}{\partial r} = \frac{r_0 - r}{u} + \frac{r}{r^2 - \phi^2} = 0$$
(7.56a)

$$\frac{\partial S_E}{\partial \phi} = \frac{\phi}{g} - \frac{\phi}{r^2 - \phi^2} = 0 \tag{7.56b}$$

We can eliminate the variable r in Eq.7.55 and solve for the solutions for ϕ and we find:

$$\phi_{1,2,3} = 0, \pm \frac{i\sqrt{g\left[(u-g)^2 - gr_0^2\right]}}{u-g}$$
(7.57)

From Eq.7.56 we find when $r_0 > \sqrt{g}(\frac{u}{g} - 1)$ or $r_0 < \sqrt{g}(1 - \frac{u}{g})$, a finite expectation value of ϕ is found, meaning the system is in the nematic phase. If we neglect all the fluctuations we can use the expression of r_0 , u and g described in Eq.7.49 and find when: $T > 1.9J_2$ or $T < 0.1J_2$, we find a finite expectation value for the nematic order parameter. But apparently and unfortunately, we find such result does not suggest the T_c for the nematic transition in a right way qualitatively.

In conclusion, we stressed the conflict between the computational and analytical results, which are related for the behavior of the nematic T_c in strong frustration regime. A toy model based on [14] for capturing the features of the critical temperature for nematic phase transition is mentioned. Nevertheless we conducted an analysis using Feynman diagram expansion up to fourth order in order to understand the characteristics of the nematic phase transition. Building upon the work of [17], we explored a similar approach to formulate the nematic order parameter for our $J_1 - J_2$ Heisenberg model in order to compute the critical temperature (T_c) for the nematic order. However, our analytical treatment gave results that deviated from those reported in previous studies, indicating the need for a more thorough investigation into the calculations and the validity of the approximations employed.

Chapter 8

Conclusion and Outlook

In conclusion, with the help of the pseudofermion representation of quantum spin, we successfully included the J_1 - J_2 quantum Heisenberg model within the framework of the path integral formalism. This adaptation provides a solid platform for conducting comprehensive investigations into the ground state properties and low-energy excitations of our many-body quantum system. Explicitly, we achieved the following key results:

- 1. In the mean field level, we found two magnetic states when tuning the ratio between J_1 and J_2 : when $\frac{J_2}{J_1} < 0.5$, the system develops a Néel state, while for $\frac{J_2}{J_1} > 0.5$, a Collinear state is favoured.
- 2. The role played by the quantum fluctuations in lower dimensions is studied: Long range magnetic orders are suppressed when the quantum fluctuations are taken into the consideration upon the saddle point approximation. Furthermore, by showing these magnetic orders can be totally destroyed by the fluctuations in the thermodynamic limit, enables us to reestablish the Mermin-Wagner theorem.
- 3. The dispersion relation of the spin wave is obtained and the corresponding Goldstone modes for both the Néel and Collinear states are found. The relation between the rate of frustration and the low-energy excitations is partially revealed.
- 4. We established the general framework of the effective theory in terms of pesudofermions, in order to capture the feature of nematic T_c for our J_1 - J_2 model.

To improve or continue with the aforementioned results, one may consider the following aspects:

- 1. To obtain a more realistic connection between the nematic T_c and $\frac{J_2}{J_1}$, it is essential to conduct a thorough investigation into potential adjustments to the prefactor (r_0) in Eq.7.43, when extending Δ_{Q_1} to $\Delta_{Q_1}(\delta q)$.
- 2. It could be worth (fun) to check the critical behavior of \mathcal{K}_{ab} and \mathcal{K}_{aa} when: $\frac{J_2}{J_1} \rightarrow 0.5$. In Appendix.E, we found the different critical behaviors of those two may lead to a change in the sign of the prefactor (g) in Eq.7.43 which may lead to phase transition of long range magnetic order from Collinear to Spin density wave phase, as described by Eq.7.47-48.

Appendix A Derivation of the Eq.6.16

In the beginning we have:

$$\sum_{\alpha} (\Pi_i^{-1})^{\tau \alpha} \chi_{ij}^{\alpha \beta} = \sum_{\alpha} (\Pi_i^{-1})^{\tau \alpha} \Pi_i^{\alpha \beta} \delta_{ij} - \sum_{\alpha} (\Pi_i^{-1})^{\tau \alpha} \sum_{\gamma,\varphi} \Pi_i^{\alpha \gamma} (\underline{\mathfrak{I}})_{ij}^{\gamma \varphi} \Pi_j^{\varphi \beta}, \tag{A.1}$$

which can be reduced as:

$$\sum_{\alpha} (\Pi_i^{-1})^{\tau \alpha} \chi_{ij}^{\alpha \beta} = \delta_{\tau \beta} \delta_{ij} - \sum_{\varphi} (\underline{\mathfrak{J}})_{ij}^{\tau \varphi} \Pi_j^{\varphi \beta}.$$
(A.2)

Then we multiply the $\sum \mathfrak{J}^{-1}$ to both sides:

$$\sum_{i,\alpha,\tau} (\underline{\mathfrak{J}}^{-1})_{pi}^{\eta\tau} (\Pi_i^{-1})^{\tau\alpha} \chi_{ij}^{\alpha\beta} = (\underline{\mathfrak{J}}^{-1})_{pj}^{\eta\beta} - \sum_{i,\varphi,\tau} (\underline{\mathfrak{J}}^{-1})_{pi}^{\eta\tau} (\underline{\mathfrak{J}})_{ij}^{\tau\varphi} \Pi_j^{\varphi\beta}, \tag{A.3}$$

which can be reduced as:

$$\sum_{i,\alpha,\tau} (\underline{\tilde{\mathfrak{Z}}}^{-1})_{pi}^{\eta\tau} (\Pi_i^{-1})^{\tau\alpha} \chi_{ij}^{\alpha\beta} = (\underline{\tilde{\mathfrak{Z}}}^{-1})_{pj}^{\eta\beta} - \Pi_j^{\eta\beta} \delta_{pj} = (\underline{\mathcal{J}}^{-1})_{pj} \delta_{\eta\beta}.$$
(A.4)

Inserting the expression of \mathfrak{J}^{-1} into Eq.A.4 we can get:

$$\sum_{i,\alpha,\tau} \left(\Pi_p^{\eta\tau} \delta_{pi} + (\underline{\mathcal{J}}^{-1})_{pi} \delta_{\eta\tau} \right) (\Pi_i^{-1})^{\tau\alpha} \chi_{ij}^{\alpha\beta} = (\underline{\mathcal{J}}^{-1})_{pj} \delta_{\eta\beta}.$$
(A.5)

