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Nematic phase transition in J_1-J_2 square lattice

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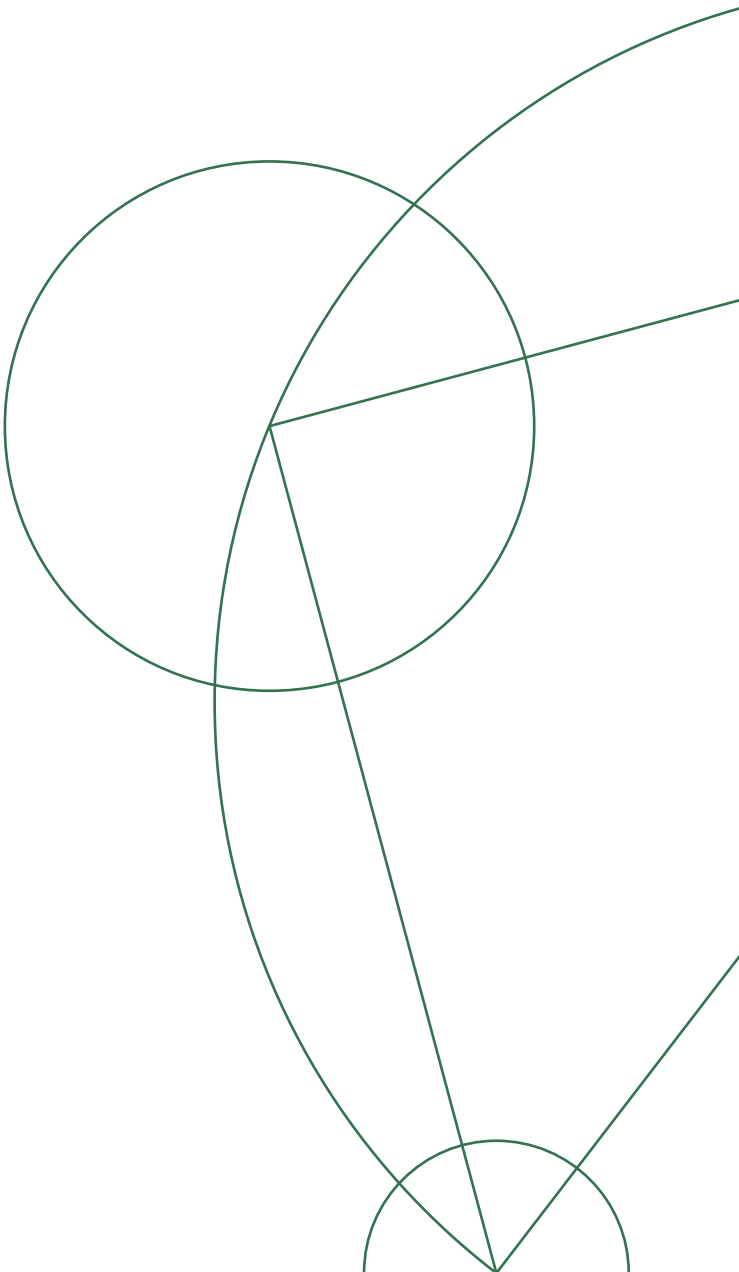

Master's thesis in Physics

Advisor: Jens Paaske

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Abstract

The two dimensional Heisenberg J_1-J_2 square lattice model with nearest- and next nearest neighbor antiferromagnetic interactions is an example of a frustrated magnetic system. The interactions tend to compete because they cannot both be minimized simultaneously. In the regime where $J_1 < 2J_2$ this leads to a highly degenerate ground state consisting of two coupled Néel lattices with an arbitrary relative angle, θ. Due to thermal and quantum fluctutations the true ground states are instead those with $\theta = 0$ or $\theta = \pi$. This is a manifestation of the phenomenon known as order by disorder. These two states break the x-y symmetry of the lattice by having ferromagnetic structure along one direction and antiferromagnetic along the other. A system displaying this symmetry breaking is said to have a finite nematic moment.
When the temperature is finite there can be no long range magnetic order in the system, but there can still be approximate magnetic order within domains of length scale Λ^{-1} as long as it satisfies $a \ll \Lambda^{-1} \ll \xi$, where ξ is the magnetic correlation length and a is the lattice constant. Within these domains spin waves exist, and they affect the long range behavior of the magnet. The magnetically ordered domains consist of two approximately Néel ordered lattices, and due to the spin waves, they minimize their energy by choosing a relative angle $\theta = 0, \pi$. They can be therefore be interpreted as nematic moments. This in turn gives rise to a nematic phase transition of the whole system at finite temperature, as shown by Chandra, Coleman and Larkin[1].
Despite the prediction of a nematic phase transition being confirmed numerically, their result for the critical temperature has been shown to be incorrect at strong frustration, $J_1/2J_2 \sim 1$. The aim of this thesis was to explore whether incorporating spin wave interactions in the domains of magnetic order minimizes the difference between the CCL and numerical result. The method for incorporating the spin wave interactions has been to make a mean field approximation inspired by the non-interacting spin wave correlation functions. While the mean field theory did lower the free energy of the system, it failed to bridge the gap between CCL and the numerical critical temperature, and either a better mean field must be utilized or another way of incorporating the interactions must be found.

Acknowledgements

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Contents

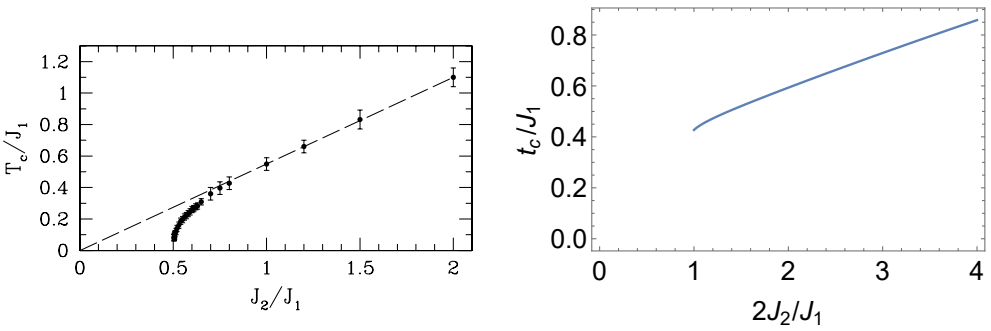
Chapter 1

Introduction

1.1 Motivation

In magnetic systems frustration, the competition between non compatible magnetic configurations, can lead to a wide variety of physical phenomena that continually elude simple descriptions. A frustrated magnet is one where the minimization of the energy of one magnetic moment precludes the minimization of the energy of another. Quite simple systems can be frustrated. One canonical example is the two-dimensional triangular lattice with antiferromagnetic nearest neighbor interactions where all three moments on a triangle cannot simultaneously anti-align. This is an example of geometric frustration. Other examples of geometrically frustrated magnets are those with kagomé and pyrochlore lattice structures[2]. One can also induce frustration through extended interactions. One example is the case of a square lattice with antiferromagnetic next nearest neighbor interactions and ferromagnetic or antiferromagnetic nearest neighbor interactions, and that particular model is called a Heisenberg J_1-J_2 square lattice model. It is easy to imagine frustration playing an important part in many physical materials when it can be achieved simply by extending the interaction beyond just nearest neighbors. Considering classical magnetic moments, when $2J_2 < J_1$ the ground state of the J_1-J_2 model is a simple Néel lattice, but when $J_1 < 2J_2$ the ground states are all the configurations of two interpenetrating Néel lattices with an arbitrary relative angle. It turns out that thermal and quantum fluctuations pick out as the ground states the two collinear antiferromagnetic configurations where the relative angle between the Néel lattices is either 0 or π, corresponding to the configurations where magnetic moments are parallel along one lattice direction and Néel ordered along the other. This is an example of a phenomenon called order by disorder[3], [4]. These states do not possess the x-y symmetry of the underlying Hamiltonian, and one can define the direction of parallel spins as the nematic moment of the states. The highly frustrated point $2J_2 = J_1$ is special and does not prefer any kind of order, but it is the point between the two phases of the magnet, and is therefore of great interest.

The J_1-J_2 square lattice is a two dimensional model and it therefore does not exhibit long range magnetic order at any finite temperature, since no continuous symmetry, such as the O(3) symmetry of a disordered spin system, may be broken in two dimensions or below as stated by the Mermin-Wagner theorem. In a pioneering paper by P. Chandra, P. Coleman and A.I. Larkin [1] it was shown that the system could have a different phase transition at a finite temperature, a nematic phase transition, where the discrete symmetry between two equivalent directions is broken. The crucial assumption is the existence of an intermediate length scale Λ^{-1} between the lattice constant (the smallest length scale of the system) and the correlation length ξ of magnetic moments. Even though the whole system is not magnetically ordered, magnons, quantized spin-waves, can exist within domains of size Λ^{-1} and their ultimate effect is the nematic ordering of the lattice below some critical temperature.



(a) (b)

Figure 1.1: Left: Monte Carlo results of the critical temperature of the nematic phase transition. For large J_2, the critical temperature scales linearly with J_2 but drops to zero with infinite slope as we approach the critical point $2J_2/J_1 = 1$. Figure taken from the paper by Weber et al.[5]. Right: CCL result for the critical temperature. The critical temperature increases as one approaches $2J_2/J_1 = 1$.

Although the idea of spin-waves being the source of a non-zero nematic order parameter is a great proof of concept, the critical temperature calculated by [1] is at odds with later numerical calculations. In a paper by Weber et al. [5], Monte Carlo calculations show that the critical temperature follows $2J_2/J_1$ linearly in the large J_2 limit as predicted by Chandra, Coleman and Larkin, but that it goes to 0 as $2J_2/J_1 \to 1$, as shown in Figure 1.1a (Figure taken from [5]). In contrast, the CCL result does not go to zero as one approaches the highly frustrated point as shown on Figure 1.1b.

The main goal of this thesis is to go beyond linear spin-wave theory and incorporate interactions between magnons through a mean-field approximation inspired by the single particle correlation functions of linear spin-wave theory. This is one of many possible mean-fields one could use, and it has the primary effect of renormalizing the on-site spin parameter S. It will be shown how this affects the magnon dispersion and by extension the critical temperature calculated by [1]. The aim is to solve the discrepancy between the CCL result and the Monte Carlo simulation or at least show that the correction betters the CCL critical temperature.

1.2 Experimental realization

Though the primary motivation of this thesis is theoretical, experimental research in the J_1-J_2 model is of course of great interest, so we mention here an experimental realization.

The two dimensional J_1-J_2 square lattice model with $0.5J_1 < J_2$ and $0 < J_2$ has been realized in AMoOPO$_4$Cl (A =K, Rb) compounds [6]. Measurements indiciate that the material can enter the collinear antiferromagnetic (CAF) state. In contrast to the Néel antiferromagnetic state, CAF is ferromagnetic along one direction and antiferromagnetic along the orthogonal direction in the crystal. The crystal is composed of MoO_5Cl octahedra connected by PO_4 tetrahedra. It is three dimensional, but is composed of stacks of bilayered sheets separated by planes of K or Rb, making interstack coupling small, and each bilayered sheet separate from the others.

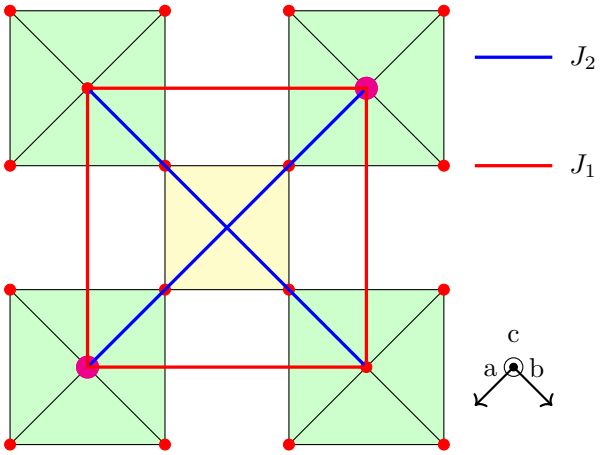


Figure 1.2: A bilayer $MoOPO_4Cl$ stack from the c direction. MoO_5Cl octahedra are green while the connecting PO_4 tetrahedron is yellow. Octahedron height is constant along a.

The interstack direction is called c. The bilayered sheet consists of rows of octahedra at two different heights, connected by tetrahedra. The direction of constant height is called a while the orthogonal is called b. Rows adjecent are of different height. Thus each stack can be considered a two dimensional square lattice. At the same time, the Mo^{5+} ions have spin 1/2, so each stack acts as a square spin lattice. Powder neutron diffraction and NMR experiments indicates [6] that the structure of the $AMoOPO_4Cl$ compounds are CAF in a regime of the H, T (external magnetic field, temperature) parameter space. This suggests a nearest neighbor (J_1) and a next nearest neighbor (J_2) interaction between spins on the lattice. Measurements of the magnetic susceptibility fits well with the J_1-J_2 model with parameters $(J_1, J_2) = (-2\text{K}, 19\text{K}), (0\text{K}, 29\text{K})$ for $A = \text{K}, \text{Rb}$ respectively. Theoretical calculations suggest CAF ground states, if taking into account order by disorder effects, for $0.5J_1 < J_2$, which fits well with these parameters. Most interestingly, the authors suggest changing parameters through crystal structure change, which could increase J_1/J_2. If that is possible when growing the crystals one could approach the highly frustrated point $J_1/J_2 = 2$ which is still not well understood theoretically.

1.3 Thesis outline

The structure of the thesis is chosen so as to give a coherent introduction to quantum magnetism. We have tried to cover a lot of ground to give a picture of the overall landscape of the field while emphasizing the points which are most relevant to the goal of the thesis.

- Chapter 2 is a brief introduction to magnetic interactions, how magnetism is inherently a quantum mechanical phenomenon and the role of quantum fluctuations.
- In chapter 3 the spin quantum partition function or spin path integral is introduced by means of spin coherent states. Several ideas, including spin quantization and classical spins, are touched upon simply because they are interesting and can help establish a coherent picture of interacting spins, but the main point of the chapter is to show how the quantum partition function naturally leads to the classical partition function in the large spin S limit.
- Classical spin systems are explored in chapter 4, the spin-wave spectrum of the J_1-J_2 model is found and the concept of order by disorder is introduced.
- In chapter 5 spin waves are quantized (magnons) using the Holstein-Primakoff (H.P.) transformation. To diagonalize the Hamiltonian the Bogoliubov transformation is employed, a procedure complicated by the fact that magnons are bosons and not fermions. The analysis is based on defining magnons on four ferromagnetic sublattices.
- In chapter 6 the system is once again analyzed with the H.P. transformation but this time on a single ferromagnetic sublattice. The eigenvectors of the Hamiltonian are found and using these the single particle correlation functions at arbitrary temperature are found.

- The next term in the large S expansion is found in chapter 7 and a mean field approximation is used to include the effect on the spin wave spectrum. The setup of the field theory calculation made by [1] is shown, and it is explored how the mean field approximated interaction term affects the critical temperature of the nematic phase transition.

Chapter 2

Basics of magnetism

One of the most widely known macroscopic manifestations of quantum physics is the phenomenon of magnetism. As well known as it is the origins of magnetic materials can be elusive. Niels Bohr, and later Hendrika van Leeuwen, famously showed[2] that magnetic materials cannot exist in classical mechanics. This was resolved with the advent of quantum mechanics and several different mechanisms are now known that lead to the *Heisenberg Hamiltonian*, one model of interactions between magnetic moments with parameters strong enough to support magnetic order at known temperatures.

2.1 Origins of magnetism

In this section we will briefly go through the argument of Bohr and van Leeuwen, go on to study the exchange interaction between two electrons and finally set up the Heisenberg Hamiltonian.

2.1.1 Bohr-van Leeuwen theorem

A magnet, both in classical and quantum mechanics, consists of a set of *magnetic moments*. In classical electrodynamics a magnetic moment, $\boldsymbol{\mu}$ is usually modeled by be a steady current flowing through a closed wire. In that case

$$\boldsymbol{\mu} = I\mathbf{a} \tag{2.1.1}$$

One can use this simple picture as a crude model of an electron moving in orbit around an atomic nucleus, at least as a first attempt at modeling magnets. In the limit where the area of the circuit vanishes, the limit of an infinitesimal magnetic moment, we denote the magnetic moment $d\boldsymbol{\mu}$. Then the total magnetization of a material of volume V is given by

$$\mathbf{M} = \int_V d\boldsymbol{\mu}. \tag{2.1.2}$$

The magnetic moment is related to its' angular momentum through the relation

$$\boldsymbol{\mu} = \gamma\mathbf{L}, \tag{2.1.3}$$

where γ is known as the gyromagnetic ratio. Finally, the moment interacts with external magnetic fields through the relation

$$E = -\boldsymbol{\mu}\cdot\mathbf{B} = -\gamma\mathbf{L}\cdot\mathbf{B} = -\gamma\mathbf{r}\times\mathbf{p}\cdot\mathbf{B}. \tag{2.1.4}$$

In other words, the energy associated with a set of magnetic moments stem from the momenta and positions of the particles giving rise to these moments. With this in mind, we take a step

back and look at the Hamiltonian for a set of such particles

$$H = \mathbf{p}^2/2m + V(\mathbf{x}). \tag{2.1.5}$$

In the presence of a magnetic field, $\mathbf{B} = \nabla \times \mathbf{A}$, the momentum is in general no longer a constant of motion. Rather the conserved quantity is the canonical momentum $\mathbf{p} - \frac{q}{c}\mathbf{A}$, and, more importantly, the Hamiltonian becomes

$$H = (\mathbf{p} - \frac{e}{c}\mathbf{A})^2/2m + V(\mathbf{x}). \tag{2.1.6}$$

This is sometimes called *minimal coupling*. The partition function of an ensemble of such particles is

$$Z = \int_{-\infty}^{\infty} d\mathbf{p} \int_{-\infty}^{\infty} d\mathbf{x} e^{-\beta\left[(\mathbf{p}-\frac{e}{c}\mathbf{A})^2/2m+V(\mathbf{x})\right]}. \tag{2.1.7}$$

The momentum can be shifted by the value of the vector potential, a change of coordinates which neither changes the measure nor the limits of the integral (since they extend to $\pm\infty$). In other words, the partition function for a set of classical particles does not change in the presence of a magnetic field. The result is that the magnetic moments of a material cannot affect each other through their magnetic fields and nor can they be affected by any external magnetic field. Assuming these are the only ways magnetic order could be formed the conclusion is that magnets do not exist.

2.1.2 Quantum magnetism

In classical mechanics no magnets exist but several different mechanisms circumvent the argument by Bohr and van Leeuwen in quantum mechanics. Most prominent is the existence of spin in quantum mechanics, an intrinsic quality of particles which resembles regular angular momentum. Spin couples directly to magnetic fields through the Zeeman interaction

$$H_Z \propto -\mathbf{S} \cdot \mathbf{B}, \tag{2.1.8}$$

a term which for electrons (and other spin-half particles) appears in the low-energy limit of the Dirac equation. Heuristically (but paradoxically) spin can be thought of as angular momentum from a non-extended object. Since it has nothing to do with position and momentum variables, the interaction cannot be produced by a minimal coupling, and will therefore appear by itself in the Hamiltonian and ultimately change the partition function. In general, the Bohr-van Leeuwen theorem does not hold in quantum mechanics.

2.1.3 The exchange interaction

The dipole-dipole interactions between two magnetic moments, due to the magnetic dipole field associated with a magnetic moment, give rise to the Hamiltonian

$$H_{\text{dip-dip}} = \frac{\mu_0}{4\pi r^3}\left(\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2 - \frac{3}{r^2}(\boldsymbol{\mu}_1 \cdot \mathbf{r})(\boldsymbol{\mu}_2 \cdot \mathbf{r})\right). \tag{2.1.9}$$

The energy typically associated with this type of interaction for moments seperated by 1Å is of order 1K. Comparing this to the temperature $T_C = 1043$K where iron loses its ferromagnetic properties, it is clear that the dipole-dipole interaction cannot account for magnetic iron, and therefore other interactions must exist.

As mentioned, there are in fact several mechanisms which lead to an effective interaction

between magnetic moments. Here we will discuss one which is due to the Coulomb interaction and the Pauli exclusion principle. Let $|\psi\rangle$ be the collective state of two electrons. The electrons are fermions meaning they change sign under exchange, and so the collective state can be written

$$|\psi\rangle = (|\chi\rangle_1 |\phi\rangle_2 \pm |\chi\rangle_2 |\phi\rangle_1) \otimes |\sigma\rangle_{s,t} \tag{2.1.10}$$

where $|\sigma\rangle$ is the spin state of the two electrons, which can either be one of the symmetric triplet states or the antisymmetric singlet state and the first parenthesis represents the spatial part of the electron state. The indices associated with the spatial part refer to each electron. If the first part of the wavefunction is symmetric in an exchange of the two electrons (relative positive sign between the terms in the parenthesis), the spin state must be a singlet state and vice versa. We now assume that the electrons do not interact directly through their spins, as they would for example do through the dipole-dipole interaction. Instead they only interact through the Coulomb interaction, $V_C = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}$, and the energy associated with this interaction is

$$\langle\psi|V_C|\psi\rangle = \frac{e^2}{4\pi\epsilon_0}\int d^3\mathbf{r}\left[\frac{|\chi(\mathbf{r}_1)|^2|\phi(\mathbf{r}_2)|^2}{|\mathbf{r}_1-\mathbf{r_2}|} \pm \frac{\chi^*(\mathbf{r}_1)\phi(\mathbf{r}_1)+\phi^*(\mathbf{r}_2)\chi(\mathbf{r}_2)}{|\mathbf{r}_1-\mathbf{r}_2|} + \text{h.c.}\right], \tag{2.1.11}$$

where the first term (and its identical hermitian conjugate) represent the "classical interaction" between the two electrons, in the sense that it depends on the overlap of the absolute square of the wave-function of the two electrons. Whether the electrons are in the singlet or triplet state is inconsequential to this term. The second term, called the exchange term, is due to quantum mechanical interference and changes sign depending on the spin state of the electrons. It is the exchange term that is of interest here. Denote it C_{ex}. We can now deduce an effective interaction between the spins of the two electrons

$$H_{\text{eff}} = -\frac{C_{\text{ex}}}{2}\left(1 + 4\mathbf{S}_1\cdot\mathbf{S}_2\right), \tag{2.1.12}$$

which, due to the singlet (triplet) state being an eigenstate of $\mathbf{S}_1\cdot\mathbf{S}_2$ with eigenvalue $-3/4$ $(1/4)$ with $\hbar = 1$, give exactly the energies from eq. (2.1.11). Thus, an effective spin-spin interaction emerges through an interplay between the Coulomb interaction and fermion statistics (the exclusion principle).

2.1.4 Heisenberg Hamilton

The general interaction between electrons of the form in eq. (2.1.12) is the Heisenberg Hamiltonian

$$H = \frac{1}{2}\sum_{ij} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j, \tag{2.1.13}$$

where i, j label the particle in question, usually the site at which a localized electron sits in a lattice, and J_{ij} is the interaction constant arising through the underlying mechanism that gives the effective interaction. The sign, range and strength of the exchange constants J_{ij} lead to a wide range of different ground states.

2.2 The ground state of the Heisenberg Hamiltonian

The information about the ground state of the Heisenberg Hamiltonian lies in the exchange constants J_{ij}[3]. In this section the terms ferromagnetic and antiferromagnetic exchange constant is defined and are used to explore the difference between the classical ground state of the Heisenberg Hamiltonian and the quantum mechanical.

2.2.1 Classical ferromagnetic and antiferromagnetic exchange

What will be called a classical spin in this section is just a three dimensional arrow $\mathbf{S}_i$ which can point in any direction. Consider a square lattice with one spin on each site, and only nearest neighbor interaction, with the exchange parameter J_{ij} constant everywhere on the lattice. Then

$$H = \frac{J}{2} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{2.2.1}$$

Now, assuming $J < 0$, the whole lattice minimizes its energy by assuming a *ferromagnetic* configuration, one in which all arrows point along the same direction. Thus, whenever J is negative it is heuristically called ferromagnetic. Note that the ground state of the system is degenerate, and an $O(3)$ rotation of the whole lattice corresponds to a rotation within the degenerate eigenspace. We can denote the state of the whole ferromagnetic lattice by a vector pointing along one of the spins. On the other hand, if $0 < J$ the system minimizes its energy by assuming an antiferromagnetic configuration, often called a Néel configuration, where arrows next to each other point in opposite directions. This can be thought of as two ferromagnetic lattices overlapping. The antiferromagnetic state can be denoted by a vector pointing along the spins *of a sublattice*. We call this the Néel vector. Note that it makes no difference in terms of energy which sublattice the Néel vector points along, which might suggest another symmetry of the system, namely invariance under sublattice exchange. This however is nothing but a π rotation in the plane of the spins.

2.2.2 Quantum ferromagnetic and antiferromagnetic exchange

To find the eigenstates of the quantum Heisenberg Hamiltonian we first rewrite it

$$H = \frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{2} \sum_{ij} J_{ij} \left[S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \right], \tag{2.2.2}$$

where $\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) = S_i^x S_j^x + S_i^y S_j^y$ is called the XY-term. For a spin state $|S, m\rangle$ where S is the total spin and m is the component in the z direction, $S^\pm |S, m\rangle \propto |S, m \pm 1\rangle$. The states are annihilated if they cannot be further raised or lowered. Now, the ferromagnetic state (here defined as states with every spin polarized in a direction defined as the z-direction) is an eigenstate of this Hamiltonian. The XY-term in the parenthesis annihilates the state and therefore has eigenvalue 0, while the state is an eigenstate of the S_i^z operators by definition. If we assume nearest neighbor coupling and $J < 0$, the ferromagnetic state is in fact the ground state. On the other hand, the Néel state is not an eigenstate, because it is not an eigenstate of the XY-term. To get a better understanding of this, we scale the lattice down to two spin-1/2 particles instead of N spin-S particles. The eigenstates of $\mathbf{S}_1 \cdot \mathbf{S}_2$ for two spin 1/2-particles are the well known singlet/triplet states. The states and their eigenvalues are

$$\begin{aligned} |\psi_T\rangle &= \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \right), & E_T = \frac{1}{4} \\ |\downarrow\downarrow\rangle \end{cases} \\ |\psi_S\rangle &= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right), \qquad E_S = -\frac{3}{4}. \end{aligned} \tag{2.2.3}$$

We now see that in the case of $0 < J$ it is the singlet state which is the ground state, and the configuration of spins in the singlet state resembles that of the Néel state. The crucial difference is that the singlet state is an antisymmetric linear combination of the two possible "Néel" states. If measuring the spin of one the particles in a series of experiments one would measure $\pm 1/2$ equally often, and in this sense the system exhibits quantum fluctuations. This generalizes to magnetic systems of more particles with general S, as we will now discuss.