Further reduced as:

$$\sum_{\alpha,\tau} \Pi_p^{\eta\tau} (\Pi_p^{-1})^{\tau\alpha} \chi_{pj}^{\alpha\beta} + \sum_{i,\alpha} (\underline{\mathcal{I}}^{-1})_{pi} (\Pi_i^{-1})^{\eta\alpha} \chi_{ij}^{\alpha\beta} = (\underline{\mathcal{I}}^{-1})_{pj} \delta_{\eta\beta},$$
(A.6)

which is:

$$\chi_{pj}^{\eta\beta} + \sum_{i,\alpha} (\underline{\mathcal{J}}^{-1})_{pi} (\Pi_i^{-1})^{\eta\alpha} \chi_{ij}^{\alpha\beta} = (\underline{\mathcal{J}}^{-1})_{pj} \delta_{\eta\beta}.$$
(A.7)

Then we multiply the $\sum \mathcal{J}$ to both sides:

$$\sum_{p} (\underline{\mathcal{J}})_{zp} \chi_{pj}^{\eta\beta} + \sum_{i,p,\alpha} (\underline{\mathcal{J}})_{zp} (\underline{\mathcal{J}}^{-1})_{pi} (\Pi_{i}^{-1})^{\eta\alpha} \chi_{ij}^{\alpha\beta} = \sum_{p} (\underline{\mathcal{J}})_{zp} (\underline{\mathcal{J}}^{-1})_{pj} \delta_{\eta\beta},$$
(A.8)

Which is reduced as:

$$\sum_{p} (\underline{\mathcal{I}})_{zp} \chi_{pj}^{\eta\beta} + \sum_{\alpha} (\Pi_{z}^{-1})^{\eta\alpha} \chi_{zj}^{\alpha\beta} = \delta_{zj} \delta_{\eta\beta}.$$
(A.9)

Then we multiply the $\sum \Pi$ to both sides:

$$\sum_{p,\eta} \Pi_z^{\xi\eta} (\underline{\mathcal{J}})_{zp} \chi_{pj}^{\eta\beta} + \sum_{\alpha,\eta} \Pi_z^{\xi\eta} (\Pi_z^{-1})^{\eta\alpha} \chi_{zj}^{\alpha\beta} = \Pi_z^{\xi\beta} \delta_{zj}, \qquad (A.10)$$

which is reduced as:

$$\sum_{p,\eta} \Pi_z^{\xi\eta} (\underline{\mathcal{J}})_{zp} \chi_{pj}^{\eta\beta} + \chi_{zj}^{\xi\beta} = \Pi_z^{\xi\beta} \delta_{zj}.$$
(A.11)

From A.11 we can easily get the expression shown in the Eq.6.16 in the Chpater 6.

Appendix B

Third order static correction to the action

Like we did in the case of second order:

$$-\frac{1}{3}\sum_{n,n',n'',\boldsymbol{k},\boldsymbol{k'},\boldsymbol{k''}}G_{0}(n,\boldsymbol{k})V_{n-n',\boldsymbol{k-k'}}G_{0}(n',\boldsymbol{k'})V_{n'-n'',\boldsymbol{k'-k''}}G_{0}(n'',\boldsymbol{k''})V_{n''-n,\boldsymbol{k''-k''}}.$$
(B.1)

Which explicitly is:

$$-\frac{1}{3N^{3}}\sum_{\substack{n,n',n'',\boldsymbol{k},\boldsymbol{k}',\boldsymbol{k}'',i,j,l,a,b,c}}G_{0}(n,k)J_{\boldsymbol{k}'-\boldsymbol{k}}^{>}\Delta_{n-n',\boldsymbol{k}-\boldsymbol{k}'}^{(i)}\sigma_{ab}^{(i)}G_{0}(n',\boldsymbol{k}')$$

$$J_{\boldsymbol{k}'-\boldsymbol{k}''}^{>}\Delta_{n'-n'',\boldsymbol{k}'-\boldsymbol{k}''}^{(j)}\sigma_{bc}^{(j)}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}}^{>}\Delta_{n''-n,\boldsymbol{k}''-\boldsymbol{k}}^{(l)}\sigma_{ca}^{(l)}.$$
(B.2)

By using the properties of the Pauli matrix: $\text{Tr}(\sigma^{(i)}\sigma^{(j)}\sigma^{(l)}) = 2i\epsilon_{ijl}$ we can further get:

$$-\frac{2i}{3N^{3}}\sum_{n,n',n'',\boldsymbol{k},\boldsymbol{k'},\boldsymbol{k''},i,j,l}\epsilon_{ijk}G_{0}(n,\boldsymbol{k})J_{\boldsymbol{k'}-\boldsymbol{k}}^{>}\Delta_{n-n',\boldsymbol{k}-\boldsymbol{k'}}^{(i)}G_{0}(n',\boldsymbol{k'})$$

$$J_{\boldsymbol{k'}-\boldsymbol{k''}}^{>}\Delta_{n'-n'',\boldsymbol{k'}-\boldsymbol{k''}}^{(j)}G_{0}(n'',\boldsymbol{k''})J_{\boldsymbol{k''}-\boldsymbol{k}}^{>}\Delta_{n''-n,\boldsymbol{k''}-\boldsymbol{k}}^{(l)}.$$
(B.3)

Then we can turn it into a contour integration:

$$-\frac{2i\beta}{3N^2} \sum_{m_1,m_2,q_1,q_2,i,j,l} \oint \frac{dz}{2\pi i} \frac{f(z)}{z(z-i\nu_{m_1})(z-i\nu_{m_1}-i\nu_{m_2})}$$
(B.4)
$$J_{q_1}^{>} J_{q_2}^{>} J_{-q_1-q_2}^{>} \epsilon_{ijl} \Delta_{m_1,q_1}^{(i)} \Delta_{m_2,q_2}^{(j)} \Delta_{-m_1-m_2,-q_1-q_2}^{(l)}.$$

Consider that: $i\nu_{m_1} = i\nu_{m_2} = 0$, or so to speak consider only the static configuration of the white-noise field, and we can carry out the contour integration:

$$-\frac{2i\beta}{3N^2} \sum_{m_1,m_2,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l} \left[\frac{J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^>}{(3-1)!} \frac{d^2 f(x)}{dz^2} \Big|_{z\to 0} \right] \epsilon_{ijl} \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)} = 0.$$
(B.5)

Appendix C

Fourth order static correction to the action

For the fourth order term we find:

$$-\frac{1}{4}\sum_{i\cdots r} (G_{0ij}V_{jk}G_{0kl}V_{lp}G_{0pq}V_{qh}G_{0hr}V_{ri}\delta_{ij}\delta_{kl}\delta_{pq}\delta_{hr}), \qquad (C.1)$$

which is simplified as:

$$-\frac{1}{4}\sum_{i,l,p,h} (G_{0i}V_{il}G_{0l}V_{lp}G_{0p}V_{ph}G_{0h}V_{hi}).$$
(C.2)