2.2.3 Quantum fluctuations

We will now turn to a general discussion of quantum fluctuations which will be connected with magnetism by the end of the discussion. The first example we will look at is the usual harmonic oscillator, the Hamiltonian of which can be written as

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{2.2.4}$$

It is worth it to emphasize that this representation of the Hamiltonian is nothing but a *choice*. It could be represented by different operators, as we shall see in a moment. What we should note is that both the momentum of a state, and its position contribute to the energy. But since momentum and position are canonically conjugate operators, the operators cannot be simultaneously diagonalized. If for example we wanted to find the lowest energy state of the momentum term, $|p = 0\rangle$, it has no well defined position and consequently is not an eigenstate of H. Therefore the classical choice minimizing both the position and momentum term at the same time is not a viable state. Instead the ground state of the harmonic oscillator (written in terms of its coordinates in the x-basis) is

$$|0\rangle = \left(\frac{m\omega}{2\pi}\right)^{1/2} \int dx\, e^{\frac{-m\omega x^2}{2}} |x\rangle\,, \tag{2.2.5}$$

which is manifestly not of well defined position, and equally not of well defined momentum. Because the ground state does not have a well defined position at $x = 0$, the position operator of H contributes a non-zero term to the energy of this state. Essentially this is the origin of zero-point energy. It manifests itself clearly when writing the Hamiltonian in terms of the operator $a = \left(\sqrt{\frac{m\omega}{2}}x + \frac{ip}{\sqrt{2m\omega}}\right)$ and its hermitian conjugate. In that case

$$H = \omega\left(a^\dagger a + \frac{1}{2}\right), \tag{2.2.6}$$

with ω real. In terms of these operators, the ground state is the state annihilated by a, and so the ground state energy is $\omega/2$. This form of the Hamiltonian is more "natural", in the sense that the operator $a^\dagger a$ has a well defined eigenbasis with one state having eigenvalue 0, and no other terms appear in the Hamiltonian which do not commute with $a^\dagger a$. Putting the Hamiltonian in this form the constant addition may seem a bit out of place. Why could we not simply start from this Hamiltonian without the constant term? In fact this is a manifestations of the ordering problem of quantum mechanics. Since the traditional way of obtaining a quantum mechanical Hamiltonian is to write up the classical counterpart and set up canonical commutation relations between classically canonically conjugate variables, we have a choice of which expression for the classical Hamiltonian we start with. For example, the classical Hamiltonian of the harmonic oscillator may just as well be written as

$$H = \omega\left(\sqrt{\frac{m\omega}{2}}x - \frac{ip}{\sqrt{2m\omega}}\right)\left(\sqrt{\frac{m\omega}{2}}x + \frac{ip}{\sqrt{2m\omega}}\right). \tag{2.2.7}$$

If we quantize $[x, p] = i$ now, eq. (2.2.7) yields.

$$H = \omega\, a^\dagger a. \tag{2.2.8}$$

In other words, the concept of a zero-point energy in the harmonic oscillator hinges on which expression of the classical Hamiltonian one quantizes. This may seem uncomfortably arbitrary but it is just an indication that the world is fundamentally quantum mechanical. In other words one should start with a quantum mechanical Hamiltonian and derive the classical Hamiltonian from it. So which of eqs. (2.2.6) and (2.2.8) is the correct quantum mechanical expression?

Canonical quantization gives no answer. To determine the answer we should turn to experiments and in the case of the electromagnetic field, which in essence is a harmonic oscillator at each point in space, the answer is eq. (2.2.6). The zero-point energy in that case gives rise to the experimentally observed phenomenon known as the Casimir effect[7].

The point of analyzing the harmonic oscillator was to show that zero-point energy arises due to the constituents of its Hamiltonian not being simultaneously diagonalizable. In the case of the harmonic oscillator the constituents of the Hamiltonian are x and p. Using another picture of the same system, formulating it through the $a^\dagger a$ operators, one can instead talk about the ground state as the vacuum of quanta or particles represented by a. Each excitation to a higher energy eigenstate is just an addition of one of these particles to the system. If instead we started with a Hamiltonian of the form

$$H = \omega(a^\dagger a + aa^\dagger) + \Delta(aa + a^\dagger a^\dagger), \tag{2.2.9}$$

the terms in the Hamiltonian no longer commute, and the previous states counting the number of a particles are no longer eigenstates. To find the eigenstates of the Hamiltonian one can instead define new particles through a Bogoliubov transformation

$$\alpha = ua^\dagger + va. \tag{2.2.10}$$

The coefficients u, v must satisfy certain relations in order for the α particles to be meaningful particles (in this case "meaningful" means that $[\alpha, \alpha^\dagger] = [a, a^\dagger]$). In the end, one finds the Hamiltonian can be written as

$$H = \tilde{\omega}\left(\alpha^\dagger\alpha + 1/2\right). \tag{2.2.11}$$

Therefore the ground state of the Hamiltonian is not the vacuum of the a particles but instead the vacuum of the α particles. Excitations from the ground state are additions of the α particles. The point is that there may now be a non-zero expectation value of the a particles *even in the ground state*. For example, in the case where u, v are real, we find

$$a^\dagger = u\alpha - v\alpha^\dagger \tag{2.2.12}$$

and so

$$\langle 0|a^\dagger a|0\rangle = u^2 \langle 0|\alpha\alpha^\dagger|0\rangle = u^2. \tag{2.2.13}$$

This we call *quantum fluctuations*, and its emergence should not surprise us too much. After all, we had no right to expect that there are no a particles in the vacuum state of the α particles from the form of H. But it does lead to a somewhat counterintuitive result for the case of a Néel state and other non-ferromagnetic states, namely that there are small fluctuations about such states (spin waves/magnons in the classical/quantum system) even in the ground state of the system, as will be shown later in the thesis. In the case of thermal fluctuations one can think of a magnon being created/destroyed in the system by its interaction with the environment. Heuristically one can have a similar picture in mind when thinking of quantum fluctuations, but it seems to be a different type of fluctuation, since nothing actually fluctuates in an eigenstate of the Hamiltonian (it is stationary).

2.3 Conclusion

The quantum mechanical origin of magnetic interactions has been discussed and a mechanism for effective spin-spin interactions has been shown (the exchange interaction). The difference

between the ferromagnetic and antiferromagnetic exchange between two spin half particles has been analysed and importantly the antiferromagnetic exchange leads to a ground state which is a superposition of two "Néel" states (the singlet state). This is an illustration of how the ground state of antiferromagnet systems, in contrast to the ferromagnetic counterparts, are manifestly non-classical. One is led to the same conclusion when considering magnons on non-ferromagnetic systems. It was illustrated in the final section how the number of magnons of a magnetic lattice may be non-zero even in the ground state as a result of magnons not diagonalizing the Hamiltonian. This will be the definition of quantum fluctuations in this thesis.

Chapter 3

Coherent state path integral

In this section the quantum mechanical system consisting of spins of size S on a lattice structure is introduced. We will consider the case where the spins interact through a general Heisenberg Hamiltonian. The quantum partition function can be written as a path integral built from coherent spin states, and it is shown how the classical partition function arises in the limit $S \to \infty$. Further, gauge-invariance, spin-quantization and a classical definition of spins are discussed. The differences between the usual coherent state path integrals of bosons and fermions and the spin coherent path integral is also explored. This chapter is mostly based on [8], and if otherwise it will be stated.

3.1 Schwinger bosons and spin coherent states

There exists a mapping from spin operators to bosons called *Schwinger bosons*, and in three dimensions it is

$$\hat{S}^+ = S_x + iS_y = a^\dagger b \tag{3.1.1}$$

$$\hat{S}^- = S_x - iS_y = b^\dagger a \tag{3.1.2}$$

$$\hat{S}^z = \frac{1}{2}\left(a^\dagger a - b^\dagger b\right). \tag{3.1.3}$$

Using the commutation relations of bosons it is straightforward to check that the spin operators satisfy the spin commutation relations

$$[S^i, S^j] = i\epsilon_{kij}S^k. \tag{3.1.4}$$

Of course such bosons act on states in an infinite dimensional Fock space and so in the boson picture the Hilbert space is much larger than in the spin state picture, which for finite S is a finite dimensional Hilbert space. There is a *physical subspace* of the Fock space in the boson picture, and there is a one to one correspondence between states in this subspace and spin states in the usual spin Hilbert space. The physical subspace of the bosonic Fock space is that which obeys the restriction

$$n_a + n_b = 2S \tag{3.1.5}$$

such that the eigenvalues of S^z are neither above S or below $-S$ in the physical subspace. The mapping between spin states and states in the Fock space is

$$|S, m\rangle_{\hat{z}} = \frac{(a^\dagger)^{(S+m)}}{\sqrt{(S+m)!}} \frac{(b^\dagger)^{(S-m)}}{\sqrt{(S-m)!}} |0\rangle, \tag{3.1.6}$$

with $|0\rangle$ being the vacuum state of Schwinger bosons.

3.1.1 Rotation of spin states

When faced with the operator corresponding to the spin in the $\hat{n}$ direction

$$\hat{S}(\theta,\phi) = \hat{\mathbf{S}} \cdot \hat{n}, \tag{3.1.7}$$

with $\hat{n} = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$, one may find the eigenstates through a rotation of, for example, the spin state fully polarized in the z-direction. Rotations are unitary transformations generated by the spin-operators and one can check that the state

$$|\mathbf{\Omega}\rangle = \mathcal{R}\,|S,S\rangle_{\hat{z}} = e^{-i\phi\hat{S}_z} e^{-i\theta\hat{S}_y} e^{-i\chi\hat{S}_z}\,|S,S\rangle_{\hat{z}}\,, \tag{3.1.8}$$

is indeed an eigenstate of $\hat{S}(\theta,\phi)$ which will be called a coherent state. Here it should be noted that the operators are spin-operators on the usual spin Hilbert space. It is clear that the first rotation simply corresponds to an arbitrary phase choice and can therefore be set to 1. The unit vector

$$\mathbf{\Omega} = \big(\sin(\theta)\cos(\phi), \quad \sin(\theta)\sin(\phi), \quad \cos(\theta)\big)\,, \tag{3.1.9}$$

parameterizes the eigenstate. Correspondingly, the Fock states transform by rotations of the operators

$$(a^\dagger)' = \mathcal{R}^{-1} a^\dagger \mathcal{R}, \qquad (b^\dagger)' = \mathcal{R}^{-1} b^\dagger \mathcal{R}. \tag{3.1.10}$$

3.1.2 Transformation of linear operators

A general bilinear operator in the second quantized form is

$$\hat{A} = a_i^\dagger A_{ij} a_j, \tag{3.1.11}$$

where A is a matrix. A linear operator generally takes the form

$$\hat{v}^\dagger = v_i a_i^\dagger. \tag{3.1.12}$$

The unitary transformation generated by $\hat{A}$ and applied to $\hat{v}^\dagger$ is

$$e^{i\theta\hat{A}}\hat{v}^\dagger e^{-i\theta\hat{A}} = \hat{v}^\dagger + i\theta[\hat{A},\hat{v}^\dagger] + \frac{(i\theta)^2}{2}[\hat{A},[\hat{A},\hat{v}^\dagger]] + ..., \tag{3.1.13}$$

where we used the Baker-Hausdorff lemma. Assuming $a_i^\dagger$ are all bosonic operators, and using the bosonic commutation relations

$$[\hat{A},\hat{v}^\dagger] = A_{ij}v_k[a_i^\dagger a_j, a_k^\dagger] = A_{ij}v_j a_i^\dagger = (A\cdot v)_i\, a_i^\dagger, \tag{3.1.14}$$

the transformed linear operator becomes

$$e^{i\theta\hat{A}}\hat{v}^\dagger e^{-i\theta\hat{A}} = \hat{v}^\dagger + i\theta\,(A\cdot v)_i\, a_i^\dagger + \frac{(i\theta)^2}{2}\,(A\cdot A\cdot v)_i\, a_i^\dagger + ... = \Big(e^{i\theta A}\cdot v\Big)_i\, a_i^\dagger, \tag{3.1.15}$$

which establishes a one-to-one mapping between the transformation of a vector v through unitary matrices generated by A and linear operators $\hat{v}^\dagger$ through unitary operators generated by $\hat{A}$.

3.1.3 Rotation of Schwinger bosons

The rotated spin eigenstates are also called spin coherent states. To write any coherent state through Schwinger bosons we must obtain an expression for the operators in eq. (3.1.10). Using the definition of Schwinger bosons the spin operators can be written as

$$\hat{S}_i = (a^\dagger, b^\dagger) \cdot S_i \cdot \begin{pmatrix} a \\ b \end{pmatrix}, \tag{3.1.16}$$

where S_i are the 2×2 Pauli matrices. Using

$$a^\dagger = \begin{pmatrix} a^\dagger, & b^\dagger \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{3.1.17}$$

and eq. (3.1.15) we find

$$\begin{aligned}
(a^\dagger)' &= \begin{pmatrix} a^\dagger, & b^\dagger \end{pmatrix} \cdot \left(e^{-i\phi S_z} e^{-i\theta S_y} e^{-i\chi S_z} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right) \\
&= e^{-i\chi/2} \begin{pmatrix} a^\dagger, & b^\dagger \end{pmatrix} \cdot \left(\begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix} \cdot \begin{pmatrix} \cos(\frac{\theta}{2}) & -\sin(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right) \\
&= e^{-i\chi/2} \begin{pmatrix} a^\dagger, & b^\dagger \end{pmatrix} \cdot \left(\begin{pmatrix} e^{-i\frac{\phi}{2}} \cos(\frac{\theta}{2}) & -e^{-i\frac{\phi}{2}} \sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}} \sin(\frac{\theta}{2}) & e^{i\frac{\phi}{2}} \cos(\frac{\theta}{2}) \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right) \\
&= e^{-i\frac{\chi}{2}} \left(a^\dagger e^{-i\frac{\phi}{2}} \cos\left(\frac{\theta}{2}\right) + b^\dagger e^{i\frac{\phi}{2}} \sin\left(\frac{\theta}{2}\right) \right).
\end{aligned} \tag{3.1.18}$$

Similarly we find

$$(b^\dagger)' = e^{i\frac{\chi}{2}} \left(b^\dagger e^{i\frac{\phi}{2}} \cos\left(\frac{\theta}{2}\right) - a^\dagger e^{-i\frac{\phi}{2}} \sin\left(\frac{\theta}{2}\right) \right). \tag{3.1.19}$$

We could rewrite this result more neatly as

$$\begin{pmatrix} (a^\dagger)' \\ (b^\dagger)' \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\chi+\phi}{2}} \cos\left(\frac{\theta}{2}\right) & e^{-i\frac{\chi-\phi}{2}} \sin\left(\frac{\theta}{2}\right) \\ -e^{i\frac{\chi-\phi}{2}} \sin\left(\frac{\theta}{2}\right) & e^{i\frac{\chi+\phi}{2}} \cos\left(\frac{\theta}{2}\right) \end{pmatrix} \cdot \begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix}. \tag{3.1.20}$$

3.1.4 Coherent States

A general coherent state can be generated through the rotation of a spin state fully polarized in the z-direction. Thus

$$|\mathbf{\Omega}\rangle = \frac{((a^\dagger)')^{2S}}{\sqrt{2S!}} |0\rangle = e^{-iS\chi} \frac{(ua^\dagger - vb^\dagger)^{2S}}{\sqrt{2S!}} |0\rangle = e^{-iS\chi} \sqrt{2S!} \sum_{m=-S}^{S} \frac{(ua^\dagger)^{S+m} (-vb^\dagger)^{S-m}}{(S+m)!(S-m)!} |0\rangle, \tag{3.1.21}$$

where $u = e^{-i\phi/2} \cos(\theta/2), v = e^{i\phi/2} \sin(\theta/2)$, and where the binomial expansion was used in the last equality. The overlap between two coherent states is then

$$\langle \mathbf{\Omega} | \mathbf{\Omega}' \rangle = e^{-iS(\chi'-\chi)} (2S)! \sum_{m=-S}^{S} \frac{(u^* u')^{S+m} (v^* v')^{S-m}}{(S+m)!(S-m)!} = e^{-iS(\chi'-\chi)} \left(u^* u' + v^* v' \right)^{2S}, \tag{3.1.22}$$

where we used the orthonormality of different Fock states. This result shows that the coherent states are not orthogonal. One can rewrite this expression such that

$$\begin{aligned}
\langle \mathbf{\Omega} | \mathbf{\Omega}' \rangle &= \left(\frac{1 + \mathbf{\Omega} \cdot \mathbf{\Omega}'}{2} \right)^S e^{iS\psi}, \\
\psi &= 2 \arctan \left[\tan\left(\frac{\phi - \phi'}{2} \right) \frac{\cos\left[\frac{1}{2}(\theta + \theta')\right]}{\cos\left[\frac{1}{2}(\theta - \theta')\right]} \right] + \chi - \chi'.
\end{aligned} \tag{3.1.23}$$

From this expression it is clear that different coherent states approach orthogonality as $S \to \infty$. By constructing the identity operator through coherent states we can show they span the whole Hilbert space. The coherent states are parametrized through continuous parameters on the unit sphere, so the identity must be an integral

$$\begin{aligned}
&\int d\mathbf{\Omega} \left|\mathbf{\Omega}\right\rangle \left\langle\mathbf{\Omega}\right| \\
&= \int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\phi \sum_{m,m'} \frac{(2S)!(\cos(\theta/2))^{2S+m+m'}(\sin(\theta/2))^{2S-m-m'} e^{i2\phi(m'-m)}}{\sqrt{(S+m)!(S+m')!(S-m)!(S-m')!}} \left|S,m\right\rangle \left\langle S,m'\right| \\
&= 2\pi \int_0^\pi d\theta \sin(\theta) \sum_m \frac{(2S)!(\cos^2(\theta/2))^{S+m}(\sin^2(\theta/2))^{S-m}}{(S+m)!(S-m)!} \left|S,m\right\rangle \left\langle S,m\right| \\
&= 2\pi \int_0^\pi d\theta \sin(\theta) \sum_m \frac{(2S)!}{(S+m)!(S-m)!} \left(\frac{1+\cos\theta}{2}\right)^{S+m} \left(\frac{1-\cos\theta}{2}\right)^{S-m} \left|S,m\right\rangle \left\langle S,m\right| .
\end{aligned} \tag{3.1.24}$$

To proceed, we must evaluate the θ integral. First of all

$$I_{S,m} = \frac{1}{2}\int_0^\pi d\theta \sin(\theta) \left(\frac{1+\cos\theta}{2}\right)^{S+m} \left(\frac{1-\cos\theta}{2}\right)^{S-m} = \int_0^1 dx\, x^{S+m}(1-x)^{S-m} . \tag{3.1.25}$$

Next we invoke the generating function

$$\begin{aligned}
f(z) &= \sum_{n=0}^{2S} \frac{(2S)!}{(2S-n)!n!} I_{S,n-S} z^n = \int_0^1 dx\, (1-x)^{2S} \sum_{n=0}^{2S} \frac{(2S)!}{(2S-n)!n!} \left(\frac{xz}{1-x}\right)^n \\
&= \int_0^1 dx\, (1-x)^{2S} \left(\frac{xz}{1-x}+1\right)^{2S} = \int_0^1 dx\, \left(x(z-1)+1\right)^{2S} \\
&= \frac{1}{(2S+1)(z-1)} \left(z^{2S+1}-1\right) = \frac{1}{2S+1} \sum_{n=0}^{2S} z^n .
\end{aligned} \tag{3.1.26}$$

By comparing the expression after the first equality with the expression after the last we find

$$\frac{(2S)!}{(2S-n)!n!} I_{S,n-S} = \frac{1}{2S+1}, \tag{3.1.27}$$

and have thus found an expression for $I_{S,m}$. Inserting this back into the expression we find

$$\int d\mathbf{\Omega} \left|\mathbf{\Omega}\right\rangle \left\langle\mathbf{\Omega}\right| = \frac{4\pi}{2S+1} \sum_m \left|S,m\right\rangle \left\langle S,m\right| = \frac{4\pi}{2S+1}, \tag{3.1.28}$$

where we used the fact that the set of states, $|S,m\rangle$ is a complete orthonormal basis. In other words,

$$\frac{2S+1}{4\pi} \int d\mathbf{\Omega} \left|\mathbf{\Omega}\right\rangle \left\langle\mathbf{\Omega}\right| = 1, \tag{3.1.29}$$

and therefore the coherent states span the Hilbert space of spin states, but does so with some degree of redundancy. In other words, the coherent states form an overcomplete basis. Eq. (3.1.29) will be one of the ingredients in constructing a path integral expression of the partition function. Another important ingredient is the equation

$$\left\langle\mathbf{\Omega}\right| \mathbf{S}_i \cdot \mathbf{S}_j \left|\mathbf{\Omega}\right\rangle = S^2 \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j, \tag{3.1.30}$$

where i, j denote spins at different sites, for instance in a lattice, and $|\mathbf{\Omega}\rangle = \prod_i |\mathbf{\Omega}\rangle_i$. To show this, we use

$$\mathbf{\Omega}_i \cdot \mathbf{S}_i \, |\mathbf{\Omega}\rangle = S \, |\mathbf{\Omega}\rangle \,, \tag{3.1.31}$$

which is true by definition of the coherent states, and can also be shown by a basis change of the vectors $\mathbf{\Omega}_i, \mathbf{S}_i$. If we let R^{-1} be the rotation matrix rotating $\hat{x}, \hat{y}, \hat{z}$ to $\hat{x}', \hat{y}', \hat{z}'$, where $\hat{z}' = \mathbf{\Omega}_i$ and $\hat{x}', \hat{y}'$ are two orthonogal unit vectors also orthogonal to $\mathbf{\Omega}_i$, then

$$\mathbf{\Omega}_i \cdot \mathbf{S}_i = (\hat{z}R) \cdot \mathbf{S}_i = \hat{z} \cdot (R\mathbf{S}_i) = \hat{S}_i^{\hat{z}'}, \tag{3.1.32}$$

which explicitly shows Eq. (3.1.31). Using this

$$\langle \mathbf{\Omega} | \mathbf{S}_i \cdot \mathbf{S}_j | \mathbf{\Omega} \rangle = R_i^{\alpha\alpha'} R_j^{\beta\beta'} \, \langle \mathbf{\Omega} | S_i^{\alpha'} S_j^{\beta'} | \mathbf{\Omega} \rangle = S^2 R_i^{\alpha,3'} R_j^{3',\beta} = S^2 \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j, \tag{3.1.33}$$

where the primed indices denote coordinates in the $\hat{x}_i', \hat{y}_i', \hat{z}_i'$ basis, and where we used $\langle \mathbf{\Omega}_i | S_i^{\alpha'} | \mathbf{\Omega}_i \rangle = \delta_{3',\alpha'} S$. This last property is derived from Eq. (3.1.31) and the fact that if a particle is in an eigenstate of the spin along some direction on the unit sphere, the expectation value along the two orthogonal directions is zero. We also used the fact that rotation matrices are orthogonal, and that the rows/columns of such a matrix is composed of the unit vectors of the basis one is rotating to. Using Eq. (3.1.29) the expectation value of the Heisenberg Hamiltonian is

$$\langle \mathbf{\Omega} | H | \mathbf{\Omega} \rangle = \frac{S^2}{2} \sum_{ij} J_{ij} \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j, \tag{3.1.34}$$

which is the classical Heisenberg Hamiltonian.