By using the properties of the Pauli matrix: $\text{Tr}(\tau_i \tau_j \tau_k \tau_l) = 2(\delta_{ij} \delta_{kl} - \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$ we can further get:

$$-\frac{1}{2N^{4}}\sum_{\boldsymbol{k}\cdots\boldsymbol{k}''',n\cdots n''',\boldsymbol{i},\boldsymbol{j}}\left[+G_{0}(n,\boldsymbol{k})J_{\boldsymbol{k}-\boldsymbol{k}'}^{\geq}\Delta_{n-n',\boldsymbol{k}-\boldsymbol{k}'}^{(i)}G_{0}(n',\boldsymbol{k}')J_{\boldsymbol{k}'-\boldsymbol{k}''}^{\geq}\Delta_{n'-n'',\boldsymbol{k}'-\boldsymbol{k}''}^{(i)}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}\Delta_{n''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{(i)}G_{0}(n''',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}\Delta_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{(j)}-G_{0}(n,\boldsymbol{k})J_{\boldsymbol{k}-\boldsymbol{k}'}^{\geq}\Delta_{n-n',\boldsymbol{k}-\boldsymbol{k}'}^{(i)}G_{0}(n',\boldsymbol{k}')J_{\boldsymbol{k}'-\boldsymbol{k}''}^{\geq}\Delta_{n''-n'',\boldsymbol{k}'-\boldsymbol{k}''}^{(j)}-G_{0}(n,\boldsymbol{k})J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}\Delta_{n''-n'',\boldsymbol{k}'-\boldsymbol{k}''}^{(i)}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}\Delta_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{(j)}-G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}\Delta_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}'}^{(j)}+G_{0}(n,\boldsymbol{k})J_{\boldsymbol{k}-\boldsymbol{k}'}^{\geq}\Delta_{n-n',\boldsymbol{k}-\boldsymbol{k}'}^{(i)}G_{0}(n',\boldsymbol{k}')J_{\boldsymbol{k}'-\boldsymbol{k}''}^{\geq}\Delta_{n''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{(j)}-G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n',\boldsymbol{k}')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{(j)}-G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{(j)}-G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n''',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}G_{0}(n'',\boldsymbol{k}'')J_{\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-\boldsymbol{k}''-\boldsymbol{k}''}^{\geq}A_{n'''-n,\boldsymbol{k}''-$$

By renaming the labels we can rewrite it as:

$$-\frac{1}{2N^{4}}\sum_{\boldsymbol{q_{1},q_{2},q_{3},n,m_{1},m_{2},m_{3},i,j}}\frac{J_{\boldsymbol{q_{1}}}^{\geq}J_{\boldsymbol{q_{2}}}^{\geq}J_{\boldsymbol{q_{3}}}^{\geq}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}}{(i\omega_{n})(i\omega_{n}-i\nu_{m_{1}})(i\omega_{n}-i\nu_{m_{1}}-i\nu_{m_{2}})(i\omega_{n}-i\nu_{m_{1}}-i\nu_{m_{2}}-i\nu_{m_{3}})}$$

$$(\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{3},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2}-m_{3},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}-\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{3},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2}-m_{3},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}-\Delta_{m_{1},\boldsymbol{q_{1}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{3},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2}-m_{3},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)})$$

$$+\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{3},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2}-m_{3},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(i)}).$$

$$(C.4)$$

By applying the contour integral method to Eq.7.40 we can get:

$$-\frac{1}{2N^{3}}\beta \sum_{\boldsymbol{q}_{1},\boldsymbol{q}_{2},\boldsymbol{q}_{3},m_{1},m_{2},m_{3},i,j} \oint \frac{dz}{2\pi i} \frac{f(z)}{z(z-i\nu_{m_{1}})(z-i\nu_{m_{1}}-i\nu_{m_{2}})(z-i\nu_{m_{1}}-i\nu_{m_{2}}-i\nu_{m_{3}})} \\ J_{\boldsymbol{q}_{1}}^{\geq} J_{\boldsymbol{q}_{2}}^{\geq} J_{\boldsymbol{q}_{3}}^{\geq} J_{-\boldsymbol{q}_{1}-\boldsymbol{q}_{2}-\boldsymbol{q}_{3}}^{\geq} (\Delta_{m_{1},\boldsymbol{q}_{1}}^{(i)}\Delta_{m_{2},\boldsymbol{q}_{2}}^{(j)}\Delta_{m_{3},\boldsymbol{q}_{3}}^{(j)}\Delta_{-m_{1}-m_{2}-m_{3},-\boldsymbol{q}_{1}-\boldsymbol{q}_{2}-\boldsymbol{q}_{3}} \\ -\Delta_{m_{1},\boldsymbol{q}_{1}}^{(i)}\Delta_{m_{2},\boldsymbol{q}_{2}}^{(j)}\Delta_{m_{3},\boldsymbol{q}_{3}}^{(j)}\Delta_{-m_{1}-m_{2}-m_{3},-\boldsymbol{q}_{1}-\boldsymbol{q}_{2}-\boldsymbol{q}_{3}} + \Delta_{m_{1},\boldsymbol{q}_{1}}^{(i)}\Delta_{m_{2},\boldsymbol{q}_{2}}^{(j)}\Delta_{m_{3},\boldsymbol{q}_{3}}^{(i)}\Delta_{-m_{1}-m_{2}-m_{3},-\boldsymbol{q}_{1}-\boldsymbol{q}_{2}-\boldsymbol{q}_{3}} \\ (C.5)$$

Now we should carefully evaluate the contour integral in Eq.C.6, first consider that $i\nu_{m_1} = i\nu_{m_2} = i\nu_{m_3} = 0$ and we can get:

$$-\frac{1}{2N^{3}}\beta\sum_{\boldsymbol{q_{1},q_{2},q_{3},i,j}}\oint \frac{dz}{2\pi i}\frac{f(z)}{z^{4}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}(\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(i)}\Delta_{0,\boldsymbol{q_{1}}}^{(j)}\Delta_{0,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)} -\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{0,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)} +\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{0,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}).$$
(C.6)

And if we rename q_2 to q_3 and q_3 to q_2 in the first term, we can further eliminate the first term and the second with each other and only left with:

$$-\frac{1}{2N^{3}}\beta\sum_{\boldsymbol{q_{1},q_{2},q_{3},i,j}}\oint\frac{dz}{2\pi i}\frac{f(z)}{z^{4}}J_{\boldsymbol{q_{1}}}^{\geq}J_{\boldsymbol{q_{2}}}^{\geq}J_{\boldsymbol{q_{3}}}^{\geq}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{\geq}\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{0,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(i)}.$$
(C.7)

Then we can carry out the contour integration to get:

$$-\frac{1}{2N^{3}}\beta\sum_{\boldsymbol{q_{1},q_{2},q_{3},i,j}}\frac{J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}}{(4-1)!}\left[\frac{d^{3}f(z)}{dz^{3}}\Big|_{z\to0}\right]\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{0,\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(i)}.$$
(C.8)

From which we get:

$$-\frac{\beta^4}{96N^3} \sum_{\boldsymbol{q_1}, \boldsymbol{q_2}, \boldsymbol{q_3}, i, j} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^> \Delta_{0, \boldsymbol{q_1}}^{(i)} \Delta_{0, \boldsymbol{q_2}}^{(j)} \Delta_{0, \boldsymbol{q_3}}^{(j)} \Delta_{0, -\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^{(i)}.$$
(C.9)

Appendix D

Non-static corrections to the action

For the Non static correction up to third order gives:

When $i\nu_{m_1} = 0$, $i\nu_{m_2} \neq 0$ we have:

$$-\frac{2i\beta}{3}\sum_{m,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l}\oint \frac{dz}{2\pi i} \frac{f(z)}{z^2(z-i\nu_m)} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^> \epsilon_{ijl} \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m,\boldsymbol{q_2}}^{(j)} \Delta_{-m,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)} \tag{D.1}$$

Which compute as:

$$-\frac{i\beta^2}{6} \sum_{m,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l} \frac{1}{i\nu_m} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^> \epsilon_{ijl} \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m,\boldsymbol{q_2}}^{(j)} \Delta_{-m,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)} (i\nu_m \neq 0)$$
(D.2)

When $i\nu_{m_1} \neq 0, i\nu_{m_2} = 0$ we have:

$$-\frac{2i\beta}{3}\sum_{m,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l}\oint \frac{dz}{2\pi i}\frac{f(z)}{z(z-i\nu_m)^2}J_{\boldsymbol{q_1}}^{\geq}J_{\boldsymbol{q_2}}^{\geq}J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^{\geq}\epsilon_{ijl}\Delta_{m,\boldsymbol{q_1}}^{(i)}\Delta_{0,\boldsymbol{q_2}}^{(j)}\Delta_{-m,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)} \tag{D.3}$$

Which compute as:

$$+\frac{i\beta^2}{6}\sum_{m,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l}\frac{1}{i\nu_m}J_{\boldsymbol{q_1}}^>J_{\boldsymbol{q_2}}^>J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^>\epsilon_{ijl}\Delta_{m,\boldsymbol{q_1}}^{(i)}\Delta_{0,\boldsymbol{q_2}}^{(j)}\Delta_{-m,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)}(i\nu_m\neq 0) \tag{D.4}$$

When $i\nu_{m_1} \neq 0, i\nu_{m_2} \neq 0, i\nu_{m_1} + i\nu_{m_2} = 0$ we have:

$$-\frac{2i\beta}{3}\sum_{m,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l}\oint \frac{dz}{2\pi i} \frac{f(z)}{z^2(z-i\nu_m)} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^> \epsilon_{ijl} \Delta_{m,\boldsymbol{q_1}}^{(i)} \Delta_{-m,\boldsymbol{q_2}}^{(j)} \Delta_{0,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)} \tag{D.5}$$

Which compute as:

$$-\frac{i\beta^2}{6}\sum_{m,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l}\frac{1}{i\nu_m}J_{\boldsymbol{q_1}}^{\geq}J_{\boldsymbol{q_2}}^{\geq}J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^{\geq}\epsilon_{ijl}\Delta_{m,\boldsymbol{q_1}}^{(i)}\Delta_{-m,\boldsymbol{q_2}}^{(j)}\Delta_{0,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)}(i\nu_m\neq 0) \tag{D.6}$$

When $i\nu_{m_1} \neq 0, i\nu_{m_2} \neq 0, i\nu_{m_1} + i\nu_{m_2} \neq 0$ we have:

$$-\frac{2i\beta}{3} \sum_{m_1,m_2,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l} \oint \frac{dz}{2\pi i} \frac{f(z)}{z(z-i\nu_{m_1})(z-i\nu_{m_1}-i\nu_{m_2})}$$
(D.7)
$$J_{\boldsymbol{q_1}}^{\geq} J_{\boldsymbol{q_2}}^{\geq} J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^{\geq} \epsilon_{ijl} \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)}$$

Which compute as:

$$-\frac{16i\beta}{3}\sum_{m_1,m_2,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l}\frac{f(0)}{(i\nu_{m_1})(i\nu_{m_1}+i\nu_{m_2})} + \frac{f(0)}{(i\nu_{m_2})(i\nu_{m_1}+i\nu_{m_2})} - \frac{f(0)}{(i\nu_{m_1}i\nu_{m_2})} \qquad (D.8)$$
$$J_{\boldsymbol{q_1}}^{>}J_{\boldsymbol{q_2}}^{>}J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^{>}\epsilon_{ijl}\Delta_{m_1,\boldsymbol{q_1}}^{(i)}\Delta_{m_2,\boldsymbol{q_2}}^{(j)}\Delta_{-m_1-m_2,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)} = 0$$

By combining above equations the third order term reads:

$$-\frac{i\beta^2}{2} \sum_{m,\boldsymbol{q_1},\boldsymbol{q_2},i,j,l} \frac{1}{i\nu_m} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}}^> \epsilon_{ijl} \Delta_{m,\boldsymbol{q_1}}^{(i)} \Delta_{-m,\boldsymbol{q_2}}^{(j)} \Delta_{0,-\boldsymbol{q_1}-\boldsymbol{q_2}}^{(l)} (i\nu_m \neq 0)$$
(D.9)

For the Non static correction up to fourth order gives:

For $i\nu_{m_1} = i\nu_{m_2} = 0$, $i\nu_{m_3} \neq 0$, by renaming m_3 as m we can get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^3(z-i\nu_m)} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> (\Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(i)} \Delta_{m,\boldsymbol{q_3}}^{(j)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(j)} \\ -\Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(j)} \Delta_{m,\boldsymbol{q_3}}^{(i)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(j)} + \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(j)} \Delta_{m,\boldsymbol{q_3}}^{(j)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(j)}$$
(D.10)

Similarly we can eliminate second term and third with each other by changing the labels:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1}, \boldsymbol{q_2}, \boldsymbol{q_3}, m, i, j} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^3 (z - i\nu_m)} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^> \Delta_{0, \boldsymbol{q_1}}^{(i)} \Delta_{0, \boldsymbol{q_2}}^{(i)} \Delta_{m, \boldsymbol{q_3}}^{(j)} \Delta_{-m, -\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^{(j)}$$
(D.11)

And we can further carry out the contour integration to get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1}, \boldsymbol{q_2}, \boldsymbol{q_3}, m, i, j} \left(\frac{1}{(3-1)!} \left[\frac{d^2}{dz^2} \frac{f(z)}{(z-i\nu_m)}\right]|_{z\to 0} + \frac{f(i\nu_m)}{(i\nu_m)^3}\right) \\ J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^> \Delta_{0, \boldsymbol{q_1}}^{(i)} \Delta_{0, \boldsymbol{q_2}}^{(j)} \Delta_{m, \boldsymbol{q_3}}^{(j)} \Delta_{-m, -\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^{(j)}$$
(D.12)