3.2 Coherent state path integral

The starting point in constructing the coherent state path integral is the partition function

$$Z = \mathrm{Tr}\left(\exp\left(-\beta H\right)\right) = \int d\mathbf{\Omega} \, \langle \mathbf{\Omega} | \exp\left(-\beta H\right) | \mathbf{\Omega} \rangle = \lim_{N_\epsilon \to \infty} \int d\mathbf{\Omega} \, \langle \mathbf{\Omega} | (1 - \epsilon H)^{N_\epsilon} | \mathbf{\Omega} \rangle \,, \tag{3.2.1}$$

where $d\mathbf{\Omega} = \prod_i d\mathbf{\Omega}_i \frac{2S+1}{4\pi}$ and $\epsilon = \beta / N_\epsilon$. One obtains this expression for the trace straightforwardly by use of the identity operator written in terms of coherent states. Next, we insert identity operators in between each parenthesis and label each with a number $n \in 0, ..., N_\epsilon$ so

$$Z = \lim_{N_\epsilon \to \infty} \int d\{\mathbf{\Omega}\}^n \, \langle \mathbf{\Omega}^{N_\epsilon} | (1 - \epsilon H) | \mathbf{\Omega}^{N_\epsilon - 1} \rangle \, \langle \mathbf{\Omega}^{N_\epsilon - 1} | (1 - \epsilon H) | \mathbf{\Omega}^{N_\epsilon - 2} \rangle \, ... \, \langle \mathbf{\Omega}^{1} | (1 - \epsilon H) | \mathbf{\Omega}^{0} \rangle \,, \tag{3.2.2}$$

where $\mathbf{\Omega}^0 \equiv \mathbf{\Omega}^{N_\epsilon}$. This means we have to evaluate the expectation values

$$\langle \mathbf{\Omega}^n | (1 - \epsilon H(\mathbf{S})) | \mathbf{\Omega}^{n-1} \rangle = \langle \mathbf{\Omega}^n | \mathbf{\Omega}^{n-1} \rangle \left(1 - \epsilon H(\mathbf{\Omega}^n, \mathbf{\Omega}^{n-1})\right), \tag{3.2.3}$$

where $H(\mathbf{\Omega}^n, \mathbf{\Omega}^{n-1}) = \frac{\langle \mathbf{\Omega}^n | H(\mathbf{S}) | \mathbf{\Omega}^{n-1} \rangle}{\langle \mathbf{\Omega}^n | \mathbf{\Omega}^{n-1} \rangle} = \frac{S^2}{2} \sum_{ij} J_{ij} \mathbf{\Omega}_i^n \mathbf{\Omega}_j^{n-1}$, which is obtained in analogy with Eq. (3.1.29). The overlap between coherent states is given by (3.1.23), and so

$$\begin{aligned} \langle \mathbf{\Omega}^n | \mathbf{\Omega}^{n-1} \rangle &= \frac{1 + \mathbf{\Omega}^n \cdot \mathbf{\Omega}^{n-1}}{2} e^{iS\psi(n,n-1)} \\ \psi(n, n+1) &= 2 \arctan\left[\tan\left(\frac{\phi^n - \phi^{n-1}}{2} \right) \frac{\cos\left[\frac{1}{2}(\theta^n + \theta^{n-1})\right]}{\cos\left[\frac{1}{2}(\theta^n - \theta^{n-1})\right]} \right] + \chi^n - \chi^{n-1}. \end{aligned} \tag{3.2.4}$$

The next step is to make the assumption, that $\Delta\mathbf{\Omega} = \mathbf{\Omega}^n - \mathbf{\Omega}^{n-1}$ is small in the limit $N_\epsilon \to \infty$. This does not seem fair, since each vector $\mathbf{\Omega}^n$ is integrated over the entire unit sphere independently of the others. As will be seen, this assumption is equivalent to assuming that smooth functions (in the sense that the function and it's first derivative are continuous) $\mathbf{\Omega}_i(\tau)$ dominate the path integral[8]. The motivation is to arrive at an expression for the action containing first derivatives of the fields, and we therefore assume$\Delta\mathbf{\Omega} \propto \epsilon + \mathcal{O}(\epsilon^2)$. Making use of this assumption we find

$$\begin{aligned}\psi(n,n-1) &= 2\arctan\left[\tan\left(\frac{\phi^n-\phi^{n-1}}{2}\right)\frac{\cos\left[\frac{1}{2}(\theta^n+\theta^{n-1})\right]}{\cos\left[\frac{1}{2}(\theta^n-\theta^{n-1})\right]}\right]+\chi^n-\chi^{n-1}\\ &\approx 2\arctan\left[\frac{\phi^n-\phi^{n-1}}{2}\frac{\cos\left[(\theta^n+\mathcal{O}(\epsilon))\right]}{1+\mathcal{O}(\epsilon^2)}\right]+\chi^n-\chi^{n-1}\\ &\approx \left(\phi^n-\phi^{n-1}\right)\cos\theta^n+\chi^n-\chi^{n-1}+\mathcal{O}(\epsilon^2),\end{aligned} \tag{3.2.5}$$

where we used that the tan-function and it's inverse are linear to small orders of it's argument. Now reinsert this expression in Z and use that to dominant order in ϵ $\mathbf{\Omega}^n\cdot\mathbf{\Omega}^{n-1}=1$. Next reexponentiate $1-\epsilon H(\mathbf{\Omega}^n,\mathbf{\Omega}^{n-1})$ (an approximation which becomes exact in the limit $N_\epsilon\to\infty$), which leads to the result

$$\begin{aligned}Z &= \lim_{N_\epsilon\to\infty}\int d\{\mathbf{\Omega}\}^n \exp\left(-\epsilon\sum_{n=1}^{N_\epsilon}\left(-iS\left[\frac{\phi^n-\phi^{n-1}}{\epsilon}\cos\theta^n+\frac{\chi^n-\chi^{n-1}}{\epsilon}\right]+\frac{1}{2}\sum_{ij}J_{ij}\mathbf{\Omega}_i^n\mathbf{\Omega}_i^{n-1}\right)\right)\\ &= \oint\mathcal{D}\mathbf{\Omega}\exp\left(-\int_0^\beta d\tau\left[-iS\dot\phi(\tau)\cos(\theta(\tau))+H(\mathbf{\Omega}(\tau))\right]\right),\end{aligned} \tag{3.2.6}$$

where the arbitrary phases χ were set to 0. The circle in the path integral is to denote the periodic boundary condition $\mathbf{\Omega}(\beta)=\mathbf{\Omega}(0)$. Also note that $\dot\phi\cos(\theta)=\sum_i\dot\phi_i\cos(\theta_i)$, where i denotes lattice site. Now note that one can reformulate this phase by making use of

$$\dot{\mathbf{\Omega}} = \dot\theta\hat\theta+\sin(\theta)\dot\phi\hat\phi. \tag{3.2.7}$$

Defining $\mathbf{A}=-\frac{\cos\theta}{\sin\theta}\hat\phi$ we can write

$$-\dot\phi\cos(\theta)=\mathbf{A}\cdot\dot{\mathbf{\Omega}}, \tag{3.2.8}$$

which yields the expression for the quantum partition function

$$Z=\oint\mathcal{D}\mathbf{\Omega}\exp\left(-\int_0^\beta d\tau\left[iS\mathbf{A}\cdot\dot{\mathbf{\Omega}}+H(\mathbf{\Omega}(\tau))\right]\right). \tag{3.2.9}$$

3.2.1 Spin coherent path integral and bosonic/fermionic coherent state path integral

At this point it might seem as if the spin coherent path integral is more or less just another path integral, and indeed the procedure for obtaining it is quite reminiscent of the procedure for obtaining the coherent state path integral of bosons and fermions

$$Z=\oint\mathcal{D}\{\overline\psi,\psi\}e^{-\int_0^\beta d\tau\int dx\ \ \overline\psi\dot\psi+H(\overline\psi,\psi)}, \tag{3.2.10}$$

where the circle in the integration symbol denotes periodicity/antiperiodicity of the bosonic/fermionic fields. Despite this, there are a few differences we should observe:

- The fields of the spin coherent path integral are defined on the base manifold S^2, the unit sphere, whereas those of the bosons and fermions are over $\mathbb{R}^n$, with n being the dimension of the system. Several things could be said about this, but one important feature of S^2 is that it cannot be covered by a single coordinate system.

- Contrary to the case of bosons and fermions, the τ-dynamics are included as a phase in the spin coherent path integral.

Turning now to the case of bosons, these are usually, if not always, defined through small distortions of an otherwise rigid ground state. The distortions are small in the sense that the energy cost associated with them are assumed to be quadratic, i.e. all distortions behave as harmonic oscillators. This, of course, is only generally valid near minima of the potential landscape. The excitations of the ground state are represented by bosons, and these are therefore only defined in the "background" of a rigid ground state. This stands in contrast to the spin coherent path integral. The degrees of freedom one integrates over are well defined even in the absence of some background ground state (although if the spins are not sitting on a lattice we might be interested also in their positional dynamics). It may be the case that some subset of states completely dominate the partition function - in that case it might be more fruitful to restrict the partition function over these states and the set of states representing small fluctuations about them. These fluctuations are called spin-waves and are the analogues of phonons of a lattice. But the point is that the spin-coherent path integral is more general than that. It is the equivalent of finding the (quantum) partition function of a set of particles *before* assuming that they crystallize.

3.2.2 Gauge invariance and spin quantization

In this subsection we touch upon the gauge invariance of the phase term in the coherent state path integral, and how this leads to spin quantization. Of course we started with a spin quantized quantum mechanical description to obtain the path integral in the first place, but it is nice to see that the path integral leads to the same results as the usual operator formalism.
As seen, we can obtain an expression for the quantum partition function of spins as an integration of classical fields over the unit sphere and the parameter τ. The term

$$\mathcal{S} = -iS \int d\tau \cos(\theta)\dot{\phi} = iS \int d\tau \dot{\phi}(1 - \cos(\theta)) \tag{3.2.11}$$

is a geometric phase, and the equality is valid as long as the trajectory of $\mathbf{\Omega}$ does not cross the domain boundary of $\phi \in [0, 2\pi)$[1]. The choice of gauge $\mathcal{S} = iS \int d\tau \dot{\phi}(1 - \cos(\theta))$ corresponds to $\mathbf{A} = \frac{1-\cos(\theta)}{\sin(\theta)}\hat{\phi}$. We choose this gauge so that $\mathbf{A}$ is singular only at the south pole. The vector potential $\mathbf{A}$ can be interpreted as the potential of a Dirac magnetic monopole, since $\mathbf{B}_m = \nabla \times \mathbf{A} = \hat{\mathbf{\Omega}}$. Of course this magnetic field seems to have a non-zero divergence and should therefore not be due solely to the curl of another field, but the fact that it can be written as such is just due to the singular behavior of $\mathbf{A}$ at the south pole. If we consider some closed path on the unit sphere, $\partial\mathcal{A}$, then we may write

$$\mathcal{S} = iS \int_0^\beta d\tau \mathbf{A} \cdot \dot{\hat{\mathbf{\Omega}}} = iS \oint_{\partial\mathcal{A}} d\mathbf{\Omega} \cdot \mathbf{A} = iS \int_{\mathcal{A}} d\mathbf{a} \cdot \mathbf{B}_m, \tag{3.2.12}$$

where the area enclosed by $\partial\mathcal{A}$ is that which does not enclose the singularity of $\mathbf{A}$. The point is that we could have chosen another gauge, $\mathbf{A} = \frac{-1-\cos(\theta)}{\sin(\theta)}\hat{\phi}$, where the singularity is on the

[1] In the case where it does cross the domain boundary, Auerbach argues that the discrepancy is resolved by deforming the path such that it goes through the north pole [8].

north pole, but which otherwise yields the same expression for the geometric phase. This seems to lead to an ambiguity in $\mathcal{S}$ since the difference between the two choices is

$$\Delta\mathcal{S} = iS\int_{A_n} d\mathbf{a}\cdot\mathbf{B}_m + iS\int_{A_s} d\mathbf{a}\cdot\mathbf{B}_m = iS\int_{S^2} da = iS4\pi, \tag{3.2.13}$$

where the first equality is due to the sign convention in Stokes theorem[2]. Thus we see that for the ambiguity in geometric phase to be resolved, the spin of a particle must be a half integer. It is in this way that the spin coherent path integral quantizes spin.

3.2.3 From the quantum to the classical and semiclassical partition function

The expression for the quantum partition function readily yields the classical partition function. We first adjust the parameters of H, namely J_{ij} such that

$$\overline{J_{ij}} = J_{ij}S^2, \tag{3.2.14}$$

where $\overline{J_{ij}}$ is independent of S. This is allowed since these are just parameters of the theory. Doing this, $H(\mathbf{\Omega})$ is just the classical Hamiltonian. In that case, by letting $S\to\infty$, no field configuration with a non-constant $\mathbf{\Omega}(\tau)$ contributes to the partition function, due to the fast oscillating term proportional to S. Thus

$$Z = \oint \mathcal{D}\mathbf{\Omega}\exp\left(-\int_0^\beta d\tau\left[iS\mathbf{A}\cdot\dot{\mathbf{\Omega}} + H(\mathbf{\Omega}(\tau))\right]\right) \longrightarrow \oint \mathcal{D}\mathbf{\Omega}\exp\left(-\beta H(\mathbf{\Omega})\right). \tag{3.2.15}$$

It is worth noting what the difference between the quantum and classical partition function is. It all lies in the τ dependency of the fields. The partition function is a sum over weights, and in the classical case these weights depend only on the *energies* associated with the coordinates on the unit sphere, of the spins in the systems. In contrast, the quantum mechanical weights depend on the whole function of $\mathbf{\Omega}(\tau)$ through *both* the energies of these *fields* and through a geometric phase. One can also make a systematic expansion in $1/S$. The first step is to rescale τ and β by S

$$\begin{aligned}\overline{\tau} &= \tau/S\\ \overline{\beta} &= \beta/S,\end{aligned} \tag{3.2.16}$$

where $\overline{\tau},\overline{\beta}$ are independent of S. We can then scale out S from the action $\mathcal{S}$

$$\mathcal{S} = S\int_0^{\overline{\beta}} d\overline{\tau}\left[i\mathbf{A}\cdot(\partial_{\overline{\tau}}\mathbf{\Omega}) + H(\mathbf{\Omega})\right]. \tag{3.2.17}$$

Now the partition function may be rewritten

$$Z = e^{-\mathcal{S}} = Z_0 Z', \tag{3.2.18}$$

where $Z_0 = \exp\left(-S\int_0^{\overline{\beta}} d\overline{\tau}\left[i\mathbf{A}\cdot(\partial_{\overline{\tau}}\mathbf{\Omega}^{cl}) + H(\mathbf{\Omega}^{cl})\right]\right)$ is the factor of the partition function due to the saddle point and Z' is the corrective factor to higher orders in $1/S$. The $1/S$ expansion also appears in a setting different from the path integral, namely in the use of the Holstein-Primakoff transformation as will be shown in chapter 5. Both in the path integral formalism and with Holstein-Primakoff bosons, the lowest order contribution in $1/S$, that is the lowest order fluctuations from the saddle point, are spin-waves.

[2] In the case where one of the areas which the path encloses contains neither the north nor south pole one can change coordinates to define the north pole within one this area.

3.3 Real time path integral

The Green functions

$$G(t,0;\mathbf{\Omega}_f,\mathbf{\Omega}_i) = \int \mathcal{D}\mathbf{\Omega} \exp\left(i\int_0^t dt\left[S\dot{\phi}\cos(\theta) - H(\mathbf{\Omega}(t))\right]\right), \tag{3.3.1}$$

is obtained in analogy with the expression for the partition function. In this case, one starts with the overlap $\langle \mathbf{\Omega}_f | \mathbf{\Omega}_i(t)\rangle$ where the time dependency is generated through the Hamiltonian in the interaction picture. Now denoting

$$q = \phi \quad p = S\cos(\theta), \tag{3.3.2}$$

it is clear that q, p make up canonical conjugate variables in the Hamiltonian, and that the action in the Green function is formulated in terms of a Legendre transformed Lagrangian $L(q,\dot{q})$.

3.3.1 Classical spin

Without dwelling too much at it, we will now see how the concept of a classical spin can be defined. While it may not be so useful at this point, it is an interesting idea and might help clarify some points of confusion when looking at classical systems of spin. Here we follow [9].

At this point we have seen how the quantum dynamics are obtained from a path integral over some action. Usually this action is the action of the classical system corresponding to the quantum mechanical system, so we could now *define* a classical spin as an arrow on the unit sphere with the action

$$\mathcal{S} = \int_0^T dt\ \left(S\dot{\mathbf{\Omega}}\cdot\mathbf{A} - H(\mathbf{\Omega})\right). \tag{3.3.3}$$

It is in fact possible to show that the Poisson brackets of the classical arrows correspond to the commutation relations of spin operators. Notice that this action stands in contrast to one of an extended object with some angular momentum. For example, a rod with moment of inertia I in a field, $\mathbf{B}$, which couples to its angular frequency, has the action

$$\mathcal{S}_{rod} = \int_0^T dt\ \left(\frac{1}{2}I\dot{\boldsymbol{\omega}}^2 + \mathbf{B}\cdot\boldsymbol{\omega}\right), \tag{3.3.4}$$

which involves the second power of the first derivative. To have any sensible dynamics in this classical theory, the moment of inertia must be non-zero, but this is not so for the classical spin. A crucial difference between the coordinates of the classical spin and those of the ordinary system of particles considered in classical mechanics, is that the classical spin is defined on the unit sphere. This manifold is non-euclidean, and a general set of coordinates, a set covering the whole sphere, does not exist. Instead one must restrict oneself to local patches on the manifold and define phase space on these. The phase space is then a symplectic manifold with a closed two-form ω (such that $\mathrm{d}\omega = 0$), and "d" is the exterior derivative defined by $\omega = \sum_i \mathrm{d}p_i \wedge \mathrm{d}q_i$, where the wedge product is the anti-symmetric product between two n-forms. We will not do a thorough examination of the generalized classical framework which makes it possible to treat such a set of coordinates, but will use some of the results of this framework. If we restrict ourselves to the parts of the sphere defined by $\phi, \theta \in (0, 2\pi), (0, \pi)$, we can use these as coordinates of the phase space. We note that the action, in terms of θ, ϕ is

$$\mathcal{S} = \int_0^T dt\ \left(S\dot{\phi}(1-\cos(\theta)) - H(\phi,\theta)\right). \tag{3.3.5}$$

This leads us to define the generalized momenta $p_\phi = -S\cos(\theta)$, $p_\theta = 0$. In terms of these (local) coordinates,

$$\omega = \frac{1}{2}\omega_{\mu\nu}\mathrm{d}q^\mu \wedge \mathrm{d}q^\nu = S\sin(\theta)\mathrm{d}\theta \wedge \mathrm{d}\phi, \tag{3.3.6}$$

with $\omega_{\theta\phi} = S\sin(\theta) = -\omega_{\phi\theta}$. The inverse matrix $\omega^{\mu\nu}$ has components $\omega^{\theta\phi} = \frac{1}{S\sin(\theta)} = -\omega^{\phi\theta}$. We need this expression because the Poisson brackets in the generalized Hamiltonian formalism is

$$\{f, g\} = \omega^{\mu\nu}(\partial_\mu f)(\partial_\nu g). \tag{3.3.7}$$

Using that $\Omega_x = \sin(\theta)\cos(\phi), \Omega_y = \sin(\theta)\sin(\phi)$, it is clear that

$$\begin{aligned}(\partial_\theta\Omega_x)(\partial_\phi\Omega_y) &= (\cos(\theta)\cos(\phi))(\sin(\theta)\cos(\phi)),\\ (\partial_\phi\Omega_x)(\partial_\theta\Omega_y) &= (-\sin(\theta)\sin(\phi))(\cos(\theta)\sin(\phi)),\end{aligned} \tag{3.3.8}$$

so

$$\{\Omega_x, \Omega_y\} = \frac{1}{S}\cos(\theta) = \frac{1}{S}\Omega_z, \tag{3.3.9}$$

which is exactly analogous to the commutation relation between spin operators in quantum mechanics.
We finally consider the case of a spin fluctuating about $\Omega_z = 1$. In that case Ω_x, Ω_y are small quantities, and to first order in these small quantities

$$\{\Omega_x, S\Omega_y\} = 1. \tag{3.3.10}$$

Due to the small fluctuations we are naturally in a local patch of the two-sphere and may consider the coordinates $\Omega_x, S\Omega_y$ as defined in the usual Euclidean space (despite the fact that the previous coordinates were not defined on the north pole, we could still have described fluctuations about another point on the two-sphere which should yield the same kind of Poisson brackets). Thus for small oscillations, $(\Omega_x, S\Omega_y) \equiv (Q, P)$ are canonically conjugate coordinates in the usual Euclidean space. It is in fact these coordinates one would use to describe spin-waves on a spin lattice.

3.4 Susceptibility from partition function

With the quantum partition function we are now in principle in a position to evaluate physical observables. One will be considered here, the magnetic- or spin-susceptibility. As will be seen, the naive approach one usually employs in calculating Gaussian integrals is obstructed due to the geometric phase in the path integral. The conclusion of this section is that other methods than the usual employment of source terms in the action must be employed to calculate correlation functions from the spin path integral. This section is based on [10], [11] and [12].

3.4.1 Spin susceptibility

The spin susceptibility is the linear response tensor of the magnetization, the average magnetic moment per site, to an external magnetic field $\mathbf{H}$. For a translationally invariant system it is defined through the relation

$$M^\mu(r_i, t) = \sum_j \int dt' \chi^{\mu\nu}(r_i - r_j, t - t')H^\nu(r_j, t'). \tag{3.4.1}$$

If the system is isotropic, the magnetization will align with the magnetic field, i.e. the susceptibility is diagonal

$$M^{\mu}(r_i,t) = \frac{1}{2\pi}\sum_j \int dt' \chi^{\mu\mu}(r_i - r_j, t-t') H^{\mu}(r_j,t'). \tag{3.4.2}$$

Thus

$$\chi^{\mu\mu}(r_i - r_j, t-t') = \frac{\delta M^{\mu}(r_i,t)}{\delta H^{\mu}(r_j,t')}_{|\mathbf{H}=0}, \tag{3.4.3}$$

$\delta/\delta H$ is a functional derivative, and where the external magnetic field is set to zero at the end of the functional differentiation reflects the fact that the susceptibility is the *linear* response function. The magnetization is itself derivable from

$$M^{\mu}(r_i,t) = -k_B T \frac{\delta \ln(Z)}{\delta H^{\mu}(r_i,t)}, \tag{3.4.4}$$

By replacing t with the parameter $i\tau$, we get an expression in the quantum partition function. In the end the real time result may be retrieved by analytical continuation. We obtain the result

$$\chi^{\mu\mu}(r_i - r_j, \tau - \tau') = \left(\frac{1}{Z[\mathbf{H}]}\frac{\delta^2 Z[\mathbf{H}]}{\delta H^{\mu}(r_i,\tau)\delta H^{\mu}(r_j,\tau')}\right)_{|\mathbf{H}=0} = \frac{1}{Z[0]}\frac{\delta^2 Z[\mathbf{H}]}{\delta H^{\mu}(r_i,\tau)\delta H^{\mu}(r_j,\tau')}_{|\mathbf{H}=0}. \tag{3.4.5}$$

An external magnetic field couples to a spin through the Zeeman Hamiltonian, and it can thus be incorporated in the coherent state path intergral through a term $\mathbf{H}\cdot\mathbf{\Omega}$ in the action

$$Z[\mathbf{H}] = \oint \mathcal{D}\mathbf{\Omega} \exp\left(-\int_0^{\beta} d\tau \left[iS\sum_i \mathbf{A}_i\cdot\dot{\mathbf{\Omega}}_i + \frac{S^2}{2}\sum_{ij} J_{ij}\mathbf{\Omega}_i\cdot\mathbf{\Omega}_j + S\sum_i \mathbf{H}_i(\tau)\cdot\mathbf{\Omega}_i(\tau)\right]\right). \tag{3.4.6}$$

Since the fields in the partition function are defined on the unit-sphere we cannot immediately use the usual procedure of Gaussian integration. To circumvent this, a constraint field, λ is introduced by the term $i\sum_i \lambda_i(|\mathbf{\Omega}_i|^2 - 1)$ in the action and the integration is relaxed to one over all of $\mathbb{R}^3$

$$\begin{aligned} Z[\mathbf{H}] = \oint \mathcal{D}\mathbf{\Omega}\mathcal{D}\lambda \exp\Bigg(-\int_0^{\beta} d\tau \Bigg[&\frac{S^2}{2}\sum_{ij} J_{ij}\mathbf{\Omega}_i\cdot\mathbf{\Omega}_j \\ &+S\sum_i \mathbf{H}_i(\tau)\cdot\mathbf{\Omega}_i(\tau) + i\mathbf{A}_i\cdot\dot{\mathbf{\Omega}}_i + i\lambda_i(|\mathbf{\Omega}_i|^2 - 1)\Bigg]\Bigg). \end{aligned} \tag{3.4.7}$$

Fourier transforming in the lattice and τ we obtain

$$\begin{aligned} Z[\mathbf{H}] = \oint \mathcal{D}\mathbf{\Omega}\mathcal{D}\lambda \exp\Bigg(-\sum_{\omega_n,q}\Bigg[&\frac{S^2}{2}J_q\mathbf{\Omega}_{-q,-\omega_n}\cdot\mathbf{\Omega}_{q,\omega_n} + \sum_{q'} i\lambda_{q-q',\omega_n-\omega_n'}(\mathbf{\Omega}_{-q',-\omega_n'}\cdot\mathbf{\Omega}_{q,\omega_n} - 1) \\ &+S\mathbf{H}_{-q,-\omega_n}\cdot\mathbf{\Omega}_{q,\omega_n} - \omega_n\mathbf{A}_{-q,-\omega_n}\cdot\mathbf{\Omega}_{q,\omega_n}]\Bigg). \end{aligned} \tag{3.4.8}$$

The action can be rewritten

$$\mathcal{S} = \frac{1}{2}\sum_{\omega_n\omega_n',qq'} \left(\mathbf{\Omega}^*_{q,\omega_n} + S\mathbf{H}^*_{q,\omega_n}\mathcal{G}^{-1}\right)\mathcal{G}(q,q';\omega_n,\omega_n')\left(\mathbf{\Omega}_{q',\omega_n'} + S\mathcal{G}^{-1}\mathbf{H}_{q',\omega_n'}\right) - \omega_n\mathbf{A}^*_{q,\omega_n}\cdot\mathbf{\Omega}_{q,\omega_n} - \frac{S^2}{2}\sum_{\omega_n\omega_n',qq'}\mathbf{H}_{q,\omega_n}\mathcal{G}^{-1}\mathbf{H}_{q',\omega_n'}. \tag{3.4.9}$$

with $\mathcal{G}(q,q';\omega_n,\omega_n') = \left(S^2J_q\delta_{qq'}\delta_{\omega_n\omega_n'} + 2i\lambda_{q-q',\omega_n-\omega_n'}\right)$. Usually one would redefine the $\mathbf{\Omega}_{q,\omega_n}$ fields, so as to incorporate the constant addition in the parenthesis and do the Gaussian integration. The problem is the vector potential $\mathbf{A}$ which depends on ϕ,θ in a not so obvious way. One can in fact write the term in a coordinate-independent way, so that it only depends on $\mathbf{\Omega}$. The first step is to expand the function $\mathbf{\Omega}_q(\tau)$ to $\mathbf{\Omega}_q(\tau,u)$, such that $\mathbf{\Omega}_q(\tau,u=1) = \mathbf{\Omega}_q(\tau)$ and $\mathbf{\Omega}_q(\tau,u=0) = (1,0,0)$. Then if we return to the original expression of the geometric phase

$$\begin{aligned} iS\int d\tau(\partial_\tau\phi)\cos(\theta) &= iS\int d\tau\int_0^1 du\partial_u\left((\partial_\tau\phi)\cos(\theta)\right) \\ &= iS\int d\tau\int_0^1 du(\partial_\tau\phi)(\partial_u\cos(\theta)) + (\partial_u\partial_\tau\phi)\cos(\theta) \\ &= iS\int d\tau\int_0^1 du(\partial_\tau\phi)(\partial_u\cos(\theta)) - (\partial_u\phi)(\partial_\tau\cos(\theta)), \end{aligned} \tag{3.4.10}$$

where we used partial integration on the last term in the last equality. The boundary term vanishes due to the periodic boundary conditions $\mathbf{\Omega}_q(\beta) = \mathbf{\Omega}_q(0)$. This is an integration over the area of a two-sphere which can be realized in the following way. The area measure on the unit sphere can be defined as

$$\mathbf{\Omega}\cdot(\partial_x\mathbf{\Omega})\times(\partial_y\mathbf{\Omega}), \tag{3.4.11}$$

with $\mathbf{\Omega}(x,y)$ a unit vector on the unit parametrized by x,y tracing out a path on the sphere. For instance, if x,y are θ,ϕ we find

$$\mathbf{\Omega}\cdot(\partial_\theta\mathbf{\Omega})\times(\partial_\phi\mathbf{\Omega}) = \sin\theta, \tag{3.4.12}$$

and so

$$\int d\theta\int d\phi\;\mathbf{\Omega}\cdot(\partial_\theta\mathbf{\Omega})\times(\partial_\phi\mathbf{\Omega}) = \int d\theta\sin\theta\int d\phi = \int d(\cos\theta)\int d\phi, \tag{3.4.13}$$

which is the usual integration over a unit sphere in polar coordinates. Letting $\cos(\theta),\phi$ be parametrized by τ,u and changing the integration over $\cos\theta,\phi$ to one over these τ,u we would obtain the last line in eq. (3.4.10), since the integrand is nothing but the Jacobian determinant between the two sets of coordinates. Since the parameters used in defining the area measure can be chosen as we want, we thus find

$$iS\int_0^\beta d\tau\int_0^1 du(\partial_\tau\phi)\cos(\theta) = iS\int_0^\beta d\tau\int_0^1 du\;\mathbf{\Omega}\cdot(\partial_\tau\mathbf{\Omega})\times(\partial_u\mathbf{\Omega}). \tag{3.4.14}$$

We now have a coordinate independent expression for the geometric phase. This unfortunately has three factors of $\mathbf{\Omega}$, making it impossible to incorporate into the quadratic term. Thus even in a coordinate independent notation, the straightforward approach to using the coherent state path integral to calculate correlation functions is not viable, and other means must be used. In chapter 7.2 it is shown how one may obtain an effective field theory in the classical limit and how this can be used to understand the J_1-J_2 model.