Which compute as:

$$-\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(i)}\Delta_{m,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}(i\nu_{m}\neq0)$$
(D.13)

For $i\nu_{m_1} = i\nu_{m_3} = 0, i\nu_{m_2} \neq 0$:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^2 (z-i\nu_m)^2} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> (\Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m,\boldsymbol{q_2}}^{(i)} \Delta_{0,\boldsymbol{q_3}}^{(j)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m,\boldsymbol{q_2}}^{(j)} \Delta_{0,\boldsymbol{q_3}}^{(j)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(i)} + \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m,\boldsymbol{q_2}}^{(j)} \Delta_{0,\boldsymbol{q_3}}^{(j)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(j)}$$

$$(D.14)$$

carry out the contour integration to get:

$$+\frac{1}{4}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{\geq}J_{\boldsymbol{q_{2}}}^{\geq}J_{\boldsymbol{q_{3}}}^{\geq}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{\geq}(\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$-\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}+\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)})$$
$$(D.15)$$

Which we can put together the first term and the third term to get:

$$+\frac{1}{2}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m,\boldsymbol{q_{2}}}^{(i)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$-\frac{1}{4}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(i)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$\tag{D.16}$$

For $i\nu_{m_2} = i\nu_{m_3} = 0, i\nu_{m_1} \neq 0$ follow the same procedure we get:

$$-\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{m,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(i)}$$
(D.17)

For $i\nu_{m_1} = 0$, $i\nu_{m_2} \neq 0$, $i\nu_{m_3} \neq 0$, from Eq.51 and rename m_2 as m_1 and m_3 as m_2 we can get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m_1,m_2,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^2(z-i\nu_{m_1})(z-i\nu_{m_1}-i\nu_{m_2})} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> \\ (\Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m_1,\boldsymbol{q_2}}^{(i)} \Delta_{m_2,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m_1,\boldsymbol{q_2}}^{(j)} \Delta_{m_2,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(j)} \\ + \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m_1,\boldsymbol{q_2}}^{(j)} \Delta_{m_2,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(i)})$$
(D.18)

When $i\nu_{m_1} + i\nu_{m_2} = 0$ we get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^3(z-i\nu_m)} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> (\Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m,\boldsymbol{q_2}}^{(i)} \Delta_{-m,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m,\boldsymbol{q_2}}^{(j)} \Delta_{-m,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(j)} + \Delta_{0,\boldsymbol{q_1}}^{(i)} \Delta_{m,\boldsymbol{q_2}}^{(j)} \Delta_{-m,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(j)}$$

$$(D.19)$$

Following similar procedure we get:

$$-\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m,\boldsymbol{q_{2}}}^{(j)}\Delta_{-m,\boldsymbol{q_{3}}}^{(j)}\Delta_{0,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(i)}(i\nu_{m}\neq0)$$
(D.20)

When $i\nu_{m_1} + i\nu_{m_2} \neq 0$. Similarly we get:

$$-\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m_{1},m_{2},i,j}}\frac{J_{\boldsymbol{q_{1}}}^{\geq}J_{\boldsymbol{q_{2}}}^{\geq}J_{\boldsymbol{q_{3}}}^{\geq}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{\geq}}{(i\nu_{m_{1}})(i\nu_{m_{1}}+i\nu_{m_{2}})}(\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{1},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$-\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{1},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{3}}}^{(i)}\Delta_{-m_{1}-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}+\Delta_{0,\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{1},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$(i\nu_{m_{1}}\neq 0, i\nu_{m_{2}}\neq 0, i\nu_{m_{1}}+i\nu_{m_{2}}\neq 0)$$
$$(D.21)$$

For $i\nu_{m_2} = 0$, $i\nu_{m_1} \neq 0$, $i\nu_{m_3} \neq 0$, rename m_3 as m_2 we can get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m_1,m_2,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z(z-i\nu_{m_1})^2(z-i\nu_{m_1}-i\nu_{m_2})} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> \\ (\Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(j)} \Delta_{m_2,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(j)} \Delta_{m_2,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(j)} \\ + \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(j)} \Delta_{m_2,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(i)}$$
(D.22)

When $i\nu_{m_1} + i\nu_{m_2} = 0$:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^2 (z-i\nu_m)^2} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> (\Delta_{m,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(i)} \Delta_{-m,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{m,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(j)} \Delta_{-m,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(j)} + \Delta_{m,\boldsymbol{q_1}}^{(i)} \Delta_{0,\boldsymbol{q_2}}^{(j)} \Delta_{-m,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(j)}$$
(D.23)

Following same procedure we can get:

$$+\frac{1}{2}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{\geq}J_{\boldsymbol{q_{2}}}^{\geq}J_{\boldsymbol{q_{3}}}^{\geq}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{\geq}\Delta_{m,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}(i\nu_{m}\neq 0)$$

$$-\frac{1}{4}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{\geq}J_{\boldsymbol{q_{2}}}^{\geq}J_{\boldsymbol{q_{3}}}^{\geq}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{\geq}\Delta_{m,\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{-m,\boldsymbol{q_{3}}}^{(j)}\Delta_{0,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}(i\nu_{m}\neq 0)$$

$$(D.24)$$

When $i\nu_{m_1} + i\nu_{m_2} \neq 0$. Similarly we can get:

$$-\frac{1}{4}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m_{1},m_{2},i,j}}\frac{1}{i\nu_{m_{1}}i\nu_{m_{2}}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$

$$+\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m_{1},m_{2},i,j}}\frac{1}{i\nu_{m_{1}}i\nu_{m_{2}}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{0,\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$

$$(i\nu_{m_{1}}\neq 0, i\nu_{m_{2}}\neq 0, i\nu_{m_{1}}+i\nu_{m_{2}}\neq 0)$$

$$(D.25)$$

For $i\nu_{m_3} = 0, i\nu_{m_1} \neq 0, i\nu_{m_2} \neq 0$, we can get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m_1,m_2,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z(z-i\nu_{m_1})(z-i\nu_{m_1}-i\nu_{m_2})^2} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> \\ (\Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{0,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{0,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(j)} \\ + \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{0,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2,-\boldsymbol{q_1-q_2-q_3}}^{(i)})$$
(D.26)

When $i\nu_{m_1} + i\nu_{m_2} = 0$:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1}, \boldsymbol{q_2}, \boldsymbol{q_3}, m, i, j} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^3 (z - i\nu_m)} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^> \Delta_{m, \boldsymbol{q_1}}^{(i)} \Delta_{-m, \boldsymbol{q_2}}^{(j)} \Delta_{0, \boldsymbol{q_3}}^{(j)} \Delta_{0, -\boldsymbol{q_1}-\boldsymbol{q_2}-\boldsymbol{q_3}}^{(j)}$$
(D.27)