3.5 Conclusion

We have established the quantum partition function for spin systems and shown various results using this. In particular it was shown how the large S limit leads to the classical, τ-independent partition function. This can be used to justify the semiclassical approximation in systems where one only wants to consider the small deviations from the classical ground state. We will use this fact in chapter 5. The other main conclusion from this chapter is that, due to the existence of the phase term in the action of the quantum partition function illustrated in equation (3.4.10) a straightforward Gaussian integration of the $\mathbf{\Omega}$ fields is not tenable. For this reason other methods must be used to calculate correlation functions of the spin system, such as considering only the classical (τ-independent) contribution or integrating out variables in a renormalization scheme. The latter is the method used in Haldanes mapping [8] from a Heisenberg antiferromagnet to the non-linear sigma model. A similar method will be used in section 7.2.

Chapter 4

Classical ground state and spin wave fluctuations

Having established that the large S limit reduces the quantum partition function to the classical partition function, we set out to find the classical ground states of magnetic systems at zero temperature. It is about this ground state that spin waves, both classical and quantum, can be defined, and it is the effect of the spin waves on the classical, magnetically ordered ground state we are interested in. In this chapter we find the classical ground state of magnetic systems, and then move on to study fluctuations about the ground state (spin waves), through which the notion of *order by disorder* is introduced. Some of the results are for general systems while we will also show how they apply to the J_1-J_2 square lattice. The chapter is based on [3], [4], [13] and [14].

4.1 Ground state for general J_{ij}

The energy of a system of classical spins in three dimensions sitting on a lattice of general dimension is

$$E = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{4.1.1}$$

where J_{ij} is invariant under translations and reflections, and the spins satisfy the local constraint

$$\mathbf{S}_i^2 = S^2. \tag{4.1.2}$$

To proceed, the constraint (4.1.2) is relaxed to $\sum_i \mathbf{S}_i^2 = NS^2$, where N is the number of lattice sites. Next, the Fourier transformed versions of the energy and the global constraint are

$$E = \sum_q J_q \mathbf{S}_{-q} \cdot \mathbf{S}_q = \sum_{qq'} (S_q^\alpha)^* \left[J_q \delta^{\alpha\beta} \delta_{qq'} \right] S_{q'}^\beta, \quad NS^2 = \sum_q \mathbf{S}_{-q} \mathbf{S}_q = \sum_q (S_q^\alpha)^* S_q^\alpha, \quad \alpha \in \{x, y, z\} \tag{4.1.3}$$

where we used the symmetries of J_{ij} and the fact that S_i^α is real. With this in mind, a new vector is defined, $\mathcal{S} = \left(\{S_q^\alpha\}\right)$, in a $3 \times N$-dimensional vector space. Note that even though S_q^α is complex, its complex-conjugate is equal to S_{-q}^α, which is the reason why the space is not $3 \times (2N)$ dimensional. The relaxed constraint is equivalent to the normalization of this vector, and the energy is equivalent to a matrix inner product. Since the only restraint on $\mathcal{S}$ is that it be normalized, we could now choose it to point along any direction $\hat{S}_q^\alpha$ we want. This is essentially the difference between the local constraint and the global constraint on the spins. The reason for doing this is that any non-zero component of $\mathcal{S}$ is associated with some energy,

which contributes to the overall energy of the system, and we can therefore minimize E by choosing only the components with the smallest J_q to be non-zero. If we choose a vector $\mathcal{S}$ where only S^α_Q, and by extension S^α_{-Q} is non-zero, the energy is of this vector is

$$E = J_Q \left(\mathbf{S}_Q \cdot \mathbf{S}_{-Q} + \mathbf{S}_{-Q} \cdot \mathbf{S}_Q\right). \tag{4.1.4}$$

The energy of the system is then minimized by choosing Q_0 to minimize J_Q[1]. Finally, this choice of $\mathcal{S}$ gives us

$$\mathbf{S}_i = \frac{1}{\sqrt{N}} \left(\mathbf{S}_Q e^{iQ\cdot R_i} + \mathbf{S}_{-Q} e^{-iQ\cdot R_i}\right), \tag{4.1.5}$$

or

$$S^\alpha_i = A^\alpha \cos(Q \cdot R_i + \phi^\alpha). \tag{4.1.6}$$

The parameters A^α, ϕ^α have up to now been chosen so as to satisfy the normalization of $\mathcal{S}$, but are otherwise arbitrary. We must now impose the full constraint (4.1.2) which fixes the parameters A^α, ϕ^α. One choice is

$$\begin{aligned} S^x_i &= S\cos(Q \cdot R_i + \phi), \\ S^y_i &= S\sin(Q \cdot R_i + \phi), \\ S^i_z &= 0, \end{aligned} \tag{4.1.7}$$

which can also be written as

$$\mathbf{S}_i/S = \mathbf{u}\cos(Q \cdot R_i) + \mathbf{v}\sin(Q \cdot R_i), \tag{4.1.8}$$

where $\mathbf{u}, \mathbf{v}$ are orthogonal unit vectors and Q is called the *structure vector* of the state.

4.1.1 Ground state of J_1-J_2 model

We will now find the ground state of the J_1-J_2 model. The Hamiltonian of the model is the Heisenberg Hamiltonian

$$H = \frac{1}{2}\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j. \tag{4.1.9}$$

defined on a two dimensional square lattice. The interactions considered are nearest neighbor (N.N.), with exchange constant J_1, and next nearest neighbor (N.N.N.), with exchange constant J_2. We will consider the case where both exchange constants are positive, and, as has previously been discussed, they are therefore called antiferromagnetic. Interactions which prefer N.N. and N.N.N. to anti-align cannot both be satisfied simultaneously. They therefore compete, as illustrated on Figure 4.1. This is an example of a phenomenon called *frustration* and it is in particular an example of *frustration through interaction*, in contrast to frustration due to lattice geometry. The Fourier transform of the exchange function is

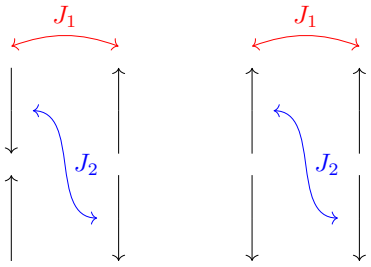
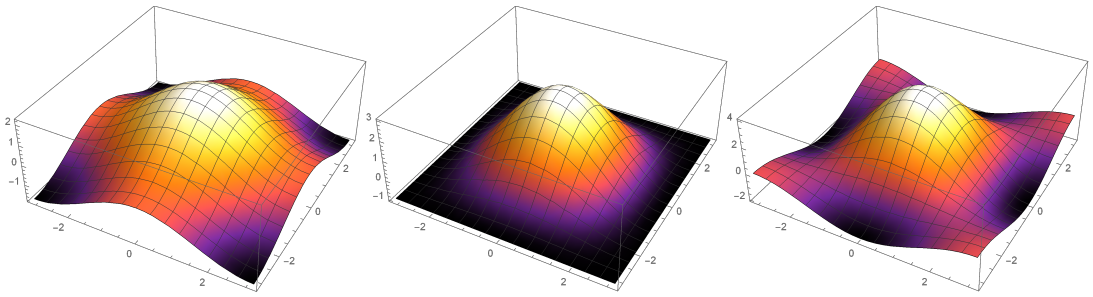


Figure 4.1: On the left, the N.N. interaction minimizes the energy of the system, at the expense of the N.N.N. interaction and vice versa on the right.

$$J_q = 2J_1\left(\cos(q_x a) + \cos(q_y a)\right) + 4J_2\cos(q_x a)\cos(q_y a), \tag{4.1.10}$$

and three representative plots for J_q are shown in Figure 4.2. As can be seen, the structure

[1] Note that it is not guaranteed that a single Q_0 minimizes the energy, i.e. the ground state may be degenerate.



(a) $J_1 = 1, J_2 = 0.2$ (b) $J_1 = 1, J_2 = 0.5$ (c) $J_1 = 1, J_2 = 1$

Figure 4.2: J_q for different values of J_1, J_2. The lattice constant a is set to one. As can be seen, at $J_2 = J_1/2$ a transition occurs, where the minimum changes position from $Q = (\pi, \pi)$ to $Q = (0, \pi), (\pi, 0)$.

vector Q_0 changes from $Q_0 = (\pi, \pi)$ to either $Q_1 = (0, \pi)$ or $Q_2 = (\pi, 0)$ as $2J_2$ is increased from $2J_2 < J_1$ to $2J_2 > J_1$. In other words, the system is now at least twice degenerate. The degeneracy is in fact even larger, due to the fact that $2Q_0$ is a reciprocal lattice vector. In such a case, the ground state is a linear combination of the solutions given by the structure vectors[3], that is

$$\mathbf{S}_i/S = \mathbf{u}\cos(Q_1 \cdot R_i)\cos(\phi) + \mathbf{v}\cos(Q_2 \cdot R_i)\sin(\phi), \tag{4.1.11}$$

where the sines of Eq. (4.1.8) are 0, due to $2Q_0 \cdot R_i = 2\pi n$, with n an integer. The ϕ is abstractly defined, since we were simply looking for some normalized linear combination of the two ground states. But it also has a physical meaning. Take a point R_i on the lattice such that $\cos(Q_1 \cdot R_i) = \cos(Q_2 \cdot R_i) = 1$, and for concreteness let this be $(0, 0)$. For the point $R_j = (1, 0)$ to the right of R_i, $\cos(Q_1 \cdot R_j) = -\cos(Q_2 \cdot R_j) = 1$. Using this we find

$$\mathbf{S}_i \cdot \mathbf{S}_j = \cos^2(\phi) - \sin^2(\phi) = \cos(2\phi). \tag{4.1.12}$$

Thus $\theta = 2\phi$ is the angle between two such neighboring spins. Furthermore, if we had chosen $R_j = (0, 1)$ we would have found that the relative angle would be $2\phi + \pi$ and for $R_j = (1, 1)$ that the relative angle would be π. Thus the ground state of the J_1-J_2 spin lattice is one of two Néel lattices with an arbitrary angle $\theta = 2\phi$ between them. When ground state is one in which $\theta = 0, \pi$ we will call it *columnar* or *collinear*. This is because the $\theta = 0$ ($\theta = \pi$) state consists of ferromagnetically aligned rows (columns) stacked antiferromagnetically.

4.2 Fluctuations - Spin waves

We will now study fluctuations about the classical ground state for both of the cases of $2Q_0$ being a reciprocal lattice vector and of $2Q_0$ not being a reciprocal lattice vector.

4.2.1 Fluctuations for $2Q_0$ not a reciprocal lattice vector

To study fluctuations about a ground state with structure vector Q_0, a state we will denote $\mathbf{S}_i^0$, we add two terms to Eq. (4.1.8) which are orthogonal to $\mathbf{S}_i^0$

$$\mathbf{S}_i = S_i^z\left(\mathbf{u}\cos(Q \cdot R_i) + \mathbf{v}\sin(Q \cdot R_i)\right) + S_i^y\left(\mathbf{u}\sin(Q \cdot R_i) - \mathbf{v}\cos(Q \cdot R_i)\right) + S_i^x\mathbf{t}, \tag{4.2.1}$$

and assume $S_y, S_x \ll S_z$. We note that the local constraint on the spin must still be respected, so

$$S_i^z = S\sqrt{1 - \left(\frac{S_i^y}{S}\right)^2 - \left(\frac{S_i^x}{S}\right)^2} \approx S\left(1 - \frac{1}{2}(Q_i^y)^2 - \frac{1}{2}(Q_i^x)^2\right), \tag{4.2.2}$$

where we defined $Q_i^a = S_i^a/S$. Up to the lowest non-zero order in the fluctuations, the energy of the system becomes

$$E = \sum_{ij} J_{ij} \left[\left(S_i^z S_j^z + S_i^y S_j^y \right) \cos(Q \cdot [R_i - R_j]) + S_i^x S_j^x - \left(S_i^z S_j^y - S_i^y S_j^z \right) \sin(Q \cdot [R_i - R_j]) \right]. \tag{4.2.3}$$

Due to translational invariance of J_{ij}, the sum over i, j could be changed for one over i, δ, with δ an index denoting the difference between two sites. It then follows straightforwardly that the factor in front of the sine term sums to zero. This, together with the fact that the ground state energy is $E_0 = S^2 \sum_{ij} J_{ij} \cos(Q \cdot [R_i - R_j])$, gives us the energy of the system up to second order in the fluctuations

$$\begin{aligned}
E &= E_0 + S^2 \sum_{ij} J_{ij} \left[\left(-\frac{1}{2} \left((Q_i^y)^2 + (Q_i^x)^2 + (Q_j^y)^2 + (Q_j^x)^2 - 2Q_i^y Q_j^y \right) \right) \cos(Q \cdot [R_i - R_j]) + Q_i^x Q_j^x \right] \\
&= E_0 - \frac{S^2}{2} \sum_{ij} J_{ij} \left[\left(\left(Q_i^y - Q_j^y \right)^2 + \left(Q_i^x - Q_j^x \right)^2 \right) \cos(Q \cdot [R_i - R_j]) \right. \\
&\qquad \left. -2Q_i^x Q_j^x \left(1 - \cos(Q \cdot [R_i - R_j]) \right) \right] \\
&= E_0 - \frac{S^2}{2N} \sum_{i\delta} J_\delta \sum_{qq'} \left[\left(Q_q^y Q_{q'}^y + Q_q^x Q_{q'}^x \right) \left(1 - e^{iq \cdot R_\delta} \right) \left(1 - e^{iq' \cdot R_\delta} \right) e^{i(q+q') \cdot R_i} \cos(Q \cdot R_\delta) \right. \\
&\qquad \left. -2Q_q^x Q_{q'}^x e^{i(q+q') \cdot R_i} e^{iq' \cdot R_\delta} \left(1 - \cos(Q \cdot R_\delta) \right) \right] \\
&= E_0 - \frac{S^2}{2} \sum_q Q_q^y Q_{-q}^y \sum_\delta J_\delta \left(2 - e^{iq \cdot R_\delta} - e^{-iq \cdot R_\delta} \right) \cos(Q \cdot R_\delta) \\
&\qquad - \frac{S^2}{2} \sum_q Q_q^x Q_{-q}^x \sum_\delta J_\delta e^{-q \cdot R_\delta} (1 - \cos(Q \cdot R_\delta)) \\
&= E_0 + S^2 \sum_q \left[\left(\frac{1}{2} \left(J_{Q+q} + J_{Q-q} \right) - J_Q \right) Q_q^y Q_{-q}^y + (J_q - J_Q) Q_q^x Q_{-q}^x \right],
\end{aligned} \tag{4.2.4}$$

where $J_q = \sum_\delta J_\delta e^{-iq \cdot R_\delta}$. Thus we have found a set of independent fluctuations that each contribute some energy to the system. To relate these to spin-waves, we must first recognize that SQ_{-q}^y and Q_q^x are canonically conjugate variables. To see this we use eq. (3.3.10). Denote $Q_q^x = Q_q$ and $SQ_{-q}^y = P_q$. Then

$$\{Q_q, P_{q'}\} = \{Q_q^x, SQ_{q'}^y\} = \frac{1}{N} \sum_{ij} e^{iq \cdot R_i} e^{iq' \cdot R_j} \{Q_i^x, SQ_j^y\} = \frac{1}{N} \sum_i e^{i(q+q') \cdot R_i} = \delta_{q,-q'}. \tag{4.2.5}$$

This can be rewritten as

$$E = E_0 + S^2 \sum_q \frac{1}{2} M_q \omega^2 Q_q Q_{-q} + \frac{P_q P_{-q}}{2S^2 M_q}, \tag{4.2.6}$$

with $M_q^{-1} = 2 \left(\frac{1}{2} \left(J_{Q+q} + J_{Q-q} \right) - J_q \right)$ and $\omega^2 = \left(\frac{1}{2} \left(J_{Q+q} + J_{Q-q} \right) - J_q \right) (J_q - J_Q)$. We now see that the energy is almost that of a set of independent harmonic oscillators. Using Hamilton's equations, we obtain the equations of motion

$$\begin{aligned}
\dot{P}_q &= S^2 M_q \omega^2 Q_{-q}, \\
\dot{Q}_q &= \frac{1}{M_q} P_{-q}.
\end{aligned} \tag{4.2.7}$$

Assuming solutions of the form $Q_q(t) = Q_q e^{i\omega' t}, P_q(t) = P_q e^{-i\omega' t}$, we obtain

$$-i\omega' P_q = S^2 M_q \omega^2 Q_{-q} = S^2 M_q \omega^2 \frac{-i}{M_{-q}\omega'} P_q \implies \omega' = \pm S\omega, \tag{4.2.8}$$

where we used $M_q = M_{-q}$. Thus the frequency of the spin-waves is

$$S|\omega_q| = S\sqrt{\left(\frac{1}{2}(J_{Q+q} + J_{Q-q}) - J_Q\right)(J_q - J_Q)}. \tag{4.2.9}$$

4.2.2 Spin-wave frequency of the J_1-J_2 model in the columnar phase

We can now apply the expression for the spin-wave frequency to the $Q = (0, \pi)$ ground state, one of the ground state structure vectors of the J_1-J_2 model with $2J_2 > J_1$. As we have seen, the Fourier transform of the exchange coupling in this model is

$$J_q = 2J_1 \left(\cos(q_x) + \cos(q_y)\right) + 4J_2 \cos(q_x)\cos(q_y), \tag{4.2.10}$$

in the case $a = 1$. Then

$$J_{Q\pm q} = 2J_1 \left(\cos(q_x) - \cos(q_y)\right) - 4J_2 \cos(q_x)\cos(q_y). \tag{4.2.11}$$

Therefore

$$\begin{aligned} \frac{1}{2}\left(J_{Q+q} + J_{Q-q}\right) - J_Q &= 4J_2 \left(1 - \cos(q_x)\cos(q_y) + \eta(\cos(q_x) - \cos(q_y))\right) \\ J_q - J_Q &= 4J_2 \left(1 + \cos(q_x)\cos(q_y) + \eta(\cos(q_x) + \cos(q_y)\right), \end{aligned} \tag{4.2.12}$$

so that we obtain the spin wave frequencies

$$\begin{aligned} 4J_2|\omega_q| &= 4J_2\sqrt{1 - \cos^2(q_x)\cos^2(q_y) + \eta^2(\cos^2(q_x) - \cos^2(q_y)) + 2\eta\cos(q_x)\sin^2(q_y)} \\ &= 4J_2\sqrt{1 - \xi_x^2\xi_y^2 + \eta^2(\xi_x^2 - \xi_y^2) + 2\eta\xi_x\overline{\xi_y}^2}, \end{aligned} \tag{4.2.13}$$

with $\eta = J_1/2J_2$ and $\xi_i = \cos(q_i a)$, $\overline{\xi}_i = \sin(q_i a)$.

4.2.3 Fluctuations for $2Q_0$ a reciprocal lattice vector

Although the method of this section follows that of the previous one, which was based on [13], [14], we have not yet seen the fluctuation spectrum derived from eq. (4.2.14) from another source.

As seen previously, when $2Q_0$ is a reciprocal lattice vector, that is when $2Q_0 \cdot R_i = 2\pi m$ with m an integer and R_i a lattice site, the ground state of the classical spin lattice is

$$\mathbf{S}_i^0/S = \mathbf{u}\cos(Q_1 \cdot R_i)\cos(\phi) + \mathbf{v}\cos(Q_2 \cdot R_i)\sin(\phi), \tag{4.2.14}$$

where Q_1, Q_2 are structure vectors with the same energy. To study fluctuations we consider the energy of the state

$$\begin{aligned} \mathbf{S}_i/S =& S_i^z \left(\mathbf{u}\cos(Q_1 \cdot R_i)\cos(\phi) + \mathbf{v}\cos(Q_2 \cdot R_i)\sin(\phi)\right) \\ &+ S_i^y \left(\mathbf{u}\cos(Q_2 \cdot R_i)\sin(\phi) + \mathbf{v}\cos(Q_1 \cdot R_i)\cos(\phi)\right) + S_i^x \mathbf{t}, \end{aligned} \tag{4.2.15}$$

where once again we assume $S_i^y, S_i^x \ll S_i^z$. Inserting this in the expression for the energy we obtain

$$E = \sum_{ij} J_{ij} \Big[(S_i^z S_j^z + S_i^y S_j^y)\mathcal{E} + S_i^x S_i^x + \cos(\phi)\sin(\phi)(S_i^z S_j^y \cos(Q_1 \cdot R_i)\cos(Q_2 \cdot R_j) - S_i^y S_j^z \cos(Q_1 \cdot R_j)\cos(Q_2 \cdot R_i)) \Big], \tag{4.2.16}$$

with $\mathcal{E} = \cos(Q_1 \cdot R_i)\cos(Q_1 \cdot R_j)\cos^2(\phi) + \cos(Q_2 \cdot R_i)\cos(Q_2 \cdot R_j)\sin^2(\phi)$. First of all, since i, j sum over the same sites they can be switched under the sum and then it is easy to see that the cross term with $S^z S^y$ cancels. Next,

$$\begin{aligned} \mathcal{E} &= \cos(Q_1 \cdot R_i)\cos(Q_1 \cdot R_j)\cos^2(\phi) + \cos(Q_2 \cdot R_i)\cos(Q_2 \cdot R_j)\sin^2(\phi) \\ &= \frac{1}{2}\left(\cos(Q_1 \cdot (R_i + R_j)) + \cos(Q_1 \cdot (R_i - R_j))\right)\cos^2(\phi) \\ &\quad + \frac{1}{2}\left(\cos(Q_2 \cdot (R_i + R_j)) + \cos(Q_2 \cdot (R_i - R_j))\right)\sin^2(\phi) \\ &= \cos(Q_1 \cdot R_\delta)\cos^2(\phi) + \cos(Q_2 \cdot R_\delta)\sin^2(\phi), \end{aligned} \tag{4.2.17}$$

where $R_\delta = R_j - R_i$ and we used $2Q_a \cdot R_i = 2\pi N$. Using that the exchange constant only depends on the distance between sites R_δ we find

$$E = \sum_{i\delta} J_\delta \left[(S_i^z S_{i+\delta}^z + S_i^y S_{i+\delta}^y)\left(\cos(Q_1 \cdot R_\delta)\cos^2(\phi) + \cos(Q_2 \cdot R_\delta)\sin^2(\phi)\right) + S_i^x S_{i+\delta}^x \right]. \tag{4.2.18}$$

Defining $E_0 = \sum_{ij} J_{ij}\mathcal{E}$ and approximating $S_i^z S_j^z \approx S^2\left(1 - \frac{1}{2}(Q_i^x + Q_{i+\delta}^x + Q_i^y + Q_{i+\delta}^y)\right)$ with $Q_i^k = S_i^k/S$, we obtain

$$\begin{aligned} E &= E_0 - \frac{S^2}{2}\sum_{i\delta} J_\delta \left[\left((Q_i^y - Q_{i+\delta}^y)^2 + (Q_i^x - Q_{i+\delta}^x)^2\right)\mathcal{E} - 2Q_i^x Q_{i+\delta}^x (1 - \mathcal{E}) \right] \\ &= E_0 - \frac{S^2}{2}\sum_{q\delta} J_\delta \left[2(Q_q^y Q_{-q}^y + Q_q^x Q_{-q}^x)(1 - \cos(q \cdot R_\delta))\mathcal{E} - 2Q_q^x Q_{-q}^x \cos(q \cdot R_\delta)(1 - \mathcal{E}) \right] \\ &= E_0 - S^2 \sum_q \left[(Q_q^y Q_{-q}^y + Q_q^x Q_{-q}^x)\left(\sum_\delta J_\delta (1 - \cos(q \cdot R_\delta))\mathcal{E}\right) - Q_q^x Q_{-q}^x \sum_\delta J_\delta \cos(q \cdot R_\delta)(1 - \mathcal{E}) \right]. \end{aligned} \tag{4.2.19}$$

Using

$$\begin{aligned} \sum_\delta J_\delta (1 - \cos(q \cdot R_\delta))\mathcal{E} &= \left[J_{Q_1} - \frac{1}{2}\left(J_{Q_1+q} + J_{Q_1-q}\right) \right]\cos^2(\phi) + \left[J_{Q_2} - \frac{1}{2}\left(J_{Q_2+q} + J_{Q_2-q}\right) \right]\sin^2(\phi), \\ \sum_\delta J_\delta \cos(q \cdot R_\delta)(1 - \mathcal{E}) &= J_q - \frac{1}{2}\left(J_{Q_1+q} + J_{Q_1-q}\right)\cos^2(\phi) - \frac{1}{2}\left(J_{Q_2+q} + J_{Q_2-q}\right)\sin^2(\phi), \end{aligned} \tag{4.2.20}$$

we find that

$$E = E_0 + S^2 \sum_q J_{Q_y} Q_q^y Q_{-q}^y + J_{Q_x} Q_q^x Q_{-q}^x, \tag{4.2.21}$$

with $J_{Q_y} = \left(\left[\frac{1}{2}\left(J_{Q_1+q} + J_{Q_1-q}\right) - J_{Q_1}\right]\cos^2(\phi) + \left[\frac{1}{2}\left(J_{Q_2+q} + J_{Q_2-q}\right) - J_{Q_2}\right]\sin^2(\phi)\right)$ and $J_{Q_x} = J_q - J_{Q_1}\cos^2(\phi) - J_{Q_2}\sin^2(\phi)$. As before, Q_q^x, SQ_{-q}^y are conjugate variables, and the spin-wave spectrum is given by

$$\omega_q^2 = S^2 J_{Q_y} J_{Q_x}, \tag{4.2.22}$$

and the system energy

$$E = E_0 + \sum_q \frac{1}{2M_q} P_q P_{-q} + \frac{1}{2} M_q \omega_q^2 Q_q Q_{-q}, \tag{4.2.23}$$

with $M_q = \frac{1}{2J_{Q_y}}$.

4.2.4 Spin-wave spectrum in the general ground state of the J_1-J_2 model

In the J_1-J_2 model the Fourier transform of the exchange coefficient is given by eq. (4.2.10). In the case $2J_2 > J_1$ the structure vectors of the ground state are $Q_1 = (0, \pi)$ and $Q_2 = (\pi, 0)$. In that case

$$\begin{aligned} &J_{Q_1} = -4J_2, \quad J_{Q_2} = -4J_2, \\ &J_{Q_1 \pm q} = 2J_1(\xi_x - \xi_y) - 4J_2 \xi_x \xi_y, \quad J_{Q_2 \pm q} = -2J_1(\xi_x - \xi_y) - 4J_2 \xi_x \xi_y, \end{aligned} \tag{4.2.24}$$

and then

$$\begin{aligned} J_{Q_x} &= 4J_2(1 + \xi_x \xi_y + \eta(\xi_x + \xi_y)) \\ J_{Q_y} &= (2J_1(\xi_x - \xi_y) - 4J_2 \xi_x \xi_y + 4J_2) \cos^2(\phi) + (-2J_1(\xi_x - \xi_y) - 4J_2 \xi_x \xi_y + 4J_2) \sin^2(\phi) \\ &= 4J_2 \left(\eta(\xi_x - \xi_y) \cos(2\phi) + 1 - \xi_x \xi_y\right), \end{aligned} \tag{4.2.25}$$

so

$$\begin{aligned} J_{Q_x} J_{Q_y} &= (4J_2)^2 \left(1 - \xi_x^2 \xi_y^2 + \cos(2\phi)\eta^2 \left(\xi_x^2 - \xi_y^2\right)\right. \\ &\quad \left. + \eta \cos(2\phi)(\xi_x(1 - \xi_y^2) - \xi_y(1 - \xi_x^2)) + \eta(\xi_y(1 - \xi_x^2) + \xi_x(1 - \xi_y^2))\right) \\ &= (4J_2)^2 \left(1 - \xi_x^2 \xi_y^2 + \cos(2\phi)\eta^2 \left(\xi_x^2 - \xi_y^2\right) + \eta(1 + \cos(2\phi))\xi_x(\bar{\xi}_y)^2 + \eta(1 - \cos(2\phi))\xi_y(\bar{\xi}_x)^2\right) \\ &= (4J_2)^2 \left(1 - \xi_x^2 \xi_y^2 + \cos(\theta)\eta^2 \left(\xi_x^2 - \xi_y^2\right) + 2\eta \left(\cos^2\left(\frac{\theta}{2}\right) \xi_x(\bar{\xi}_y)^2 + \sin^2\left(\frac{\theta}{2}\right) \xi_y(\bar{\xi}_x)^2\right)\right), \end{aligned} \tag{4.2.26}$$

where in the last line we wrote the expression in terms of the relative angle between the Néel lattices θ. Thus we have obtained the spin wave frequency

$$4J_2 S|\omega_q| = 4J_2 S \sqrt{1 - \xi_x^2 \xi_y^2 + \cos(\theta)\eta^2 \left(\xi_x^2 - \xi_y^2\right) + 2\eta \left(\cos^2\left(\frac{\theta}{2}\right) \xi_x(\bar{\xi}_y)^2 + \sin^2\left(\frac{\theta}{2}\right) \xi_y(\bar{\xi}_x)^2\right)}. \tag{4.2.27}$$

In the case where $\theta = 0$ we obtain the spin-wave frequency of the columnar phase, eq. (4.2.13).

4.3 Order by disorder - classical free energy

The classical partition function of a spin lattice is

$$Z = \int \mathcal{D}\mathbf{S} e^{-\beta \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j}, \tag{4.3.1}$$

with $\int \mathcal{D}\mathbf{S}$ denoting integration over all spin configurations at each site. Assuming the system is a J_1-J_2 spin lattice, the ground states are those of two interpenetrating Néel lattices with

an arbitrary angle between them. Let us approximate the partition function with one for the ground states and the small oscillations (spin waves) about these.

$$\int_0^{2\pi} d\theta Z(\theta), \quad Z(\theta) = e^{-\beta E_0} \int \mathcal{D}P\mathcal{D}Q e^{-\beta \sum_q \left(\frac{1}{2M_q} P_q^* P_q + \frac{1}{2} M_q (4J_2 S)^2 \omega_q^2 Q_q^* Q_q\right)}$$
$$= e^{-\beta E_0} \prod_q (2\pi M_q T) \left(\frac{2\pi T}{(4J_2 S)^2 M_q \omega_q^2}\right) = e^{-\beta E_0} \left(\frac{\pi T}{2J_2 S^2}\right)^{2N} \prod_q \frac{1}{\omega_q^2(\theta)}, \tag{4.3.2}$$

where we have carried out a Gaussian integration over P, Q. Strictly speaking, the integral should not be over a large range since we have assumed P, Q to be small numbers, but for large values of P, Q the exponent is small anyway, so the Gaussian integral is approximately equal to the partition function. The free energy is then

$$F(\theta) = -T \ln(Z(\theta)) = E_0 - 2NT \ln\left(\frac{\pi T}{2J_2 S^2}\right) + 2T \sum_q \ln(\omega_q(\theta)). \tag{4.3.3}$$

As seen, an entropy term dependent on θ emerges in the free energy. Letting

$$\sum_q \ln(\omega_q(\theta)) = N \int \frac{d^2q}{(2\pi)^2} \ln(\omega_q(\theta)), \tag{4.3.4}$$

and expanding the integrand in η we obtain

$$\ln(\omega_q(\theta)) \approx \frac{1}{2} \ln\left(1 - \xi_x^2 \xi_y^2\right) + \frac{\cos^2(\theta/2)\xi_x \bar{\xi}_y^2 + \sin^2(\theta/2)\xi_y \bar{\xi}_x^2}{1 - \xi_x^2 \xi_y^2} \eta$$
$$+ \left[\frac{\cos(\theta)(\xi_x^2 - \xi_y^2)}{2(1 - \xi_x^2 \xi_y^2)} - \frac{(\cos^2(\theta/2)\xi_x \bar{\xi}_y^2 + \sin^2(\theta/2)\xi_y \bar{\xi}_x^2)^2}{(1 - \xi_x^2 \xi_y^2)^2}\right] \eta^2. \tag{4.3.5}$$

The first order term integrates to zero due to the factors of sine- and cosine functions and the fact that the Brillouin zone extends over $(-\pi, \pi)$ in both directions. Also, because the the integration is invariant under an exchange $x \leftrightarrow y$, the first term in the square bracket η^2 also integrates to zero. Finally

$$(\cos^2(\theta/2)\xi_x \bar{\xi}_y^2 + \sin^2(\theta/2)\xi_y \bar{\xi}_x^2)^2 = \cos^4(\theta/2) \left(\xi_x \bar{\xi}_y^2\right)^2 + \sin^4(\theta/2) \left(\xi_y \bar{\xi}_x^2\right)^2$$
$$+ 2\cos^2(\theta/2) \sin^2(\theta/2) \xi_x \xi_y \bar{\xi}_x^2 \bar{\xi}_y^2, \tag{4.3.6}$$

where the cross term integrates to zero. Under the integration the integrand becomes

$$\ln(\omega_q) \approx \frac{1}{2} \ln\left(1 - \xi_x^2 \xi_y^2\right) - \frac{\eta^2(1 + \cos^2\theta)}{4} \frac{\left(\xi_x \bar{\xi}_y^2\right)^2 + \left(\xi_y \bar{\xi}_x^2\right)^2}{(1 - \xi_x^2 \xi_y^2)^2}. \tag{4.3.7}$$

Since

$$\int \frac{d^2q}{(2\pi)^2} \ln\left(1 - \xi_x^2 \xi_y^2\right) = -0.22, \quad \int \frac{d^2q}{(2\pi)^2} \frac{1}{2} \frac{\left(\xi_x \bar{\xi}_y^2\right)^2 + \left(\xi_y \bar{\xi}_x^2\right)^2}{(1 - \xi_x^2 \xi_y^2)^2} = 0.318, \tag{4.3.8}$$

we find to lowest order in η the θ dependent free energy term

$$F(\theta, \eta) - F(\theta, 0) = -0.318 \; NT \; \eta^2(1 + \cos^2\theta). \tag{4.3.9}$$

Thus we have found that when coupling the two interpenetrating Néel lattices with a coupling factor η, the free energy of the system is minimized if their relative angle is either $\theta = 0$ or $\theta = \pi$. In other words the disorder due to thermal fluctuations (spin wave fluctuations) lifts the continuous θ degeneracy of the ground state energy and replaces it with a discrete symmetry between the $\theta = 0$ and $\theta = \pi$ state.

4.4 Conclusion

The ground state of classical spin (arrow) systems have been found, and it has been shown how the J_1-J_2 square lattice has a ground state manifold consisting of coupled Néel lattices with an energetically arbitrary relative angle θ. Importantly, this ground state will be used in the next chapter to define Holstein-Primakoff bosons. It was also shown how spin waves affect the free energy of the system. In particular it was shown that a temperature dependent term arises which lifts the continuous ground state degeneracy. The new ground states are those with $\theta = 0, \pi$, and this is a manifestation of the order by disorder phenomenon.

Chapter 5

Quantized spin waves: magnons

In this section we explore quantum mechanical spin-wave excitations of the classical, degenerate ground state of the J_1-J_2 model. We have seen that in the regime $0 < J_1 < 2J_2$, the classical ground states of the frustrated lattice are those of two coupled Néel lattices, where the coupling is characterized by $\eta = J_1/(2J_2)$. The angle between the two lattices distinguishes the different ground states and does not affect the energy. As will be shown, the ground state of the quantum system is not the vacuum of quantized spin waves. This fact leads to a zero-point energy which prefers collinear states with the relative angles $\theta = 0, \pi$. Thus, similar to temperature fluctuations of the classical spin system, the "disorder" of vacuum fluctuations picks two system states from the degenerate classical subspace of ground states. This section is based on [8], [15] and appendix A of [16].

5.1 Holstein-Primakoff representation of spin-operators

We consider a square lattice with N.N. and N.N.N. coupling, $0 < J_1 < 2J_2$. The system is a Heisenberg model

$$H = \frac{1}{2}\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j. \tag{5.1.1}$$

The Holstein-Primakoff bosons (H.P. bosons) are defined through the relations

$$S^z = S - b^\dagger b, \qquad S^+ = \sqrt{2S - b^\dagger b}\, b, \qquad S^- = b^\dagger \sqrt{2S - b^\dagger b}, \tag{5.1.2}$$

which preserve the spin-algebra. As can be seen, each boson lowers the spin along the z direction by 1 and can be thought of as spin 1 bosons. As with Schwinger bosons, the Fock space associated with the bosons is larger than the Hilbert space of spin-states. The physical subspace (P.S.) of the Fock space is the space of states for which

$$\langle\rangle\, b^\dagger b\, |n\rangle = n\, |n\rangle\,, \quad n \leq 2S \;\; \forall\, |n\rangle \in \text{P.S.}. \tag{5.1.3}$$

This representation has general applicability, but is quite hard to work with due to the square root in the definition. It is useful in the case where one can make an expansion of the square root, treating $b^\dagger b/2S$ as a small parameter. To this end, one assumes some lattice configuration, usually motivated by other methods (for instance a classical calculation), and then assumes $\langle b^\dagger b\rangle /2S \ll 1$ for the states of interest. At the end of the program one must therefore make sure that this assumption is still valid. To this end, we consider a spin-configuration corresponding to a ground state of the classical system, as illustrated in Fig. 5.1, and define local frames in which the z-axes are parallel to the spins. It is with respect to these axes that the H.P. bosons are defined.

$$H = \frac{1}{2}\sum_{\substack{ij\\ab}} J_{ij}^{ab}\tilde{S}_k^{i,a} R_{kl}^{i,a} (R^{-1})_{lm}^{j,b} \tilde{S}_m^{j,b}, \tag{5.1.4}$$

where we have introduced the Euler-rotation matrices

$$\begin{aligned} R^{i,a} &= R_{xy}(\phi_{i,a})R_{yz}(\theta_{i,a}) \\ &= \begin{pmatrix} \cos\phi_i & -\sin\phi_i & 0 \\ \sin\phi_i & \cos\phi_i & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_{i,a} & -\sin\theta_{i,a} \\ 0 & \sin\theta_{i,a} & \cos\theta_{i,a} \end{pmatrix}, \\ &= \begin{pmatrix} \cos\phi_{i,a} & -\sin\phi_{i,a}\cos\theta_{i,a} & \sin\phi_{i,a}\sin\theta_{i,a} \\ \sin\phi_{i,a} & \cos\phi_{i,a}\cos\theta_{i,a} & -\cos\phi_{i,a}\sin\theta_{i,a} \\ 0 & \sin\theta_{i,a} & \cos\theta_{i,a} \end{pmatrix}, \end{aligned} \tag{5.1.5}$$

and $\tilde{\mathbf{S}}$ are spin-operators defined through the local frame of reference. The $\tilde{\mathbf{S}}$ operators fulfill the same commutation relations as the $\mathbf{S}$, since

$$\begin{aligned} [\tilde{S}^i, \tilde{S}^j] &= R^{il}R^{jm}[S^l, S^m] = i\epsilon_{lmn}R^{il}R^{jm}S^n \\ &= i\epsilon_{lmn}R^{il}R^{jm}R^{kn}\tilde{S}^k = i\epsilon_{ijk}\tilde{S}^k, \end{aligned} \tag{5.1.6}$$

where we used $\epsilon_{lmn}R^{il}R^{jm}R^{kn} = \epsilon_{ijk}\det(R) = \epsilon_{ijk}$. We have also introduced the indices ab which sum over different sublattices (i.e. $a \in 1, ..., 4$) with $a = a + 4$. For the degenerate ground state, we choose $\phi_i = 0$, which means the rotation matrices become particularly simple and, due to the property

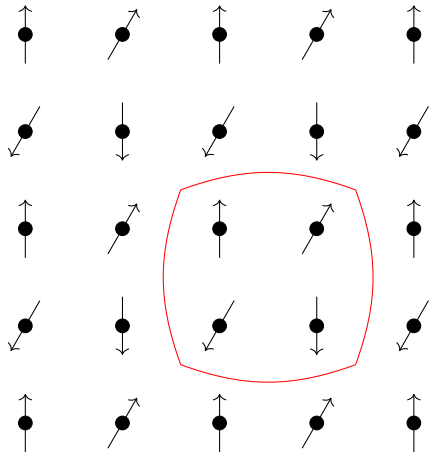


Figure 5.1: Member of the degenerate space of ground states. Inside red boundary is site i of a superlattice. The sublattice index increases in the counterclockwise direction starting topleft.

$$R_{yz}(\theta_i)R_{yz}^{-1}(\theta_j) = R_{yz}(\theta_i - \theta_j), \tag{5.1.7}$$

it is only the relative angle between the spins that is important. We will denote the angle between the upper left spin and upper right spin in the unit cell θ.

5.1.1 Nearest neighbor contribution

We now consider the N.N. coupling and denote its contribution to the Hamiltonian H_1.

$$\begin{aligned} H_1 &= \frac{J_1}{2} \sum_{\langle (i,a),(j,b)\rangle} \tilde{S}_k^{i,a} \left(R(\theta_{i,a})(R^{-1})(\theta_{j,b})\right)_{km} \tilde{S}_m^{j,b} \\ &= \frac{J_1}{2} \sum_{\langle (i,a),(j,b)\rangle} \tilde{S}_1^{i,a}\tilde{S}_1^{j,b} + \cos(\theta_{i,a} - \theta_{j,b}) \left(\tilde{S}_2^{i,a}\tilde{S}_2^{j,b} + \tilde{S}_3^{i,a}\tilde{S}_3^{j,b}\right) \\ &\qquad - \sin(\theta_{i,a} - \theta_{j,b}) \left(\tilde{S}_2^{i,a}\tilde{S}_3^{j,b} - \tilde{S}_3^{i,a}\tilde{S}_2^{j,b}\right). \end{aligned} \tag{5.1.8}$$

The two cross-terms between different components of the spin-operators is zero. To see this we note that for any (i, a) in the sum,

$$\sin(\theta_{(i,a)+\delta} - \theta_{i,a}) = \begin{cases} \sin(\pi - \theta) = \sin(\theta) & \text{if } R_{i,a} + \delta \text{ is above or below } R_{i,a} \\ \sin(-\theta) = -\sin(\theta) & \text{if } R_{i,a} + \delta \text{ is to the right or left of } R_{i,a} \end{cases}. \tag{5.1.9}$$

Where δ is a vector from site (i, a) to one of its' N.N.. Therefore, we might as well pull out the sine-function in the sum, letting the sign depend on δ and then sum over i. Now we see that the terms from a particular site coupled to the the site above it will cancel due to the relative sign between the two cross terms. This is also true of any site and the site to the right of it, and since we assume a translationally invariant system (e.g. by periodic boundaries) the whole

sum is zero.
Making a large-S approximation to order $\mathcal{O}((1/S)^{-1})$, such that

$$\tilde{S}_1^{i,a}\tilde{S}_1^{j,b} = \frac{1}{4}\left(S_+^{i,a}+S_-^{i,a}\right)\left(S_+^{j,b}+S_-^{j,b}\right) \approx \frac{S}{2}\left(b_{i,a}^\dagger b_{j,b} + b_{j,b}^\dagger b_{i,a} + b_{i,a}b_{j,b} + b_{i,a}^\dagger b_{j,b}^\dagger\right) \tag{5.1.10}$$

$$\tilde{S}_2^{i,a}\tilde{S}_2^{j,b} = \frac{-1}{4}\left(S_+^{i,a}-S_-^{i,a}\right)\left(S_+^{j,b}-S_-^{j,b}\right) \approx \frac{S}{2}\left(b_{i,a}^\dagger b_{j,b} + b_{j,b}^\dagger b_{i,a} - b_{i,a}b_{j,b} - b_{i,a}^\dagger b_{j,b}^\dagger\right) \tag{5.1.11}$$

$$\tilde{S}_3^{i,a}\tilde{S}_3^{j,b} \approx -S(b_{i,a}^\dagger b_{i,a} + b_{j,b}^\dagger b_{j,b}) + S^2, \tag{5.1.12}$$

the Hamiltonian can be written

$$H_1 = \frac{J_1}{2}\sum_{\langle(i,a),(j,b)\rangle} S\left[\frac{1+\cos(\theta_{j,b}-\theta_{i,a})}{2}\left(b_{i,a}^\dagger b_{j,b} + b_{j,b}^\dagger b_{i,a}\right) + \frac{1-\cos(\theta_{j,b}-\theta_{i,a})}{2}\left(b_{i,a}b_{j,b} + b_{j,b}^\dagger b_{i,a}^\dagger\right)\right]$$
$$+ S^2\cos(\theta_{j,b}-\theta_{i,a}) - S\cos(\theta_{j,b}-\theta_{i,a})\left(b_{i,a}^\dagger b_{i,a} + b_{j,b}^\dagger b_{j,b}\right) \tag{5.1.13}$$

We next evaluate the classical contribution to the energy, and see if there is a preferred θ that minimizes the energy. This term is the only one which is not proportional to the boson operators:

$$E_1^{cl} = \frac{J_1 S^2}{2}\sum_{\langle(i,a),(j,b)\rangle}\cos(\theta_{j,b}-\theta_{i,a}) = 0. \tag{5.1.14}$$

due to the fact that

$$\cos(\theta_{j,b}-\theta_{i,a}) = \begin{cases}\cos(\pi-\theta) = -\cos(\theta) & \text{if } R_{j,b} \text{ is above or below } R_{i,a}\\ \cos(-\theta) = \cos(\theta) & \text{if } R_{j,b} \text{ is to the right or left of } R_{i,a}\end{cases}. \tag{5.1.15}$$

This, together with the fact that the N.N.N. term in the Hamiltonian never depends on θ (this term represents a coupling between each AFM-sublattice with itself), shows that the classical ground state does not depend on θ, in correspondence with the result from chapter 4. Thus the Hamiltonian becomes

$$H_1 = \frac{J_1 S}{2}\sum_{ia,\delta}\left[\cos^2\left(\frac{\theta_{j,b}-\theta_{i,a}}{2}\right)\left(b_{i,a}^\dagger b_{j,b} + b_{j,b}^\dagger b_{i,a}\right) + \sin^2\left(\frac{\theta_{j,b}-\theta_{i,a}}{2}\right)\left(b_{i,a}b_{j,b} + b_{j,b}^\dagger b_{i,a}^\dagger\right)\right.$$
$$\left. -2\cos(\theta_{j,b}-\theta_{i,a})\left(b_{i,a}^\dagger b_{i,a} + b_{j,b}^\dagger b_{j,b}\right)\right], \tag{5.1.16}$$

where we let δ be a vector from the site (i,a) to any of its N.N., and we let b depend on the choice of δ. Next we note that the choice of δ to be horizontal or vertical corresponds to choosing sines of θ with different phases as seen from (5.1.15). Thus

$$H_1 = \frac{J_1 S}{2}\sum_{ia,\delta}\left[\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right)\left(b_{i,a}^\dagger b_{j,b} + b_{j,b}^\dagger b_{i,a}\right) + \sin^2\left(\frac{\theta+\phi(\delta)}{2}\right)\left(b_{i,a}b_{j,b} + b_{j,b}^\dagger b_{i,a}^\dagger\right)\right.$$
$$\left. -2\cos(\theta+\phi(\delta))\left(b_{i,a}^\dagger b_{i,a} + b_{j,b}^\dagger b_{j,b}\right)\right], \tag{5.1.17}$$

with $\phi(\delta) = \begin{cases} 0, & \delta = (\pm 1, 0) \\ \pi, & \delta = (0, \pm 1) \end{cases}$. Then we decompose our operators into their Fourier components:

$$\begin{aligned} H_1 = \frac{J_1 S}{2N} \sum_{ia,\delta} \sum_{qq'} \Bigg[& \cos^2\left(\frac{\theta + \phi(\delta)}{2}\right) b^\dagger_{q,a} b_{q',b} e^{i(q-q')\cdot R_{i,a}} \left(e^{-iq'\cdot\delta} + e^{iq'\cdot\delta}\right) \\ & + \sin^2\left(\frac{\theta + \phi(\delta)}{2}\right) \left(b_{q,a} b_{q',b} e^{-i(q+q)\cdot R_{i,a}} e^{-iq'\cdot\delta} + e^{i(q+q)\cdot R_{i,a}} b^\dagger_{q',b} b^\dagger_{q,a} e^{iq'\cdot\delta}\right) \\ & -4\cos(\theta + \phi(\delta)) e^{i(q-q')\cdot R_{i,a}} b^\dagger_{q,a} b_{q',a} \Bigg], \end{aligned} \tag{5.1.18}$$

where we used $b^\dagger_{q,a} b_{q',b} = b^\dagger_{q,b} b_{q',a}$ under the summation in question. Doing the i sum we obtain

$$\begin{aligned} H_1 = \frac{J_1 S}{2} \sum_{qa,\delta} \Bigg[& 2\cos^2\left(\frac{\theta + \phi(\delta)}{2}\right) \cos(q\cdot\delta) b^\dagger_{q,a} b_{q,b} + \sin^2\left(\frac{\theta + \phi(\delta)}{2}\right) \left(b_{q,a} b_{-q,b} e^{iq\cdot\delta} + b^\dagger_{-q,b} b^\dagger_{q,a} e^{-iq\cdot\delta}\right) \\ & -4\cos(\theta + \phi(\delta)) b^\dagger_{q,a} b_{q,a} \Bigg]. \end{aligned} \tag{5.1.19}$$

Finally we must do the δ sum, the result of which becomes

$$\begin{aligned} H_1 = \frac{J_1 S}{2} \sum_{qa} \Bigg[& 4\left(\cos^2\left(\frac{\theta}{2}\right) \cos(q_x) b^\dagger_{q,a} b_{q,a+\sigma(a)} + \sin^2\left(\frac{\theta}{2}\right) \cos(q_y) b^\dagger_{q,a} b_{q,a-\sigma(a)}\right) \\ & + 2\sin^2\left(\frac{\theta}{2}\right) \left(b_{q,a} b_{-q,a+\sigma(a)} + b^\dagger_{-q,a+\sigma(a)} b^\dagger_{q,a}\right) \cos(q_x) \\ & + 2\cos^2\left(\frac{\theta}{2}\right) \left(b_{q,a} b_{-q,a-\sigma(a)} + b^\dagger_{-q,a-\sigma(a)} b^\dagger_{q,a}\right) \cos(q_y) \Bigg]. \end{aligned} \tag{5.1.20}$$

Where we have defined

$$\sigma(a) = \begin{cases} 1 \text{ if even } a \\ -1 \text{ if odd } a \end{cases}.$$

The rationale behind this is that if a is odd, then a horizontal δ will connect the boson on a with one on $a-1$ and a vertical δ with one $a+1$. Vice versa for a even. We can write the Hamiltonian in a much neater form by using a vector notation

$$H_1 = \frac{J_1 S}{2} \sum_q \mathbf{b}^\dagger_q \mathbf{T}_1 \mathbf{b}_q, \tag{5.1.21}$$

with

$$\mathbf{b}^T_q = \left(b_{q,1}, ...b_{q,4}, b^\dagger_{-q,1}, ..., b^\dagger_{-q,4}\right), \quad \mathbf{T}_1 = \begin{pmatrix} \mathbf{T}_n & \mathbf{T}_{an} \\ \mathbf{T}_{an} & \mathbf{T}_n \end{pmatrix}, \tag{5.1.22}$$

and

$$\mathbf{T}_n = \begin{pmatrix} 0 & T_v & 0 & T_h \\ T_v & 0 & T_h & 0 \\ 0 & T_h & 0 & T_v \\ T_h & 0 & T_v & 0 \end{pmatrix}, \quad \mathbf{T}_{an} = \begin{pmatrix} 0 & T_{av} & 0 & T_{ah} \\ T_{av} & 0 & T_{ah} & 0 \\ 0 & T_{ah} & 0 & T_{av} \\ T_{ah} & 0 & T_{av} & 0 \end{pmatrix}, \tag{5.1.23}$$

where $T_h = 2\cos^2\left(\frac{\theta}{2}\right)\cos(q_x)$, $T_v = 2\sin^2\left(\frac{\theta}{2}\right)\cos(q_y)$ and $T_{ah} = 2\sin^2\left(\frac{\theta}{2}\right)\cos(q_x)$, $T_{av} = 2\cos^2\left(\frac{\theta}{2}\right)\cos(q_y)$

5.1.2 Next nearest neighbor contribution

Before continuing, we derive the expression for the N.N.N. contribution to the Hamiltonian, H_2. The relative angle between a spin and all of its' N.N.N. is π, and so the Hamiltonian, to the relevant order, is

$$\begin{aligned}
H_2 &= \frac{J_2}{2} \sum_{\langle\langle (i,a),(j,b)\rangle\rangle} S_x^{i,a} S_x^{j,b} - S_y^{i,a} S_y^{j,b} - S_z^{i,a} S_z^{j,b} \\
&= \frac{J_2}{2} \sum_{\substack{i\delta a \\ b=a+2}} \frac{2S}{2} \left(b_{i,a} b_{j,b} + b_{i,a}^\dagger b_{j,b}^\dagger \right) - S^2 + S(b_{i,a}^\dagger b_{i,a} + b_{j,b}^\dagger b_{j,b}) \\
&= E_2^{cl} + \frac{J_2 S}{2} \sum_{\substack{i\delta a \\ b=a+2}} \left(b_{i,a} b_{j,b} + b_{i,a}^\dagger b_{j,b}^\dagger + b_{i,a}^\dagger b_{i,a} + b_{j,b}^\dagger b_{j,b} \right) \\
&= E_2^{cl} + \frac{J_2 S}{2N} \sum_{\substack{i\delta a, qq' \\ b=a+2}} \Big[b_{a,q}^\dagger b_{a,q'} e^{i(q-q')\cdot R_{i,a}} \left(1 + e^{i(q-q')\cdot\delta} \right) \\
&\qquad\qquad + e^{-i(q+q')\cdot R_{i,a}} \left(b_{a,q} b_{b,q'} e^{iq'\cdot\delta} + b_{b,q'}^\dagger b_{a,q}^\dagger e^{-iq'\cdot\delta} \right) \Big] \\
&= E_2^{cl} + \frac{J_2 S}{2} \sum_{qa\delta} 2 b_{a,q}^\dagger b_{a,q} + \left(b_{a,q} b_{a+2,-q} e^{-iq\cdot\delta} + b_{a+2,-q}^\dagger b_{a,q}^\dagger e^{iq\cdot\delta} \right) \\
&= E_2^{cl} + \frac{J_2 S}{2} \sum_{qa} 8 b_{a,q}^\dagger b_{a,q} + 4 \left(b_{a,q} b_{a+2,-q} + b_{a+2,-q}^\dagger b_{a,q}^\dagger \right) \cos q_x \cos q_y,
\end{aligned} \tag{5.1.24}$$

with δ being a vector from site (i,a) to one of its' N.N.N. and $E_2^{cl} = -8NJ_2S^2$. To add it to the N.N. term we also write H_2 as an inner product:

$$\begin{aligned}
H_2 &= E_2^{cl} - 8J_2SN + \frac{J_2 S}{2} \sum_q \mathbf{b}_q^\dagger \mathbf{T}_2 \mathbf{b}_q \\
&\equiv E_2^{cl} + \frac{J_2 S}{2} \sum_q \mathbf{b}_q^\dagger \mathbf{T}_2 \mathbf{b}_q,
\end{aligned} \tag{5.1.25}$$

where we redefined $E_2^{cl} = -8J_2NS(S+1)$. Note that N is the number of unit cells shown in Fig. 5.1.

$$\mathbf{T}_2 = \begin{pmatrix} 4\mathbf{I} & \mathbf{T}_{an,2} \\ \mathbf{T}_{an,2} & 4\mathbf{I} \end{pmatrix}, \tag{5.1.26}$$

where $\mathbf{I}$ is the 4-by-4 identity and

$$\mathbf{T}_{an,2} = \begin{pmatrix} 0 & 0 & T_2 & 0 \\ 0 & 0 & 0 & T_2 \\ T_2 & 0 & 0 & 0 \\ 0 & T_2 & 0 & 0 \end{pmatrix}, \tag{5.1.27}$$

with $T_2 = 4\cos(q_x)\cos(q_y)$.