Which compute as:

$$-\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{m,\boldsymbol{q_{1}}}^{(i)}\Delta_{-m,\boldsymbol{q_{2}}}^{(i)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{0,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}(i\nu_{m}\neq0)$$
(D.28)

When $i\nu_{m_1} + i\nu_{m_2} \neq 0$. Similarly we can get:

$$+\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m_{1},m_{2},i,j}}\frac{J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}(\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)})$$
$$-\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}+\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{0,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1}-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)})$$
$$(i\nu_{m_{1}}\neq 0, i\nu_{m_{2}}\neq 0, i\nu_{m_{1}}+i\nu_{m_{2}}\neq 0)$$
$$(D.29)$$
For $i\nu_{m_1} \neq 0$, $i\nu_{m_2} \neq 0$, $i\nu_{m_3} \neq 0$, we can get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m_1,m_2,m_3,i,j}} \oint \frac{dz}{2\pi i} \frac{J_{\boldsymbol{q_1}}^2 J_{\boldsymbol{q_2}}^2 J_{\boldsymbol{q_3}}^2 J_{-\boldsymbol{q_1-q_2-q_3}}^2 f(z)}{z(z-i\nu_{m_1}-i\nu_{m_2})(z-i\nu_{m_1}-i\nu_{m_2}-i\nu_{m_3})} \\ (\Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{m_3,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2-m_3,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{m_3,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2-m_3,-\boldsymbol{q_1-q_2-q_3}}^{(j)} \\ + \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{m_3,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1-m_2-m_3,-\boldsymbol{q_1-q_2-q_3}}^{(i)} \right)$$
(D.30)

When $i\nu_{m_1} + i\nu_{m_2} = 0$ we get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m_1,m_3,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^2(z-i\nu_{m_1})(z-i\nu_{m_3})} J_{\boldsymbol{q_1}}^{\geq} J_{\boldsymbol{q_2}}^{\geq} J_{\boldsymbol{q_3}}^{\geq} J_{-\boldsymbol{q_1-q_2-q_3}}^{\geq} (\Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{-m_1,\boldsymbol{q_2}}^{(j)} \Delta_{m_3,\boldsymbol{q_3}}^{(j)} \Delta_{-m_3,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{-m_1,\boldsymbol{q_2}}^{(j)} \Delta_{m_3,\boldsymbol{q_3}}^{(j)} \Delta_{-m_3,-\boldsymbol{q_1-q_2-q_3}}^{(i)} + \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{-m_1,\boldsymbol{q_2}}^{(j)} \Delta_{m_3,\boldsymbol{q_3}}^{(j)} \Delta_{-m_3,-\boldsymbol{q_1-q_2-q_3}}^{(i)})$$
(D.31)

When $i\nu_{m_1} = i\nu_{m_3}$ we further get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^2(z-i\nu_m)^2} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> \\ (\Delta_{m,\boldsymbol{q_1}}^{(i)} \Delta_{-m,\boldsymbol{q_2}}^{(j)} \Delta_{m,\boldsymbol{q_3}}^{(j)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{m,\boldsymbol{q_1}}^{(i)} \Delta_{-m,\boldsymbol{q_2}}^{(j)} \Delta_{m,\boldsymbol{q_3}}^{(j)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(j)} \\ + \Delta_{m,\boldsymbol{q_1}}^{(i)} \Delta_{-m,\boldsymbol{q_2}}^{(j)} \Delta_{m,\boldsymbol{q_3}}^{(j)} \Delta_{-m,-\boldsymbol{q_1-q_2-q_3}}^{(i)})$$
(D.32)

Which compute as:

$$+\frac{1}{2}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{m,\boldsymbol{q_{1}}}^{(i)}\Delta_{-m,\boldsymbol{q_{2}}}^{(j)}\Delta_{m,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}(i\nu_{m}\neq 0)$$

$$-\frac{1}{4}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m,i,j}}\frac{1}{(i\nu_{m})^{2}}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}\Delta_{m,\boldsymbol{q_{1}}}^{(i)}\Delta_{-m,\boldsymbol{q_{2}}}^{(j)}\Delta_{m,\boldsymbol{q_{3}}}^{(j)}\Delta_{-m,-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}(i\nu_{m}\neq 0)$$

$$(D.33)$$

When $i\nu_{m_1} \neq i\nu_{m_3}$. We get:

$$+\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m_{1},m_{2},i,j}}\frac{1}{(i\nu_{m_{1}})(i\nu_{m_{2}})}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}(\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{-m_{1},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$-\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{-m_{1},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}+\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{-m_{1},\boldsymbol{q_{2}}}^{(j)}\Delta_{m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{2},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$(i\nu_{m_{1}}\neq i\nu_{m_{2}},i\nu_{m_{1}}\neq 0,i\nu_{m_{2}}\neq 0)$$
$$(D.34)$$

When $i\nu_{m_1} + i\nu_{m_2} \neq 0$ while $i\nu_{m_1} + i\nu_{m_2} + i\nu_{m_3} = 0$ we get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m_1,m_2,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z^2(z-i\nu_{m_1})(z-i\nu_{m_1}-i\nu_{m_2})} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> \\ (\Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{-m_1-m_2,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{-m_1-m_2,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(i)} \\ + \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{-m_1-m_2,\boldsymbol{q_3}}^{(j)} \Delta_{0,-\boldsymbol{q_1-q_2-q_3}}^{(i)})$$
(D.35)

Which compute as:

$$+\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q}_{1},\boldsymbol{q}_{2},\boldsymbol{q}_{3},m_{1},m_{2},i,j}\frac{J_{\boldsymbol{q}_{1}}^{\geq}J_{\boldsymbol{q}_{2}}^{\geq}J_{\boldsymbol{q}_{3}}^{\geq}J_{-\boldsymbol{q}_{1}-\boldsymbol{q}_{2}-\boldsymbol{q}_{3}}^{\geq}}{(i\nu_{m_{1}})(i\nu_{m_{1}}+i\nu_{m_{2}})}(\Delta_{m_{1},\boldsymbol{q}_{1}}^{(i)}\Delta_{m_{2},\boldsymbol{q}_{2}}^{(j)}\Delta_{-m_{1}-m_{2},\boldsymbol{q}_{3}}^{(j)}\Delta_{0,-\boldsymbol{q}_{1}-\boldsymbol{q}_{2}-\boldsymbol{q}_{3}}^{(j)}$$
$$-\Delta_{m_{1},\boldsymbol{q}_{1}}^{(i)}\Delta_{m_{2},\boldsymbol{q}_{2}}^{(j)}\Delta_{-m_{1}-m_{2},\boldsymbol{q}_{3}}^{(j)}\Delta_{0,-\boldsymbol{q}_{1}-\boldsymbol{q}_{2}-\boldsymbol{q}_{3}}^{(j)}+\Delta_{m_{1},\boldsymbol{q}_{1}}^{(i)}\Delta_{m_{2},\boldsymbol{q}_{2}}^{(j)}\Delta_{-m_{1}-m_{2},\boldsymbol{q}_{3}}^{(j)}\Delta_{0,-\boldsymbol{q}_{1}-\boldsymbol{q}_{2}-\boldsymbol{q}_{3}}^{(i)})$$
$$(i\nu_{m_{1}}+i\nu_{m_{2}}\neq 0, i\nu_{m_{1}}\neq 0, i\nu_{m_{2}}\neq 0)$$
$$(D.36)$$