5.1.3 Full Hamiltonian

Collecting the two terms we obtain the full Hamiltonian

$$H = E_0^{cl} + \frac{S}{2} \sum_q \mathbf{b}_q^\dagger \left(J_1 \mathbf{T}_1 + J_2 \mathbf{T}_2 \right) \mathbf{b}_q \equiv E_0^{cl} + \frac{S}{2} \sum_q \mathbf{b}_q^\dagger \mathbf{H}(q) \mathbf{b}_q, \tag{5.1.28}$$

where $E_0^{cl} = E_1^{cl} + E_2^{cl} = -8J_2NS(S+1)$.

5.2 Canonical diagonalization

In this subsection the Hamiltonian will be diagonalized. Since $\mathbf{H}$ is a hermitian matrix, the Hamiltonian can straightforwardly be diagonalized by inserting factors of the unitary diagonalizing matrix U in the Hamiltonian

$$\mathbf{b}_q^\dagger UU^\dagger \mathbf{H}(q) UU^\dagger \mathbf{b}_q \equiv \mathbf{a}_q^\dagger \mathbf{D} \mathbf{a}_q, \tag{5.2.1}$$

with $\mathbf{a}_q = U^\dagger \mathbf{b}_q$. The issue with this procedure is that the new operators $\mathbf{a}_q$ are not bosonic, as can be straightforwardly shown. To sensibly diagonalize the Hamiltonian, that is in terms of bosonic operators, another procedure for diagonalization must be used, *canonical diagonalization*, and the transformation we will use to do this is called a *Bogoliubov transformation*. The procedure is as follows: arbitrary transformation matrices are defined and we will put constraints on these so as to ensure that the operators defined through these matrices are bosonic. Due to these constraints, the matrices will have certain properties and these kinds of matrices can be chosen so as to diagonalize $\mathbf{H}$ [15] .

5.2.1 Bogoliubov transformation

The first step is to define new operators and demand they be bosonic. We define the following two 8×8-matrices in terms of four 4×4-matrices

$$\begin{aligned} \mathcal{A} &= \begin{pmatrix} \mathcal{U}(q) & \mathcal{S}(q) \\ \mathcal{V}(q) & \mathcal{T}(q) \end{pmatrix} \\ \mathcal{A}' &= \begin{pmatrix} \tilde{\mathcal{U}}(q) & \tilde{\mathcal{V}}(q) \\ \tilde{\mathcal{S}}(q) & \tilde{\mathcal{T}}(q) \end{pmatrix}, \end{aligned} \tag{5.2.2}$$

where $\mathcal{U}, \mathcal{V}, \mathcal{S}, \mathcal{T}$ and $\tilde{\mathcal{U}}, \tilde{\mathcal{V}}, \tilde{\mathcal{S}}, \tilde{\mathcal{T}}$ are 4×4 matrices. Through these matrices we define new boson operators

$$\begin{aligned} \boldsymbol{\beta}_q^\dagger &= \left(\beta_{1,q}^\dagger, ..., \beta_{4,q}^\dagger, \beta_{1,-q}, ..., \beta_{4,-q}\right) = \mathbf{b}_q^\dagger \mathcal{A} \\ \boldsymbol{\alpha}_q &= \left(\alpha_{1,q}, ..., \alpha_{4,q}, \alpha_{1,-q}^\dagger, ..., \alpha_{4,-q}^\dagger\right) = \mathcal{A}' \mathbf{b}_q. \end{aligned} \tag{5.2.3}$$

Then the new operators can be written (using implicit summation of repeated indices) as

$$\begin{aligned} \beta_{i,q}^\dagger &= b_{j,q}^\dagger \mathcal{U}_{ji}(q) + b_{j,-q} \mathcal{V}_{ji}(q), \quad \beta_{i,-q} = b_{j,q}^\dagger \mathcal{S}_{ji}(q) + b_{j,-q} \mathcal{T}_{ji}(q) \\ \alpha_{i,q} &= \tilde{\mathcal{U}}_{ij}(q) b_{j,q} + \tilde{\mathcal{V}}_{ij}(q) b_{j,-q}^\dagger, \quad \alpha_{i,-q}^\dagger = \tilde{\mathcal{S}}_{ij}(q) b_{j,q} + \tilde{\mathcal{T}}_{ij}(q) b_{j,-q}^\dagger. \end{aligned} \tag{5.2.4}$$

These matrices are going to be used to diagonalize the Hamiltonian, in the same way as unitary matrices U are usually used. Therefore, since $\mathbf{H}(q) = \mathbf{H}(-q)$, it must be such that $\mathcal{A}(q) = \mathcal{A}(-q)$ and similarly for $\mathcal{A}'$. The following things are required for the new operators to be bosonic:

- $\beta_{i,q} = \alpha_{i,q}, \;\; \beta_{i,q}^\dagger = \alpha_{i,q}^\dagger$
- $(\beta_{i,q})^\dagger = \beta_{i,q}^\dagger$
- $[\beta_{i,q}, \beta_{j,q'}^\dagger] = \delta_{ij}\delta_{qq'}$ and $[\beta_{i,q}, \beta_{j,q'}] = [\beta_{i,q}^\dagger, \beta_{j,q'}^\dagger] = 0$.

First we demand that

$$\begin{aligned} \alpha_{i,q} &= \tilde{\mathcal{U}}_{ij}(q) b_{j,q} + \tilde{\mathcal{V}}_{ij}(q) b_{j,-q}^\dagger = b_{j,-q}^\dagger \mathcal{S}_{ji}(-q) + b_{j,q} \mathcal{T}_{ji}(-q) = \beta_{i,q} \\ \alpha_{i,q}^\dagger &= \tilde{\mathcal{S}}_{ij}(-q) b_{j,-q} + \tilde{\mathcal{T}}_{ij}(-q) b_{j,q}^\dagger = b_{j,q}^\dagger \mathcal{U}_{ji}(q) + b_{j,-q} \mathcal{V}_{ji}(q) = \beta_{i,q}^\dagger. \end{aligned} \tag{5.2.5}$$

This yields

$$(\tilde{\mathcal{V}})^T(q) = \mathcal{S}(-q),\ \ (\tilde{\mathcal{U}})^T(q) = \mathcal{T}(-q),\ \ (\tilde{\mathcal{S}})^T(q) = \mathcal{V}(-q),\ \ (\tilde{\mathcal{T}})^T(q) = \mathcal{U}(-q). \tag{5.2.6}$$

This, together with the fact that the matrices are even around $q = 0$ means they can be written

$$\mathcal{A} = \begin{pmatrix} \mathcal{U} & \tilde{\mathcal{V}}^T \\ \mathcal{V} & \tilde{\mathcal{U}}^T \end{pmatrix}, \quad \mathcal{A}' = \begin{pmatrix} \tilde{\mathcal{U}} & \tilde{\mathcal{V}} \\ \mathcal{V}^T & \mathcal{U}^T \end{pmatrix}, \tag{5.2.7}$$

where the q dependency is implicit. Then the second requirement also yields the constraint

$$(\beta_{i,q})^\dagger = (\tilde{\mathcal{U}}_{ij} b_{j,q} + \tilde{\mathcal{V}}_{ij} b^\dagger_{j,-q})^\dagger = \tilde{\mathcal{U}}^*_{ij} b^\dagger_{j,q} + \tilde{\mathcal{V}}^*_{ij} b_{j,-q} = b^\dagger_{j,q} \mathcal{U}_{ji} + b_{j,-q} \mathcal{V}_{ji} = \beta^\dagger_{i,q}, \tag{5.2.8}$$

such that

$$\tilde{\mathcal{U}}^\dagger = \mathcal{U}, \quad \tilde{\mathcal{V}}^\dagger = \mathcal{V}, \tag{5.2.9}$$

and

$$\mathcal{A} = \begin{pmatrix} \mathcal{U} & \mathcal{V}^* \\ \mathcal{V} & \mathcal{U}^* \end{pmatrix}, \quad \mathcal{A}' = \begin{pmatrix} \mathcal{U}^\dagger & \mathcal{V}^\dagger \\ \mathcal{V}^T & \mathcal{U}^T \end{pmatrix}, \tag{5.2.10}$$

where we note that we have obtained

$$\mathcal{A}' = \mathcal{A}^\dagger. \tag{5.2.11}$$

If we define $\mathcal{F} = \begin{pmatrix} 0 & \mathcal{I} \\ \mathcal{I} & 0 \end{pmatrix}$, where $\mathcal{I}$ is the 4×4 identity matrix, we also note that

$$\mathcal{F}\mathcal{A}\mathcal{F} = \mathcal{A}^*. \tag{5.2.12}$$

This property we call $\mathcal{F}$-canonical conjugacy of the vectors making up the columns of $\mathcal{A}$. Finally we need the third criterion to be met

$$\begin{aligned} \delta_{ij} = [\beta_{i,q}, \beta^\dagger_{j,q}] &= \left[\mathcal{U}^*_{ik} b_{k,q} + \mathcal{V}^*_{ik} b^\dagger_{k,-q}, b^\dagger_{l,q} \mathcal{U}_{lj} + b_{l,-q} \mathcal{V}_{lj}\right] \\ &= \mathcal{U}^*_{ik} \mathcal{U}_{kj} - \mathcal{V}^*_{ik} \mathcal{V}_{kj}, \end{aligned} \tag{5.2.13}$$

or simply

$$\mathcal{U}^\dagger \mathcal{U} - \mathcal{V}^\dagger \mathcal{V} = \mathcal{I}, \tag{5.2.14}$$

for any q. Also we see that

$$\begin{aligned} 0 = [\beta_{i,q}, \beta_{j,-q}] &= \left[\mathcal{U}^*_{ik} b_{k,q} + \mathcal{V}^*_{ik} b^\dagger_{k,-q}, \mathcal{U}^*_{jl} b_{l,-q} + \mathcal{V}^*_{jl} b^\dagger_{l,q}\right] \\ &= -\mathcal{V}^*_{ik} \mathcal{U}^*_{jk} + \mathcal{U}^*_{ik} \mathcal{V}^*_{jk} \implies \mathcal{V}\mathcal{U}^T - \mathcal{U}\mathcal{V}^T = 0, \end{aligned} \tag{5.2.15}$$

From these equations, we make the observation that

$$\mathcal{A}^\dagger \mathcal{G} \mathcal{A} = \mathcal{G}, \tag{5.2.16}$$

where

$$\mathcal{G} = \begin{pmatrix} \mathcal{I} & 0 \\ 0 & -\mathcal{I} \end{pmatrix}. \tag{5.2.17}$$

which, using $\mathcal{G}^2 = \mathcal{I}$, is straightforwardly seen to be equivalent to

$$\mathcal{A}^{-1} = \mathcal{G}\mathcal{A}^\dagger\mathcal{G}, \quad \mathcal{A}\mathcal{G}\mathcal{A}^\dagger = \mathcal{G}. \tag{5.2.18}$$

Due to these properties we call $\mathcal{A}$ $\mathcal{G}$-paraunitary. Thus we have seen that imposing the constraint on the new operators that they be bosonic is equivalent to assuming that the transformation matrices, $\mathcal{A}$, are $\mathcal{G}$-paraunitary and $\mathcal{F}$-canonically consistent.

Now, if $\mathcal{A}$ is $\mathcal{G}$-paraunitary and is made of columns of $\mathcal{F}$-canonically consistent vectors, then so is $\mathcal{G}\mathcal{A}\mathcal{G}$. Thus we could define a new matrix

$$\mathcal{B} = \mathcal{G}\mathcal{A}\mathcal{G}, \tag{5.2.19}$$

which is also $\mathcal{G}$-paraunitary and $\mathcal{F}$-canonically consistent, since

$$\mathcal{F}\mathcal{B}\mathcal{F} = \mathcal{F}\mathcal{G}\mathcal{F}\mathcal{F}\mathcal{A}\mathcal{F}\mathcal{F}\mathcal{G}\mathcal{F} = (-1)^2\mathcal{G}\mathcal{A}^*\mathcal{G} = (\mathcal{G}\mathcal{A}\mathcal{G})^* = \mathcal{B}^*. \tag{5.2.20}$$

Therefore we have a set of matrices obeying the following relations

$$\begin{aligned} \mathcal{B} &= \mathcal{G}\mathcal{A}\mathcal{G}, \quad & \mathcal{B}^{-1} &= \mathcal{A}^\dagger \\ \mathcal{A} &= \mathcal{G}\mathcal{B}\mathcal{G}, \quad & \mathcal{A}^{-1} &= \mathcal{B}^\dagger. \end{aligned} \tag{5.2.21}$$

Also note that if either $\mathcal{A}$ or $\mathcal{B}$ has an inverse, the other one is guaranteed to have an inverse. Assuming for example $\mathcal{B}$ to have an inverse:

$$1 = \mathcal{B}^{-1}\mathcal{B} = \mathcal{B}^{-1}\mathcal{G}\mathcal{A}\mathcal{G} \implies 1 = (\mathcal{G}\mathcal{B}^{-1}\mathcal{G})\mathcal{A}, \tag{5.2.22}$$

i.e. $\mathcal{A}^{-1} = \mathcal{G}\mathcal{B}^{-1}\mathcal{G}$.

5.2.2 Diagonalizing H

Having established the necessary qualities of the transformation matrices, the expression for the Hamiltonian is rewritten

$$H = E_0^{cl} + \frac{S}{2}\sum_q \mathbf{b}_q^\dagger\mathcal{G}\mathbf{M}\mathbf{b}_q \tag{5.2.23}$$

where $\mathbf{M} \equiv \mathcal{G}\mathbf{H}$. One can prove[15] that such a matrix $\mathbf{M}$ may be diagonalizable with a $\mathcal{G}$-orthonormal basis. The eigenbasis can also be chosen to be $\mathcal{F}$-canonically consistent if

$$\mathbf{M}^* = -\mathcal{F}\mathbf{M}\mathcal{F} \implies \mathbf{H}^* = \mathbf{H} = \mathcal{F}\mathbf{H}\mathcal{F}, \tag{5.2.24}$$

which is true of our Hamiltonian matrix. In this case, the eigenvalues of $\mathbf{M}$ come in pairs with opposite sign, and the eigenvectors associated with each eigenvalues have opposite $\mathcal{G}$-norm, defined for a vector $\mathbf{v}$ as

$$\mathbf{v}^\dagger \cdot (\mathcal{G}\mathbf{v}) = \pm 1. \tag{5.2.25}$$

Notice that it is not guaranteed that the eigenvector with positive $\mathcal{G}$-norm has a positive eigenvalue. One caveat to the proof, associated with this fact, will be considered in a moment. With this in mind we insert factors of the $\mathcal{G}$-orthonormal, $\mathcal{F}$-canonically consistent matrix $\mathcal{B}$ *which diagonalizes* $\mathbf{M}$ and whose first four column vectors have positive $\mathcal{G}$-norm, into H,:

$$\begin{aligned} H &= E_0^{cl} + \frac{S}{2}\sum_q \mathbf{b}_q^\dagger\mathcal{G}\mathcal{B}\mathcal{B}^{-1}\mathbf{M}\mathcal{B}\mathcal{B}^{-1}\mathbf{b}_q = E_0^{cl} + \frac{S}{2}\sum_q \mathbf{b}_q^\dagger\mathcal{G}\mathcal{B}\begin{pmatrix}\boldsymbol{\omega} & 0\\ 0 & -\boldsymbol{\omega}\end{pmatrix}\mathcal{B}^{-1}\mathbf{b}_q \\ &= E_0^{cl} + \frac{S}{2}\sum_q \mathbf{b}_q^\dagger\mathcal{A}\mathcal{G}\begin{pmatrix}\boldsymbol{\omega} & 0\\ 0 & -\boldsymbol{\omega}\end{pmatrix}\mathcal{A}^\dagger\mathbf{b}_q = E_0^{cl} + \frac{S}{2}\sum_q \boldsymbol{\beta}_q^\dagger\begin{pmatrix}\boldsymbol{\omega} & 0\\ 0 & \boldsymbol{\omega}\end{pmatrix}\boldsymbol{\beta}_q \\ &= E_0^{cl} + S\sum_{a,q}\omega_{a,q}\left(\beta_{a,q}^\dagger\beta_{a,q} + 1/2\right), \end{aligned} \tag{5.2.26}$$

where $\omega_{a,q}$, the elements of $\boldsymbol{\omega}$, are the eigenvalues associated with the positive $\mathcal{G}$-norm eigenvectors of $\mathbf{M}$, where we used $\omega_{a,q} = \omega_{a,-q}$ and where $\mathcal{A} = \mathcal{G}\mathcal{B}\mathcal{G}$. As we have shown, $\mathcal{A}$ defined like this is $\mathcal{G}$-orthonormal and $\mathcal{F}$-canonically consistent, and the new operators are therefore genuine bosonic operators. Now comes the caveat of the diagonalization procedure. It is now clear that it is essential that $\omega_{a,q}$ all be positive. If they are not, the system is unstable towards creation of the quasi-particles, signaling that this type of diagonalization is not possible.

A few notes before moving on. We have to choose $\mathcal{B}$ to be the matrix that diagonalizes $\mathbf{M}$ such that the first four columns of $\mathcal{B}$ have positive $\mathcal{G}$-norm, and the last four have negative $\mathcal{G}$-norm. This is due to (5.2.14). Then, if the first four columns have positive $\mathcal{G}$-norm, the last four will have negative $\mathcal{G}$-norm. This is because the last four columns are the $\mathcal{F}$-canonically conjugate of the first four, and the because $\mathcal{F}$-switches the sign of a vectors' $\mathcal{G}$-norm, due to $\mathcal{F}\mathcal{G}\mathcal{F} = -\mathcal{G}$.
We finally note, that the a index no longer can refer to a specific sublattice, since the Bogoliubov quasiparticles are linear combinations of the H.P. bosons defined on different sublattices. We thus simply treat a as another quantum number.

5.2.3 Eigenvalues

We now set out to find the eigenvalues of $\mathbf{M}$. The first step is to write out the Hamiltonian matrix $\mathbf{H}$ in terms of Pauli-matrices in three different two dimensional spaces. We will denote Pauli matrices in these spaces σ, τ, λ, and as usual a zero index denotes the identity. Then

$$\begin{aligned}\mathbf{T}_1 &= \mathbf{T}_n \otimes \lambda_0 + \mathbf{T}_{an} \otimes \lambda_1,\\ \mathbf{T}_n &= T_h\sigma_1 \otimes \tau_1 + T_v\sigma_1 \otimes \tau_0\\ \mathbf{T}_{an} &= T_{ah}\sigma_1 \otimes \tau_1 + T_{av}\sigma_1 \otimes \tau_0,\end{aligned} \tag{5.2.27}$$

and

$$\begin{aligned}\mathbf{T}_2 &= 4\sigma_0 \otimes \tau_0 \otimes \lambda_0 + \mathbf{T}_{an,2} \otimes \lambda_1\\ \mathbf{T}_{an,2} &= T_2\sigma_0 \otimes \tau_1.\end{aligned} \tag{5.2.28}$$

One can then write $\mathbf{H} = J_1\mathbf{T}_1 + J_2\mathbf{T}_2$. But we are interested in $\mathbf{M}$ and, as one can straightforwardly check from $\mathcal{G}\mathbf{H} = \mathbf{M}$, this can be written as

$$\mathbf{M} = J_1\left(\mathbf{T}_n \otimes \lambda_3 + \mathbf{T}_{an} \otimes (i\lambda_2)\right) + J_2\left(4\sigma_0 \otimes \tau_0 \otimes \lambda_3 + \mathbf{T}_{an,2} \otimes (i\lambda_2)\right). \tag{5.2.29}$$

From now on we will omit the $\otimes$ symbol and let it be implicit. Also, if no Pauli-matrices appear in a term, it is implicitly multiplied by all three identities. Next we square $\mathbf{M}$:

$$\begin{aligned}\mathbf{M}^2 = J_1^2\left[\left(\mathbf{T}_n^2 - \mathbf{T}_{an}^2\right)\lambda_0 + \mathbf{T}_n\mathbf{T}_{an}\lambda_3(i\lambda_2) + \mathbf{T}_{an}\mathbf{T}_n(i\lambda_2)\lambda_3\right] + J_2^2\left[(4^2 - \mathbf{T}_{an,2}^2)\lambda_0 - \mathbf{T}_{an,2}\{\lambda_3, (i\lambda_2)\}\right]\\ + J_1J_2\left[2(4\mathbf{T}_n)\lambda_0 + \mathbf{T}_n\mathbf{T}_{an,2}\lambda_3(i\lambda_2) + \mathbf{T}_{an,2}\mathbf{T}_n(i\lambda_2)\lambda_3 + 4\mathbf{T}_{an,2}\{i\lambda_2, \lambda_3\} - \{\mathbf{T}_{an}, \mathbf{T}_{an,2}\}\lambda_0\right].\end{aligned} \tag{5.2.30}$$

We will now make use of the identity

$$AB\sigma_i\sigma_j + BA\sigma_j\sigma_i = AB\{\sigma_i, \sigma_j\} - [A, B]\sigma_i\sigma_j, \tag{5.2.31}$$

where A and B are matrices in the space and σ are Pauli-matrices in a different space. Using this the following relations are true

$$\begin{aligned}&[\mathbf{T}_n, \mathbf{T}_{an}] = T_hT_{ah} + T_vT_{av} + (T_vT_{ah} + T_hT_{av})\sigma_0\tau_1 - (T_hT_{ah} + T_vT_{av} + (T_vT_{ah} + T_hT_{av})\sigma_0\tau_1) = 0\\ &[\mathbf{T}_n, \mathbf{T}_{an,2}] = T_2T_h\left[\sigma_1\tau_1, \sigma_0\tau_1\right] + T_2T_v\left[\sigma_1\tau_0, \sigma_0\tau_1\right] = 0\\ &\{\mathbf{T}_{an}, \mathbf{T}_{an,2}\} = T_2T_h\{\sigma_1\tau_1, \sigma_0\tau_1\} + T_2T_{ah}\{\sigma_1\tau_0, \sigma_0\tau_1\} = 2T_2\left(T_{ah}\sigma_1\tau_0 + T_{av}\sigma_1\tau_1\right).\end{aligned} \tag{5.2.32}$$

Using all of this, together with the fact that different Pauli-matrices anti-commute we obtain

$$\mathbf{M}^2 = \left(J_1^2\left[\mathbf{T}_n^2 - \mathbf{T}_{an}^2\right] + J_2^2\left[4^2 - \mathbf{T}_{an,2}^2\right] + J_1J_2\left[2(4\mathbf{T}_n) - 2T_2\left(T_{ah}\sigma_1\tau_0 + T_{av}\sigma_1\tau_1\right)\right]\right)\lambda_0. \tag{5.2.33}$$