Nblue When $i\nu_{m_1}+i\nu_{m_2}\neq 0$, $i\nu_{m_1}+i\nu_{m_2}+i\nu_{m_3}\neq 0$ while $i\nu_{m_2}+i\nu_{m_3}=0$ we get:

$$-\frac{1}{2}\beta \sum_{\boldsymbol{q_1,q_2,q_3,m_1,m_2,i,j}} \oint \frac{dz}{2\pi i} \frac{f(z)}{z(z-i\nu_{m_1})^2(z-i\nu_{m_1}-i\nu_{m_2})} J_{\boldsymbol{q_1}}^> J_{\boldsymbol{q_2}}^> J_{\boldsymbol{q_3}}^> J_{-\boldsymbol{q_1-q_2-q_3}}^> \\ (\Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{-m_2,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1,-\boldsymbol{q_1-q_2-q_3}}^{(j)} - \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{-m_1,-\boldsymbol{q_1-q_2-q_3}}^{(j)} \\ + \Delta_{m_1,\boldsymbol{q_1}}^{(i)} \Delta_{m_2,\boldsymbol{q_2}}^{(j)} \Delta_{-m_2,\boldsymbol{q_3}}^{(j)} \Delta_{-m_1,-\boldsymbol{q_1-q_2-q_3}}^{(i)})$$
(D.37)

Which compute as:

$$-\frac{1}{8}\beta^{2}\sum_{\boldsymbol{q_{1},q_{2},q_{3},m_{1},m_{2},i,j}}\frac{1}{(i\nu_{m_{1}})(i\nu_{m_{2}})}J_{\boldsymbol{q_{1}}}^{>}J_{\boldsymbol{q_{2}}}^{>}J_{\boldsymbol{q_{3}}}^{>}J_{-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{>}(\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{-m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$-\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{-m_{2},\boldsymbol{q_{3}}}^{(j)}\Delta_{-m_{1},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}+\Delta_{m_{1},\boldsymbol{q_{1}}}^{(i)}\Delta_{m_{2},\boldsymbol{q_{2}}}^{(j)}\Delta_{-m_{1},-\boldsymbol{q_{1}-q_{2}-q_{3}}}^{(j)}$$
$$(i\nu_{m_{1}}+i\nu_{m_{2}}\neq 0, i\nu_{m_{1}}\neq 0, i\nu_{m_{2}}\neq 0)$$
$$(D.38)$$

When $i\nu_{m_1} + i\nu_{m_2} \neq 0$, $i\nu_{m_1} + i\nu_{m_2} + i\nu_{m_3} \neq 0$ while $i\nu_{m_2} + i\nu_{m_3} \neq 0$ we get:

$$-\frac{f(0)}{i\nu_{m_1}(i\nu_{m_1}+i\nu_{m_2})(i\nu_{m_1}+i\nu_{m_2}+i\nu_{m_3})} + \frac{f(i\nu_{m_1})}{i\nu_{m_1}i\nu_{m_2}(i\nu_{m_2}+i\nu_{m_3})} + \frac{f(i\nu_{m_1}+i\nu_{m_2}+i\nu_{m_3})}{i\nu_{m_3}(i\nu_{m_2}+i\nu_{m_3})(i\nu_{m_1}+i\nu_{m_2}+i\nu_{m_3})} - \frac{f(i\nu_{m_1}+i\nu_{m_2})}{i\nu_{m_2}i\nu_{m_3}(i\nu_{m_1}+i\nu_{m_2})}$$

Using the periodicity of the fermi-function: $f(i\nu_n) = f(0)$ so that we can have:

$$-\frac{f(0)}{i\nu_{m_{1}}(i\nu_{m_{1}}+i\nu_{m_{2}})(i\nu_{m_{1}}+i\nu_{m_{2}}+i\nu_{m_{3}})} + \frac{f(0)}{i\nu_{m_{1}}i\nu_{m_{2}}(i\nu_{m_{2}}+i\nu_{m_{3}})} + \frac{f(0)}{i\nu_{m_{3}}(i\nu_{m_{2}}+i\nu_{m_{3}})(i\nu_{m_{1}}+i\nu_{m_{2}}+i\nu_{m_{3}})} - \frac{f(0)}{i\nu_{m_{2}}i\nu_{m_{3}}(i\nu_{m_{1}}+i\nu_{m_{2}})} = 0$$

$$(i\nu_{m_{1}}+i\nu_{m_{2}}\neq 0, i\nu_{m_{2}}+i\nu_{m_{3}}\neq 0, i\nu_{m_{1}}+i\nu_{m_{2}}+i\nu_{m_{3}}\neq 0, i\nu_{m_{1}}\neq 0, i\nu_{m_{2}}\neq 0, i\nu_{m_{3}}\neq 0)$$

$$(D.39)$$

While the non-static part up to fourth order reads:

$$\begin{split} &+\frac{1}{4}N_{s}i\beta^{2}\sum_{m,\mathbf{q}_{1},\mathbf{q}_{2},ij,l}\frac{1}{i\nu_{m}}J_{\mathbf{q}_{1}}^{s}J_{\mathbf{q}_{2}}^{s}J_{-\mathbf{q}_{1}-\mathbf{q}_{2}}^{s}\epsilon_{ijl}\Delta_{m,\mathbf{q}_{1}}^{(i)}\Delta_{-m,\mathbf{q}_{2}}^{(j)}\Delta_{0,-\mathbf{q}_{1}-\mathbf{q}_{2}}^{(i)}(i\nu_{m}\neq 0) \\ &+\frac{1}{4}N_{s}\beta^{2}\sum_{\mathbf{q}_{1},\mathbf{q}_{2},\mathbf{q}_{3},m_{1},m_{2},i,j}\frac{1}{i\nu_{m_{1}}i\nu_{m_{2}}}J_{\mathbf{q}_{1}}^{s}J_{\mathbf{q}_{2}}^{s}J_{\mathbf{q}_{3}}^{s}J_{-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}\Delta_{m,\mathbf{q}_{1},\mathbf{q}_{1}}^{(i)}\Delta_{0,\mathbf{q}_{2}}^{(j)}\Delta_{m_{2},\mathbf{q}_{3}}^{(j)}\Delta_{-m_{1}-m_{2},-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}} \\ &\quad (i\nu_{m_{1}}\neq 0,i\nu_{m_{2}}\neq 0,i\nu_{m_{1}}+i\nu_{m_{2}}\neq 0) \\ &-\frac{1}{8}N_{s}\beta^{2}\sum_{\mathbf{q}_{1},\mathbf{q}_{2},\mathbf{q}_{3},m_{1},i,j}\frac{1}{i\nu_{m_{1}}i\nu_{m_{2}}}J_{\mathbf{q}_{1}}^{s}J_{\mathbf{q}_{2}}^{s}J_{\mathbf{q}_{3}}^{s}J_{-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}\Delta_{m,\mathbf{q}_{1}}^{(i)}\Delta_{0,\mathbf{q}_{2}}\Delta_{0,\mathbf{q}_{3}}^{(j)}\Delta_{-m,-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}^{(j)} \\ &-N_{s}\beta^{2}\sum_{\mathbf{q}_{1},\mathbf{q}_{2},\mathbf{q}_{3},m_{1},i,j}\frac{1}{(i\nu_{m})^{2}}J_{\mathbf{q}_{1}}^{s}J_{\mathbf{q}_{2}}J_{\mathbf{q}_{3}}^{s}J_{-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}\Delta_{m,\mathbf{q}_{1}}^{(i)}\Delta_{0,\mathbf{q}_{2}}\Delta_{0,\mathbf{q}_{3}}^{(j)}\Delta_{-m,-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}^{(i)} \\ &+N_{s}\beta^{2}\sum_{\mathbf{q}_{1},\mathbf{q}_{2},\mathbf{q}_{3},m_{1},i,j}\frac{1}{(i\nu_{m})^{2}}J_{\mathbf{q}_{1}}^{s}J_{\mathbf{q}_{2}}J_{\mathbf{q}_{3}}^{s}J_{-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}\Delta_{m,\mathbf{q}_{1}}\Delta_{0,\mathbf{q}_{2}}\Delta_{0,\mathbf{q}_{3}}\Delta_{0,-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}^{(i)}(i\nu_{m}\neq 0) \\ &+N_{s}\beta^{2}\sum_{\mathbf{q}_{1},\mathbf{q}_{2},\mathbf{q}_{3},m_{1},i,j}\frac{1}{(i\nu_{m})^{2}}J_{\mathbf{q}_{1}}J_{\mathbf{q}_{2}}J_{\mathbf{q}_{3}}J_{\mathbf{q}_{2}}J_{\mathbf{q}_{3}}J_{-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}\Delta_{m,\mathbf{q}_{1}}\Delta_{0,\mathbf{q}_{2}}\Delta_{0,\mathbf{q}_{3}}\Delta_{0,-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}^{(i)}(i\nu_{m}\neq 0) \\ &+\frac{3}{8}N_{s}\beta^{2}\sum_{\mathbf{q}_{1},\mathbf{q}_{2},\mathbf{q}_{3},m_{1},i,j}\frac{J_{\mathbf{q}_{1}}J_{\mathbf{q}_{2}}J_{\mathbf{q}_{3}}J_{\mathbf{q}_{2}}J_{\mathbf{q}_{2}-\mathbf{q}_{2}-\mathbf{q}_{3}}\Delta_{0,-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}\Delta_{0,-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}^{(i)}(i\nu_{m}\neq 0) \\ &-\frac{3}{8}N_{s}\beta^{2}\sum_{\mathbf{q}_{1},\mathbf{q}_{2},\mathbf{q}_{3},m_{1},i,j}\frac{J_{\mathbf{q}_{2}}J_{\mathbf{q}_{3}}J_{\mathbf{q}_{2}}J_{\mathbf{q}_{2}}J_{\mathbf{q}_{2}-\mathbf{q}_{2}-\mathbf{q}_{3}}+\Delta_{0,i,j}^{(i)}\Delta_{m,i,\mathbf{q}_{2}}\Delta_{m,j,\mathbf{q}_{3}}\Delta_{-m,-\mathbf{q}_{1}-\mathbf{q}_{2}-\mathbf{q}_{3}}}(i\nu_{m},\mathbf{q}_{2})J_{\mathbf{q}_{2}}J_{\mathbf{q}$$

Appendix E Critical behavior of \mathcal{K}_{ab} compared to \mathcal{K}_{aa}

Now we take the fluctuations around $(\pi, 0)$ and $(0, \pi)$ into consideration. These fluctuations maybe come from quantum fluctuations or the thermal fluctuations. Here we only consider fluctuations that live in a small energy window that corresponds to the 1/1000 of the peak intensity. As we shown in Table.E.1, when we tuning the ratio of $\frac{J_2}{J_1}$ close to the 0.5, the coefficient \mathcal{K}_{ab} shrinks significantly compared to the rest of the coefficients which roughly acquires the same value as in the case neglecting all the fluctuations. It can be seen in the Eq.7.63, Collinear phase is less favoured when the value of \mathcal{K}_{ab} is decreasing while the value of \mathcal{K}_{aa} stays the same. In order to illustrated this idea more clearly, we shall do the contour plot once again in the ratio of $\frac{J_2}{J_1}$ close to the 0.5.

$\frac{J_2}{J_1}$	\mathcal{K}_1	\mathcal{K}_2	\mathcal{K}_{aa}	\mathcal{K}_{ab}
0.5005	0.5002	0.2502	0.0626	0.0083
0.5006	0.5003	0.2503	0.0626	0.0189
0.5007	0.5004	0.2504	0.0627	0.0243
0.5008	0.5005	0.2505	0.0627	0.0282
0.5009	0.5006	0.2506	0.0628	0.0315
0.501	0.5007	0.2507	0.0628	0.0339
0.505	0.5048	0.2548	0.0648	0.0583
0.51	0.5097	0.2598	0.0674	0.0642
0.6	0.5997	0.3596	0.1292	0.1286
1	0.9995	0.9990	0.9970	0.9962
2	1.9990	3.9960	15.9521	15.9500

Table E.1: A table for normalized coefficients that are described in Eq.7.59.

Shown in the Fig.E.1, Collinear phase is not favoured when we take the effect of fluctuations into consideration. The reason for that is the sign of g is changed from positive to negative, so fluctuation that are equally strong in both X or Y direction is more favoured in order to minimizing the free energy, and this kind of fluctuation can lead to the emergency of the Spin density wave phase. From the Fig.E.2 we infer that a phase transition from Collinear phase to Spin density wave phase may happen around at $\frac{J_2}{J_1} = 0.5008$ base on above approximation.



Figure E.1: The contour plot of $S_E[\Delta_X^2, \Delta_Y^2]$ when T = 0.1 in the regime of $\frac{J_2}{J_1} = 0.5005$. (a)Neglect all fluctuations (b)Include fluctuations.



Figure E.2: The contour plot of $S_E[\Delta_X^2, \Delta_Y^2]$ when T = 0.1 (a)in the regime of $\frac{J_2}{J_1}$ = 0.5008. (b)in the regime of $\frac{J_2}{J_1}$ = 0.5009.

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