Next we find

$$\mathbf{T}_n^2 = T_h^2 + T_v^2 + 2T_hT_v\sigma_0\tau_1 \qquad \mathbf{T}_{an}^2 = T_{ah}^2 + T_{av}^2 + 2T_{ah}T_{av}\sigma_0\tau_1, \tag{5.2.34}$$

and using $T_hT_v = T_{ah}T_{av}$, it is clear that

$$\mathbf{T}_n^2 - \mathbf{T}_{an}^2 = T_h^2 + T_v^2 - T_{ah}^2 - T_{av}^2 = 4\left(\cos^4(\theta/2) - \sin^4(\theta/2)\right)\left(\xi_x^2 - \xi_y^2\right) = 4\cos(\theta)\left(\xi_x^2 - \xi_y^2\right), \tag{5.2.35}$$

where $\xi_i = \cos(q_i)$. Also

$$\mathbf{T}_{an,2}^2 = T_2^2 = 4^2\xi_x^2\xi_y^2. \tag{5.2.36}$$

Putting this together we find

$$\begin{aligned}\mathbf{M}^2 &= M_0 + 2J_1J_2\left[(4T_v - T_2T_{ah})\sigma_1\tau_0 + (4T_h - T_2T_{av})\sigma_1\tau_1\right]\lambda_0 \\ &\equiv M_0 + 2J_1J_2\left[\kappa_v\sigma_1\tau_0 + \kappa_h\sigma_1\tau_1\right]\lambda_0,\end{aligned} \tag{5.2.37}$$

and $M_0 = 4J_1^2\cos(\theta)\left(\xi_x^2 - \xi_y^2\right) + (4J_2)^2(1 - \xi_x^2\xi_y^2)$. Then

$$(\mathbf{M}^2 - M_0)^2 = 4J_1^2J_2^2\left[\kappa_h^2 + \kappa_v^2 + 2\kappa_h\kappa_v\sigma_0\tau_1\right] = M_1 + 4J_1^2J_2^2(2\kappa_h\kappa_v)\sigma_0\tau_1. \tag{5.2.38}$$

Therefore

$$((\mathbf{M}^2 - M_0)^2 - M_1)^2 = (4J_1^2J_2^2)^2\kappa_h^2\kappa_v^2 \implies (\mathbf{M}^2 - M_0)^2 = M_1 \pm 4J_1^2J_2^2\kappa_h\kappa_v = (2J_1J_2)^2\left(\kappa_h \pm \kappa_v\right)^2. \tag{5.2.39}$$

Using

$$\kappa_h = 4T_h - T_2T_{av} = 8\cos^2(\theta/2)\xi_x(1 - \xi_y^2), \qquad \kappa_v = 4T_v - T_2T_{ah} = 8\sin^2(\theta/2)\xi_y(1 - \xi_x^2), \tag{5.2.40}$$

and defining $(\overline{\xi}_i)^2 = 1 - \xi_i^2$, we obtain

$$\begin{aligned}\mathbf{M}^2 &= M_0 \pm 2J_1J_2(\kappa_h \pm \kappa_v) \\ &= 4J_1^2\cos(\theta)\left(\xi_x^2 - \xi_y^2\right) + (4J_2)^2(1 - \xi_x^2\xi_y^2) \pm 16J_1J_2\left(\cos^2(\theta/2)\xi_x(\overline{\xi}_y)^2 \pm \sin^2(\theta/2)\xi_y(\overline{\xi}_x)^2\right) \\ &= (4J_2)^2\left(\left(\frac{J_1}{2J_2}\right)^2\cos(\theta)\left(\xi_x^2 - \xi_y^2\right) + (1 - \xi_x^2\xi_y^2) \pm 2\frac{J_1}{2J_2}\left(\cos^2(\theta/2)\xi_x(\overline{\xi}_y)^2 \pm \sin^2(\theta/2)\xi_y(\overline{\xi}_x)^2\right)\right) \\ &= (4J_2)^2\left((1 - \xi_x^2\xi_y^2) + \eta^2\cos(\theta)\left(\xi_x^2 - \xi_y^2\right) \pm 2\eta\left(\cos^2(\theta/2)\xi_x(\overline{\xi}_y)^2 \pm \sin^2(\theta/2)\xi_y(\overline{\xi}_x)^2\right)\right).\end{aligned} \tag{5.2.41}$$

This implies the eigenvalues of $\mathbf{M}$ are the positive and negative square root of the expression on the right side of Eq. (5.2.41). The energies of the bosons is the positive choice of the square root, which is

$$\begin{aligned}&4J_2\ \omega_{a,q}(\theta) \\ &\quad = 4J_2\sqrt{\left(1 - \xi_x^2\xi_y^2\right) + \eta^2\cos(\theta)\left(\xi_x^2 - \xi_y^2\right) \pm 2\eta\left(\cos^2(\theta/2)\xi_x\left(\overline{\xi_y}\right)^2 \pm \sin^2(\theta/2)\xi_y\left(\overline{\xi_x}\right)^2\right)},\end{aligned} \tag{5.2.42}$$

with $\eta = \frac{J_1}{2J_2}$, $\xi_i = \cos(q_i)$ and $\overline{\xi_i} = \sin(q_i)$.

What should be noted at this point, is that within the reduced Brillouin zone $q \in (\pi/2, \pi/2)$, the four spectra overlap. That is taking one of the spectra, say the one with only positive signs for each term, and folding it into the reduced Brillouin zone by the identification $q_i = q_i + \pi$, we obtain the same bands as in the case of folding all four spectra into the reduced zone. Note that the spectrum is equivalent to the classical spectrum in the reduced zone, as it should be.

5.2.4 Vacuum fluctuations and breaking degeneracy

As seen before, the classical contribution to the energy of the system is not affected by the relative angle θ between the two AFM sublattices. The spectra of the bosonic excitations, however, do depend on θ and therefore so does the zero-point energy of each excitation mode. The collective zero-point energy can be evaluated numerically, resulting in the energies shown in Fig. 5.2

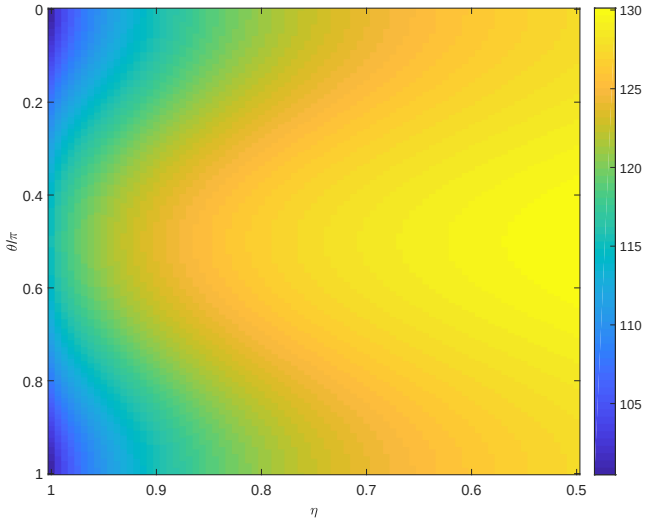
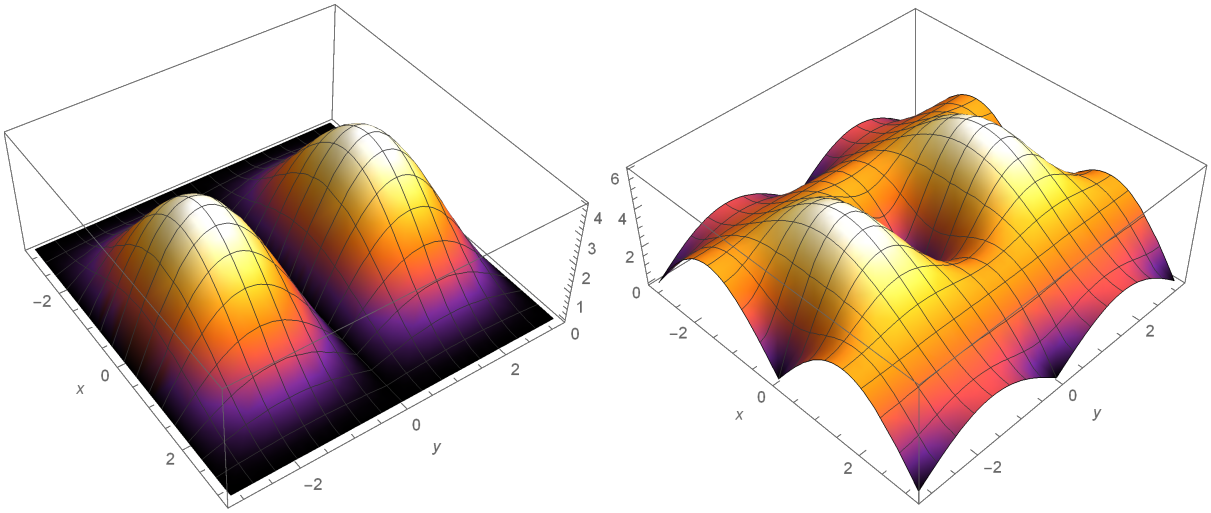


Figure 5.2: Plot of the results of a numerical integration of the sum of the energy spectra. Here J_1=1, and θ is the relative angle between sublattices. Minimum for all η is at $\theta = 0$, and $\theta = \pi$. As can be seen, it becomes less energetically advantageous to be at an optimal θ as η decreases, reflecting the decoupling of the two AFM sublattices for large η.

We can also expand the zero-point energy to smallest non-zero order in η

$$\begin{aligned} 2J_2S\sum_{q,a}\omega_{a,q} &\approx 4N2J_2S\int\frac{d^2q}{(2\pi)^2}\left[\sqrt{1-\xi_x^2\xi_y^2}-\eta^2(1+\cos^2\theta)\frac{(\xi_x(\overline{\xi}_y)^2)^2+(\xi_y(\overline{\xi}_y)^2)^2}{8(1-\xi_x^2\xi_y^2)^{3/2}}\right] \\ &= 4N2J_2S[\kappa_Q-\eta^2(1+\cos^2\theta)\frac{\gamma_Q}{2}], \end{aligned} \tag{5.2.43}$$

with $\kappa_Q = 0.842$ and $\gamma_Q = 0.130$. The factor of 4 in front of N is from summing all four spectra. We conclude that the quantum fluctuations pick out the states with $\theta = 0, \pi$ as the two degenerate ground states for the system. As η decreases, the coupling between the two AFM sublattices becomes still more negligible, and therefore the ground state depends less and less on θ. On Fig. 5.3 is shown the spectrum of one of the bosonic excitations with $\theta = 0$.



(a) $\eta = 1$ (b) $\eta = 0.5$

Figure 5.3: Energy spectrum with the choice of two positive relative signs in the expression for $\omega_{a,q}$. Here $\theta = 0$. A choice of $\theta = \pi$ will in general flip the figure 90 degrees counterclockwise.

5.2.5 Group velocity of low energy modes

Let us for a moment consider only the low energy eigenstates of the system, and let us restrict ourselves to $\theta = 0$ based on the results of the effect of vacuum fluctuations in section 5.2.4. We could analyse the spectrum in the proximity of either of the points $q = (0,0), (\pi,0), (0,\pi), (\pi,\pi)$ but for now we consider $q = (0,0)$. The results for other momenta are similar, since a shift $q_i \to q_i + \pi$ at most changes signs of ξ_i. Then we find

$$\omega_{a,q} \approx \sqrt{q^2 - \eta^2(q_x^2 - q_y^2) \pm 2\eta q_y^2} = \sqrt{(1-\eta^2)q^2 + 2(\eta^2 \pm \eta)q_y^2}. \tag{5.2.44}$$

There is manifestly a difference between the x-, and y-directions in the energy, which is a result of the choice of $\theta = 0$ and not $\theta = \pi$. Notice, that when $\eta = 1$, the highly frustrated point, there is no energy dependence on q_x. That is, we get a whole spectrum of zero-energy modes, which is worrisome when considering the validity of the large-S expansion. Let us now look at the group velocity of the system excitations,

$$\begin{aligned} v_y &= \frac{\partial \omega_{a,q}}{\partial q_y} = \frac{1}{\omega_{a,q}}(1 - \eta^2 + 2\eta^2 \pm 2\eta)q_y = \frac{1}{\omega_{a,q}}(1 \pm \eta)^2 q_y \\ v_x &= \frac{\partial \omega_{a,q}}{\partial q_x} = \frac{1}{\omega_{a,q}}(1 - \eta^2)q_x. \end{aligned} \tag{5.2.45}$$

First of all, in every expression so far we have set $a = \hbar = 1$ for simplicity, with a being the lattice constant. To get back to regular units, we must multiply the velocity with $4J_2\hbar a$. Next, notice that, at $q_x = 0$

$$v_y = \frac{1}{\sqrt{(1 \pm \eta)^2 q_y^2}}(1 \pm \eta)^2 q_y = 1 \pm \eta, \tag{5.2.46}$$

that is, we have a linear dispersion for $q_x = 0$ and q_y small. Similarly for $q_y = 0$

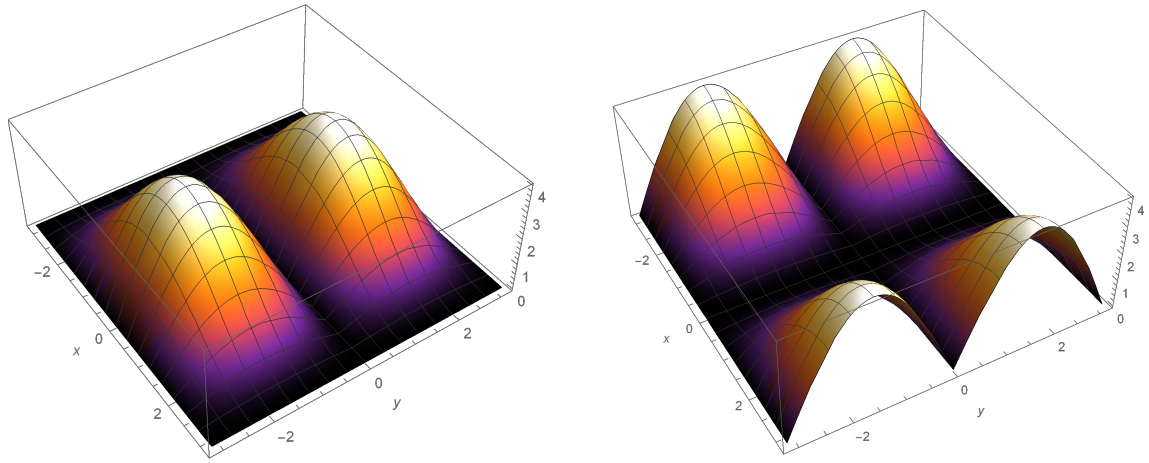
$$v_x = \sqrt{1 - \eta^2}. \tag{5.2.47}$$

What we see now is, that as $\eta \to 1$ the velocity along x goes to zero, but for two of the spectra, those that have group velocity $v_y = 1 + \eta$, the velocity goes to 2. Thus, as we enter the strongly

frustrated region, only two low-energy excitations have a finite velocity, and this will be constant in the y-direction. More generally, we may look at the fraction

$$\frac{v_y}{v_x} = \frac{1 \pm \eta}{1 \mp \eta} \frac{q_y}{q_x}, \tag{5.2.48}$$

where the sign in the denominator depends on the sign in the numerator. This shows, that when keeping q_y, q_x fixed and non-zero, v_y becomes much greater than v_x as $\eta \to 1$ for the excitations with positive sign choice in their eigenvalue. All in all, the quasi-particles move only in the y-direction at the fully frustrated point $\eta = 1$.



(a) ω^+-spectrum (b) ω^--spectrum

Figure 5.4: Dispersion relation for the excitations. Here $\theta = 0$ and $\eta = 1$ for greater illustrative effect. As can be seen, near $q = (0,0), (\pi,0), (0,\pi), (\pi,\pi)$, in the q_x direction the band is always flat.

5.3 Order by disorder - quantum free energy

Just like in the classical case, we will now consider the partition function and the contribution to the free energy due to spin waves. Assuming that a set of ground states exist composed of two decoupled, Néel ordered sublattices, these states will dominate in the low temperature limit. The partition function is again an integral over the partition functions for each of these ground states and their excitations. Thus we need to find

$$Z(\theta) = e^{-E_0^{cl}} \oint \mathcal{D}\{\phi^*, \phi\} \exp\left(-S \sum_{q,\omega_n} \phi^*_{q,\omega_n} (-i\omega_n + 4J_2\omega_q(\theta))\phi_{q,\omega_n} + 2J_2\beta\omega_q(\theta) \right), \tag{5.3.1}$$

where the summation over sublattices is implicit. Evaluating the path integral yields

$$Z(\theta) = e^{-\beta E_0^{cl}} \prod_{q,\omega_n} e^{-\beta 2J_2 S\omega_q(\theta)} \frac{1}{S\beta(-i\omega_n + 4J_2\omega_q(\theta))}. \tag{5.3.2}$$

Instead of evaluating the product, we go directly to the free energy which is

$$\begin{aligned} F(\theta) &= E_0^{cl} + 2J_2 S \sum_{\alpha,q} \omega_{q,\alpha}(\theta) + \frac{1}{\beta} \sum_{q,\omega_n} \ln\left(\beta S(-i\omega_n + 4J_2\omega_q(\theta))\right) \\ &= E_0^{cl} + 2J_2 S \sum_{q} \omega_q(\theta) + \frac{1}{\beta} \sum_{q} \ln\left(1 - e^{-\beta S 4 J_2 \omega_q}\right), \end{aligned} \tag{5.3.3}$$

where what is a product in the partition function is a Matsubara sum in the free energy and has been evaluated by the standard method of integration over the complex plane with the summand expanded to an integrand with an additional factor of a Bose-function. At this point it is useful to scale out S by the identification $J_i S^2 = \overline{J_i}$. Since the parameters are free for us to choose, we can choose them such that $\overline{J_i}$ is independent of S. Then the free energy is

$$F(\theta) = E_0^{cl} + \frac{2\overline{J_2}}{S}\sum_q \omega_q(\theta) + \frac{1}{\beta}\sum_q \ln\left(1 - e^{-\frac{\beta}{S}4\overline{J_2}\omega_q}\right). \tag{5.3.4}$$

We may now consider the classical limit,

$$\overline{J_2}\beta/S \ll 1 \implies \overline{J_2} \ll TS, \tag{5.3.5}$$

such that the relevant temperature is in fact TS and the classical limit may be reached by either increasing T or S. Thus in the large S limit we find

$$\begin{aligned} F(\theta) &\approx E_0^{cl} + \frac{\overline{2J_2}}{S}\sum_q \omega_q(\theta) + \frac{1}{\beta}\sum_q \ln\left(4\overline{J_2}\beta\omega_q(\theta)/S\right) \\ &= E_0^{cl} + NT\ln\left(4\overline{J_2}/TS\right) + \frac{2\overline{J_2}}{S}\sum_q\left(\omega_q(\theta) + \frac{TS}{2\overline{J_2}}\ln(\omega_q(\theta))\right) \\ &\equiv E_0^{cl} + NT\ln\left(4\overline{J_2}/TS\right) + F_Q(\theta) + F_T(\theta). \end{aligned} \tag{5.3.6}$$

As we see, we obtain two terms, one identical to the free energy from classical spin waves, and one from the magnon zero point energy. Note that this is only the case in the large TS limit, where bosonic statistics approaches classical statistics of distinguishable particles. We also see a contribution to the free energy solely due to quantum fluctuations which does not depend on temperature. The free energy may also be written in the more compact form

$$F(\theta) = E_0^{cl} + NT\ln(2) + T\sum_q \ln\left(\sinh\left(\frac{2\overline{J_2}\omega_q}{TS}\right)\right). \tag{5.3.7}$$

By expanding eq. (5.3.6) in η and keeping only lowest non-zero orders in η, similar to how it was done in eq. (4.3.9), we find that

$$F(\theta,\eta) - F(\theta,0) \approx -(4N)(2\overline{J_2})\ \eta^2(1+\cos^2\theta)\left(\gamma_Q\frac{1}{2S} + \gamma_T\frac{T}{2\overline{J_2}}\right), \tag{5.3.8}$$

where $\gamma_Q = 0.130$ and $\gamma_T = 0.159$. The factor of four in front of N is due to the implicit summation over sublattice indices. We now see that for any finite T, the large S limit will render the thermal contribution to the free energy dominant already seen for classical spin-waves. The free energy is now minimized both due to quantum and thermal fluctuations.

5.4 Symmetries and the eigenvectors

As seen, the system minimizes its ground-state energy by choosing $\theta = 0, \pi$, where θ is the relative angle between Néel sublattices. Assuming it has picked one of these states, we can go back to the Hamiltonian (or $\mathbf{M}$) and find its' eigenvectors. Choose $\theta = 0$. Then $T_h = 2\cos(q_x)$, $T_{av} = 2\cos(q_y)$ and $T_v = T_{ah} = 0$, and this yields

$$\begin{aligned}\mathbf{M} &= T_h\sigma_1\tau_1\lambda_3 + T_{av}\sigma_1\tau_0(i\lambda_2) + (4J_2)\,\sigma_0\tau_0\lambda_3 + T_2\sigma_0\tau_1(i\lambda_2)\\ &= (2J_1\xi_x)\,\sigma_1\tau_1\lambda_3 + (2J_1\xi_y)\,\sigma_1\tau_0(i\lambda_2) + (4J_2)\,\sigma_0\tau_0\lambda_3 + 4J_2\xi_x\xi_y\sigma_0\tau_1(i\lambda_2).\end{aligned} \tag{5.4.1}$$

What is apparent now, is that $\mathbf{M}$ commutes with the following operators

$$A = \sigma_3\tau_3\lambda_3 \tag{5.4.2}$$
$$B = \sigma_1\tau_0\lambda_0 \tag{5.4.3}$$
$$C = \sigma_0\tau_1\lambda_0. \tag{5.4.4}$$

We can use these symmetries to provide constraints on the eigenvectors of $\mathbf{M}$, and ultimately find an expression for these. As will be seen, this is only possible because $\mathbf{M}$ is reducible from an 8×8 matrix to a 2×2 matrix in the cases $\theta = 0, \pi$. This is what we should expect since in these cases the unit cell has been reduced from four spins to two. We could also find an expression for H in the case $\theta = 0, \pi$ and Bogoliubov transform this expression to find the eigenvectors.

5.4.1 Eigenvectors

Since $\theta = 0$, we see from Eq. (5.2.42) that every eigenvalue is twice degenerate. When we say $\mathbf{M}$ is diagonalizable we assume that the whole vector space is spanned by the eigenvectors. This means first that each eigenspace of the twice degenerate eigenvalues must be two-dimensional, and second that the two dimensional subspaces of each degenerate eigenvalue span the whole vector space. Now take an eigenvector of $\mathbf{M}$ with eigenvalue ω, and assume it to be in the very general form

$$\mathbf{v}^T = \begin{pmatrix} a & b & c & d & e & f & g & h\end{pmatrix} \tag{5.4.5}$$

Then, since A commutes with $\mathbf{M}$

$$\mathbf{M}\,(A\mathbf{v}) = A\mathbf{M}\mathbf{v} = \omega\,(A\mathbf{v})\,. \tag{5.4.6}$$

That is $A\mathbf{v}$ lives in the eigenspace of ω. The explicit form of this vector is

$$(A\mathbf{v})^T = \begin{pmatrix} a & -b & -c & d & -e & f & g & -h\end{pmatrix}. \tag{5.4.7}$$

Now we can make a much simpler eigenvector of $\mathbf{M}$ which also has eigenvalue ω:

$$\mathbf{v}' = \frac{1}{2}(\mathbf{v} + A\mathbf{v}) = \begin{pmatrix} a & 0 & 0 & d & 0 & f & g & 0\end{pmatrix}. \tag{5.4.8}$$

Next, use that B, C also commute with $\mathbf{M}$. Then

$$\begin{aligned}CB\mathbf{v}' &= \begin{pmatrix} d & 0 & 0 & a & 0 & g & f & 0\end{pmatrix},\\ B\mathbf{v}' &= \begin{pmatrix} 0 & a & d & 0 & f & 0 & 0 & g\end{pmatrix}\end{aligned} \tag{5.4.9}$$

both live in the eigenspace with eigenvalue ω. The second of these two vectors is orthogonal to $\mathbf{v}'$, and these two vectors could therefore make up a nice basis for the eigenspace. The next step is to create two new vectors

$$\begin{aligned}\mathbf{v}_1 &= \mathbf{v}' + CB\mathbf{v}' = \begin{pmatrix} a+d & 0 & 0 & d+a & 0 & f+g & g+f & 0\end{pmatrix}\\ \mathbf{v}_2 &= \mathbf{v}' - CB\mathbf{v}' = \begin{pmatrix} a-d & 0 & 0 & d-a & 0 & f-g & g-f & 0\end{pmatrix}.\end{aligned} \tag{5.4.10}$$

These vectors are orthogonal and both are orthogonal to $B\mathbf{v}'$. The subspace is two dimensional, so one of the three vectors must be the zero vector. If $B\mathbf{v}'$ is, all of them are, so either $\mathbf{v}_1$ or $\mathbf{v}_2$ must be zero. This is equivalent to the condition

$$a = d, f = g \text{ or } a = -d, f = -g. \tag{5.4.11}$$

Thus we conclude that an eigenvector of the subspace associated with ω can be written as

$$\mathbf{v}' = \begin{pmatrix} a & 0 & 0 & \pm a & 0 & b & \pm b & 0 \end{pmatrix}. \tag{5.4.12}$$

where we renamed f. For each of the two possible eigenspaces with positive eigenvalue, an eigenvector of the form $\mathbf{v}'$ can be chosen, and an orthogonal one with the same eigenvalue may be made through the B-operator. Each of these four eigenvectors in turn generate a new eigenvector (with an eigenvalue of opposite sign) through the operator $\mathcal{F}$ which anticommutes with $\mathbf{M}$. Thus we have reduced the problem of finding eight-eigenvectors, with 32 independent parameters, to finding just 4 independent parameters.
We end this subsection by noting the following properties of A on the eigenvectors

$$\begin{aligned} A\mathbf{v}' &= \mathbf{v}' \\ A\left(B\mathbf{v}'\right) &= -BA\mathbf{v}' = -B\mathbf{v}'. \end{aligned} \tag{5.4.13}$$

The last equation is due to $\{A, B\} = 0$.

5.4.2 Finding a, b

To find a, b we start by noting, that the 8×8 representation of $\mathbf{M}$ must obviously be reducible due to the form of the eigenvectors. In fact, the eigenvalue equation is reducible to two equivalent 4×4 matrix equations, namely

$$\begin{pmatrix} 4J_2 & T_h & T_{av} & T_2 \\ T_h & 4J_2 & T_2 & T_{av} \\ -T_{av} & -T_2 & -4J_2 & -T_h \\ -T_2 & -T_{av} & -T_h & -4J_2 \end{pmatrix} \cdot \begin{pmatrix} a \\ \pm a \\ b \\ \pm b \end{pmatrix} = \lambda^{\pm} \begin{pmatrix} a \\ \pm a \\ b \\ \pm b \end{pmatrix}. \tag{5.4.14}$$

This can be reduced further to

$$\begin{pmatrix} 4J_2 \pm T_h & T_{av} \pm T_2 \\ -\left(T_{av} \pm T_2\right) & -\left(4J_2 \pm T_h\right) \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} M_3^{\pm} & M_2^{\pm} \\ -M_2^{\pm} & -M_3^{\pm} \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} = \lambda^{\pm} \begin{pmatrix} a \\ b \end{pmatrix}. \tag{5.4.15}$$

There are two eigenvalues of this matrix, with the same length but opposite sign. The positive eigenvalue is

$$\begin{aligned} \lambda^{\pm} &= \sqrt{(M_3^{\pm})^2 - (M_2^{\pm})^2} = \sqrt{(4J_2 \pm T_h)^2 - (T_{av} \pm T_2)^2} \\ &= \sqrt{(4J_2 \pm T_h + T_{av} \pm T_2)\,(4J_2 \pm T_h - T_{av} \mp T_2)} \\ &= 4J_2\sqrt{1 - \xi_x^2\xi_y^2 + \eta^2\left(\xi_x^2 - \xi_y^2\right) \pm \frac{1}{(4J_2)^2}\left(\left(T_h + T_{av}\right)\left(4J_2 \mp T_2\right) + \left(T_h - T_{av}\right)\left(4J_2 \pm T_2\right)\right)} \\ &= 4J_2\sqrt{1 - \xi_x^2\xi_y^2 + \eta^2\left(\xi_x^2 - \xi_y^2\right) \pm \eta\left(\left(\xi_x + \xi_y\right)\left(1 \mp \xi_x\xi_y\right) + \left(\xi_x - \xi_y\right)\left(1 \pm \xi_x\xi_y\right)\right)} \\ &= 4J_2\sqrt{1 - \xi_x^2\xi_y^2 + \eta^2\left(\xi_x^2 - \xi_y^2\right) \pm 2\eta\xi_x(1 - \xi_y^2)} = 4J_2\sqrt{1 - \xi_x^2\xi_y^2 + \eta^2\left(\xi_x^2 - \xi_y^2\right) \pm 2\eta\xi_x(\overline{\xi}_y)^2}, \end{aligned} \tag{5.4.16}$$

gives us exactly the eigenvalues we expect in the case of $\theta = 0$. Thus we see $\lambda^{\pm} = 4J_2\omega^{\pm}$, the two positive eigenvalues of $\mathbf{M}$. Furthermore, the (unnormalized) eigenvector with this eigenvalue is

$$\psi_+ = \begin{pmatrix} M_3^{\pm} + \lambda^{\pm} \\ -M_2^{\pm} \end{pmatrix}. \tag{5.4.17}$$

Thus we have found

$$a = M_3^{\pm} + \lambda^{\pm}, \quad b = -M_2^{\pm}. \tag{5.4.18}$$

We could now check whether it is in fact true, that all positive eigenvalue eigenstates have positive $\mathcal{G}$-norm. This amounts to checking whether

$$2\left(a^2 - b^2\right) = 2\left((M_3^{\pm} + \lambda^{\pm})^2 - (M_2^{\pm})^2\right) = 4\left((\lambda^{\pm})^2 + M_3^{\pm}\lambda^{\pm}\right) = 4\lambda^{\pm}\left(\lambda^{\pm} + M_3^{\pm}\right), \tag{5.4.19}$$

is positive. Now $\lambda^{\pm}$ is always positive, and since $M_3^{\pm} = 4J_2\left(1 \pm \eta\cos(q_x)\right)$, we conclude $\lambda^{\pm}\left(\lambda^{\pm} + M_3^{\pm}\right) \geq 0$. Thus, the positive eigenvalue eigenstates do in fact have positive $\mathcal{G}$-norm. Note however that states with zero eigenvalue have zero $\mathcal{G}$-norm[1]. The eigenvectors generated by $\mathcal{F}$ have $\mathcal{G}$-norm

$$2\left(b^2 - a^2\right), \tag{5.4.20}$$

which is then automatically negative or zero. To sum up we have found that indeed the eigenvectors of positive $\mathcal{G}$-norm have positive eigenvalues, and that therefore $\mathbf{M}$ is diagonalizable, with a $\mathcal{G}$-normalized eigenbasis, except for the points where $\omega^{\pm} = 0$. In fact, since our current analysis was based on the eigenstates being only twice degenerate, we cannot extend this solution of eigenvectors to the case of $\omega^{\pm} = 0$. For all cases with twice-degenerate eigenvalues, the eigenvectors have been found, and with $\mathcal{G}$-normalization we found that

$$a = 1/4\lambda^{\pm}, \quad b = -\frac{M_2^{\pm}}{4\lambda^{\pm}(\lambda^{\pm} + M_3^{\pm})} \tag{5.4.21}$$

5.4.3 The case of four-times degenerate eigenvalues

Had we picked the specific values of $q = (q_x, 0), (q_x, \pi)$, the eigenvalues would have in fact been four times degenerate. We used twofold degeneracy in arguing why either $\mathbf{v}_1$ or $\mathbf{v}_2$ must be zero. The symmetries still hold, so we may assume again that

$$\begin{aligned} \mathbf{v}' &= \begin{pmatrix} a & 0 & 0 & d & 0 & f & g & 0 \end{pmatrix} \\ CB\mathbf{v}' &= \begin{pmatrix} d & 0 & 0 & a & 0 & g & f & 0 \end{pmatrix}. \end{aligned} \tag{5.4.22}$$

Either $CB\mathbf{v}'$ is proportional to $\mathbf{v}'$, in which case we are back to the situation from earlier, or it is not. Assuming it is not, we may generate two new vectors

$$\begin{aligned} \mathbf{v}_1 &= \mathbf{v}' + CB\mathbf{v}' = \begin{pmatrix} a+d & 0 & 0 & d+a & 0 & f+g & g+f & 0 \end{pmatrix} \\ \mathbf{v}_2 &= \mathbf{v}' - CB\mathbf{v}' = \begin{pmatrix} a-d & 0 & 0 & d-a & 0 & f-g & g-f & 0 \end{pmatrix} \end{aligned} \tag{5.4.23}$$

These two vectors are both orthogonal

$$\mathbf{v}_1^{\dagger} \cdot \mathbf{v}_2 = (a^* + d^*)(a - d) + (a^* + d^*)(d - a) + (f^* + g^*)(f - g) + (f^* + g^*)(g - f) = 0 \tag{5.4.24}$$

and $\mathcal{G}$ orthogonal

$$\mathbf{v}_1^{\dagger} \cdot \mathcal{G}\mathbf{v}_2 = (a^* + d^*)(a - d) + (a^* + d^*)(d - a) - (f^* + g^*)(f - g) - (f^* + g^*)(g - f) = 0, \tag{5.4.25}$$

and they are exactly of the same form as the vectors considered earlier. What is different is that now we cannot assume either one to be zero. But this does not matter. Before we had a two dimensional subspace, and we showed that in that subspace, an eigenvector must have the form of $\mathbf{v}'$, and proceeded from there. Now we a have four dimensional subspace, and since we have no restriction that either $\mathbf{v}_1$ or $\mathbf{v}_2$ are zero, and they are orthogonal, they are simply two eigenvectors spanning half the eigenspace. We generate the two others through B, and the four vectors of the other eigenspace through $\mathcal{F}$. From there we may then continue the analysis as before.

[1] It is unclear at this point how to deal with this in a rigorous way. We will not discuss it further in this thesis.

5.4.4 The $\mathcal{U}_q, \mathcal{V}_q$-matrices

Now that we know the explicit form of the eigenvectors, we may construct explicitly the matrix $\mathcal{B}$ and by extension $\mathcal{A}$. The columns of $\mathcal{B}$ are the eigenvectors of $\mathbf{M}$ so

$$\begin{pmatrix} \mathcal{U}_q \\ -\mathcal{V}_q \end{pmatrix} = \begin{pmatrix} \frac{M_3^+ + \lambda^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & \frac{M_3^- + \lambda^-}{4\lambda^-(\lambda^- + M_3^-)} & 0 \\ 0 & \frac{M_3^+ + \lambda^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & \frac{M_3^- + \lambda^-}{4\lambda^-(\lambda^- + M_3^-)} \\ 0 & \frac{M_3^+ + \lambda^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & -\frac{M_3^- + \lambda^-}{4\lambda^-(\lambda^- + M_3^-)} \\ \frac{M_3^+ + \lambda^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & -\frac{M_3^- + \lambda^-}{4\lambda^-(\lambda^+ + M_3^-)} & 0 \\ 0 & -\frac{M_2^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & -\frac{M_2^-}{4\lambda^+(\lambda^- + M_3^-)} \\ -\frac{M_2^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & -\frac{M_2^-}{4\lambda^-(\lambda^- + M_3^-)} & 0 \\ -\frac{M_2^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & \frac{M_2^-}{4\lambda^-(\lambda^- + M_3^-)} & 0 \\ 0 & -\frac{M_2^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & \frac{M_2^-}{4\lambda^-(\lambda^- + M_3^-)} \end{pmatrix}, \tag{5.4.26}$$

or

$$\mathcal{U}_q = \begin{pmatrix} \frac{1}{4\lambda^+} & 0 & \frac{1}{4\lambda^-} & 0 \\ 0 & \frac{1}{4\lambda^+} & 0 & \frac{1}{4\lambda^-} \\ 0 & \frac{1}{4\lambda^+} & 0 & -\frac{1}{4\lambda^-} \\ \frac{1}{4\lambda^+} & 0 & -\frac{1}{4\lambda^-} & 0 \end{pmatrix}$$

$$\mathcal{V}_q = \begin{pmatrix} 0 & \frac{M_2^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & \frac{M_2^-}{4\lambda^-(\lambda^- + M_3^-)} \\ \frac{M_2^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & \frac{M_2^-}{4\lambda^-(\lambda^- + M_3^-)} & 0 \\ \frac{M_2^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & -\frac{M_2^-}{4\lambda^-(\lambda^- + M_3^-)} & 0 \\ 0 & \frac{M_2^+}{4\lambda^+(\lambda^+ + M_3^+)} & 0 & -\frac{M_2^-}{4\lambda^-(\lambda^- + M_3^-)} \end{pmatrix}. \tag{5.4.27}$$

The matrices $\mathcal{V}_q\mathcal{V}_q^\dagger$ and $-\mathcal{V}_q\mathcal{U}_q^\dagger$ tell us about spin-spin correlations, as is shown in appendix C, and are therefore written for future reference.

$$\mathcal{V}_q\mathcal{V}_q^\dagger = \begin{pmatrix} V_+ & 0 & 0 & V_- \\ 0 & V_+ & V_- & 0 \\ 0 & V_- & V_+ & 0 \\ V_- & 0 & 0 & V_+ \end{pmatrix}, \tag{5.4.28}$$

and

$$V_\pm = \frac{(T_{av} + T_2)^2}{4\lambda^+(\lambda^+ + M_3^+)} \pm \frac{(T_{av} - T_2)^2}{4\lambda^-(\lambda^- + M_3^-)}, \tag{5.4.29}$$

due to the normalization of the eigenvectors. Similarly

$$\mathcal{V}_q\mathcal{U}_q^\dagger = \begin{pmatrix} 0 & U_+ & U_- & 0 \\ U_+ & 0 & 0 & U_+ \\ U_- & 0 & 0 & U_- \\ 0 & U_+ & U_- & 0 \end{pmatrix}. \tag{5.4.30}$$

Again

$$U_\pm = \frac{(T_{av} + T_2)}{4\lambda^+} \pm \frac{(T_{av} - T_2)}{4\lambda^-} \tag{5.4.31}$$

5.5 Conclusion

We have used Holstein-Primakoff bosons to find the magnon excitations of the classical ground state of the $J_1 - J_2$ square lattice. Just as in the classical case, the magnonic fluctuations pick out the angles $\theta = 0, \pi$ between the Néel lattices as the ground states of the system. Contrary to the classical case where only thermal fluctuations existed, the quantum fluctuations pick out these angles even at zero temperature. It was also seen that the four independent spectra we found are equivalent when folded into the reduced Brillouin zone, going from $q_i = -\pi/2$ to $q_i = \pi/2$ suggesting we could abandon the four sublattice picture altogether and just define H.P. bosons on a single lattice. This we will do in the next chapter to solve for the eigenvectors of a general (arbitrary θ) state.

Chapter 6

Magnons on one lattice

Having established that the sublattice picture yields four copies of the same spectrum in the reduced Brillouin zone, we will replicate the analysis based on Holstein-Primakoff bosons on a single lattice. This analysis yields much simpler expressions which we aim to use to tackle the first non-linear term in the $1/S$-expansion.

As will be shown, quantum fluctuations do not destroy long range magnetic order for $\eta < 1$ but steadily become stronger as $\eta \longrightarrow 1$ and eventually destroy magnetic order at $\eta = 1$. On the other, hand thermal fluctuations destroy the order for any η, in compliance with the Mermin-Wagner theorem. By introducing an infrared cutoff, magnetic order is preserved even for thermal fluctuations, but only when $\eta < 1$. At the fully frustrated point $\eta = 1$ the magnetic order is destroyed both by quantum and thermal fluctuations and this cannot be mitigated by any cutoff. The role of the infrared cutoff will be more fully explored in section 7.2, but amounts to assuming the system is finite sized.

6.1 Canonical diagonalization

Starting from a Hamiltonian identical to the one in eq (5.1.4) except without sublattice indices, and carrying out a similar analysis one finds the expression

$$\begin{aligned} H &= E_0^{cl} + \frac{S}{2}\sum_q \left(b_q^\dagger b_q + b_{-q} b_{-q}^\dagger\right) J_n + \left(b_q b_{-q} + b_{-q}^\dagger b_q^\dagger\right) J_{an} \\ &= E_0^{cl} + \frac{S}{2}\sum_q \left(b_q^\dagger, b_{-q}\right) \begin{pmatrix} J_n & J_{an} \\ J_{an} & J_n \end{pmatrix} \begin{pmatrix} b_q \\ b_{-q}^\dagger \end{pmatrix} = E_0^{cl} + \frac{S}{2}\sum_q \left(b_q^\dagger, b_{-q}\right) \mathcal{G} \begin{pmatrix} J_n & J_{an} \\ -J_{an} & -J_n \end{pmatrix} \begin{pmatrix} b_q \\ b_{-q}^\dagger, \end{pmatrix} \end{aligned} \tag{6.1.1}$$

where

$$\begin{aligned} J_n &= J_1\left(\cos(q_x) + \cos(q_y) + \cos(\theta)(\cos(q_x) - \cos(q_y))\right) + 4J_2 \\ J_{an} &= J_1\left(\cos(q_x) + \cos(q_y) - \cos(\theta)(\cos(q_x) - \cos(q_y))\right) + 4J_2\cos(q_x)\cos(q_y), \end{aligned} \tag{6.1.2}$$

$E_0^{cl} = -2NJ_2S(S+1)$ and $\mathcal{G} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Analogously to what was done in the case of four sublattices, we now diagonalize $\mathbf{M} = \begin{pmatrix} J_n & J_{an} \\ -J_{an} & -J_n \end{pmatrix}$. One can check that the unnormalized (with respect to $\mathcal{G}$) eigenvectors are

$$\psi_+ = \begin{pmatrix} J_n + 4J_2\omega_q \\ -J_{an} \end{pmatrix}, \quad \psi_- = \mathcal{F}\psi_+ = \begin{pmatrix} -J_{an} \\ J_n + 4J_2\omega_q \end{pmatrix}, \tag{6.1.3}$$

where

$$\omega_q = \sqrt{J_n^2 - J_{an}^2}/4J_2 = \sqrt{1 - \xi_x^2\xi_y^2 + \eta^2\cos(\theta)(\xi_x^2 - \xi_y^2) + 2\eta\left(\cos^2(\theta/2)\xi_x\overline{\xi}_y^2 + \sin^2(\theta/2)\xi_y\overline{\xi}_x^2\right)}, \tag{6.1.4}$$

and the eigenvalues of $\psi_\pm$ are $\pm 4J_2\omega_q$. These eigenvalues are easily found by squaring $\mathbf{M}$, similarly to what was done in the case of four sublattices. As can be seen, ω_q is identical to one of the four spectra found in the four sublattice picture. Next, the $\mathcal{G}$ norm of the eigenvectors are

$$\mathcal{N}_\pm = \langle\psi_\pm|\mathcal{G}\psi_\pm\rangle = \pm 2(4J_2\omega_q)(J_n + 4J_2\omega_q). \tag{6.1.5}$$

It is the $\mathcal{G}$-normalized eigenvectors that constitute the columns of the diagonalizing matrices. Note that the vectors are normalized with respect to the absolute value of their $\mathcal{G}$-norm, which in this case is common between the two eigenvectors. We denote this $\mathcal{N}$. Defining

$$\mathcal{B} = \frac{1}{\sqrt{\mathcal{N}}}\begin{pmatrix} J_n + 4J_2\omega_q & -J_{an} \\ J_{an} & J_n + 4J_2\omega_q \end{pmatrix}, \tag{6.1.6}$$

we can diagonalize the Hamiltonian

$$\begin{aligned} H &= E_0^{cl} + 2J_2S\sum_q \left(b_q^\dagger, b_{-q}\right)\mathcal{G}\mathcal{B}\begin{pmatrix}\omega_q & 0\\ 0 & -\omega_q\end{pmatrix}\mathcal{B}^{-1}\begin{pmatrix} b_q \\ b_{-q}^\dagger\end{pmatrix} \\ &= E_0^{cl} + 2J_2S\sum_q \left(b_q^\dagger, b_{-q}\right)\mathcal{A}\begin{pmatrix}\omega_q & 0\\ 0 & \omega_q\end{pmatrix}\mathcal{A}^\dagger\begin{pmatrix} b_q \\ b_{-q}^\dagger\end{pmatrix} \\ &= E_0^{cl} + 4J_2S\sum_q \omega_q\left(\beta_q^\dagger\beta_q + \frac{1}{2}\right), \end{aligned} \tag{6.1.7}$$

where $\mathcal{A} = \mathcal{G}\mathcal{B}\mathcal{G}$ and we used that $\mathbf{M}(q) = \mathbf{M}(-q)$. The new operators are defined as

$$\left(\beta_q^\dagger, \beta_{-q}\right) = \left(b_q^\dagger, b_{-q}\right)\mathcal{A} = \frac{1}{\sqrt{\mathcal{N}}}\left((J_n + 4J_2\omega_q)b_q^\dagger + J_{an}b_{-q}, J_{an}b_q^\dagger + (J_n + 4J_2\omega_q)b_{-q}\right), \tag{6.1.8}$$

and one can check that these are in fact bosonic. Using $\mathcal{A}^{-1} = \mathcal{G}\mathcal{A}^\dagger\mathcal{G}$, we find the opposite relation

$$\left(b_q^\dagger, b_{-q}\right) = \frac{1}{\sqrt{\mathcal{N}}}\left((J_n + 4J_2\omega_q)\beta_q^\dagger - J_{an}\beta_{-q}, -J_{an}\beta_q^\dagger + (J_n + 4J_2\omega_q)\beta_{-q}\right) \tag{6.1.9}$$

The ground state of the system is the vacuum of the Bogoliubov operators β, i.e. the state annihilated by all Bogoliubov annihilation operators.

6.2 Magnon expectation values

Having found the ground state as the vacuum of Bogoliubov particles we may calculate expectation values of magnons (the H.P. bosons). For notational simplicity we redefine $J_n, J_{an} \longrightarrow (4J_2)J_n, (4J_2)J_{an}$ and so $\mathcal{N} \longrightarrow (4J_2)^2\omega_q(J_n + \omega_q)$. Using now that $J_n^2 - J_{an}^2 = \omega_q^2$, we find

$$\langle b_q^\dagger b_{q+Q}\rangle\,(T=0) = \frac{J_{an}^2}{\mathcal{N}(q)}\,\langle\beta_{-q}\beta_{-q}^\dagger\rangle\,\delta_{Q,0} = \frac{(J_n + \omega_q)(J_n - \omega_q)}{\mathcal{N}(q)}\delta_{Q,0} = \left[\frac{J_n}{2\omega_q} - 1/2\right]\delta_{Q,0}, \tag{6.2.1}$$

$$\langle b_q b_{-q+Q}\rangle\,(T=0) = -\frac{(J_n + \omega_q)J_{an}}{\mathcal{N}(q)}\,\langle\beta_q\beta_q^\dagger\rangle\,\delta_{Q,0} = -\frac{J_{an}}{2\omega_q}\delta_{Q,0}. \tag{6.2.2}$$

These are the expectation values in the ground state of the system, and is thus what we should expect at zero temperature. Going instead to finite temperatures the number of Bogoliubov particles follow the Bose-distribution

$$\langle \beta_q^\dagger \beta_q \rangle = n_B(\beta 4 J_2 S \omega_q) = \frac{1}{e^{\beta 4 J_2 S \omega_q} - 1}. \tag{6.2.3}$$

In that case

$$\begin{aligned}
\langle b_q^\dagger b_{q+Q} \rangle (T) &= \frac{1}{\mathcal{N}(q)} \left\langle (J_n + \omega_q)^2 \beta_q^\dagger \beta_q + J_{an}^2 \beta_{-q} \beta_{-q}^\dagger \right\rangle \delta_{Q,0} \\
&= n_B(\beta 4 J_2 S \omega_q) \frac{(J_n + \omega_q)^2 + J_{an}^2}{\mathcal{N}(q)} \delta_{Q,0} + \langle b_q^\dagger b_q \rangle (T = 0) \\
&= \delta_{Q,0} \left[n_B(\beta 4 J_2 S \omega_q) + \coth(\beta 2 J_2 S \omega_q) \left(\frac{J_n}{2\omega_q} - 1/2 \right) \right] \\
&= \delta_{Q,0} \left[\coth(\beta 2 J_2 S \omega_q) \frac{J_n}{2\omega_q} - 1/2 \right] \qquad (6.2.4) \\
\langle b_q b_{-q+Q} \rangle (T) &= -\frac{(J_n + \omega_q) J_{an}}{\mathcal{N}(q)} \left\langle \beta_q \beta_q^\dagger + \beta_{-q}^\dagger \beta_{-q} \right\rangle \\
&= -\coth(\beta 2 J_2 S \omega_q) \frac{(J_n + \omega_q) J_{an}}{\mathcal{N}(q)} \delta_{Q,0} \\
&= -\delta_{Q,0} \coth(\beta 2 J_2 S \omega_q) \frac{J_{an}}{2\omega_q} = \langle b_{-q+Q}^\dagger b_q^\dagger \rangle (T). \qquad (6.2.5)
\end{aligned}$$

These results indicate that the expectation value of the magnon number operator does not only depend on the usual Bose-function but is increased due to terms proportional to the quantum fluctuations. If the quantum fluctuations were zero, the expectation value would be proportional to n_B as usual. On the contrary, the anomalous expectation values are only non-zero when quantum fluctuations are non-zero, as one would expect.

6.3 Lowest order magnetization correction

The lattice averaged staggered magnetization correction of the whole lattice due to magnons is to the lowest order given by [8]

$$\Delta m_z = -\langle b_i^\dagger b_i \rangle = -\frac{1}{N} \sum_k \langle b_k^\dagger b_k \rangle . \tag{6.3.1}$$

It is the correction to the spin polarization at each site due to magnons. Since the large S expansion hinges on the spin lattice being ordered with only small fluctuations about the ordered state we have implicitly assumed

$$\sum_k \langle b_k^\dagger b_k \rangle \ll NS. \tag{6.3.2}$$

In general Δm_z is non-zero both to temperature and quantum fluctuations. The quantum fluctuations arise, as we have seen, due to the fact that magnons (represented by H.P. operators) do not diagonalize the Hamiltonian, and the ground state of the excitations that do (Bogoliubov particles) has a non-zero magnon number expectation value.

6.3.1 Zero temperature correction

Assuming we are at $T = 0$, only the quantum fluctuations give rise to a non-zero Δm_z, and as we have seen, the expectation value is given by eq. (6.2.1). Thus

$$\begin{aligned} -\frac{1}{N}\sum_k \langle b_k^\dagger b_k\rangle &= -\frac{1}{N}\sum_k\left[\frac{J_n}{2\omega_k} - 1/2\right] = \frac{1}{2} - \frac{1}{8\pi^2}\int d^2k \frac{J_n}{\omega_k} \\ &= \frac{1}{2} - \frac{1}{8\pi^2}\int d^2k \frac{\left[\eta\left(\xi_x\cos^2\left(\frac{\theta}{2}\right) + \xi_y\sin^2\left(\frac{\theta}{2}\right)\right)+1\right]}{\sqrt{1-\xi_x^2\xi_y^2+\eta^2\cos(\theta)(\xi_x^2-\xi_y^2)+2\eta\left(\cos^2(\theta/2)\xi_x\bar{\xi}_y^2+\sin^2(\theta/2)\xi_y\bar{\xi}_x^2\right)}}, \end{aligned} \tag{6.3.3}$$

where the integrand diverges at the points of vanishing energy. The divergence must be characterized to understand whether the whole integral diverges. We will first consider the fraction near the point $k = (0, 0)$. In that case

$$\xi_i = \cos(k_i) \approx 1 - \frac{1}{2}k_i^2, \qquad \bar{\xi}_i = \sin(k_i) \approx k_i, \tag{6.3.4}$$

and so the numerator is

$$\begin{aligned} J_n &= \eta\left(\xi_x\cos^2\left(\frac{\theta}{2}\right) + \xi_y\sin^2\left(\frac{\theta}{2}\right)\right) + 1 \approx \eta\left(1 - \frac{1}{2}(k_x^2\cos^2(\theta/2) + k_y^2\sin^2(\theta/2))\right) + 1 \\ &= \eta + 1 - \frac{\eta}{2}\left(\cos^2(\phi)\cos^2(\theta/2) + \sin^2(\phi)\sin^2(\theta/2)\right)k^2 = \eta + 1 - \frac{\eta}{4}[1+\cos(2\phi)\cos(\theta)]k^2, \end{aligned} \tag{6.3.5}$$

where in the second line the k-vector is written in polar coordinates and $k^2 = k_x^2 + k_y^2$. Next we find

$$\begin{aligned} \omega_k^2 &= 1 - \xi_x^2\xi_y^2 + \eta^2\cos(\theta)(\xi_x^2 - \xi_y^2) + 2\eta\left(\cos^2(\theta/2)\xi_x\bar{\xi}_y^2 + \sin^2(\theta/2)\xi_y\bar{\xi}_x^2\right) \\ &\approx k_x^2 + k_y^2 - \eta^2\cos(\theta)(k_x^2 - k_y^2) + 2\eta\left(k_y^2\cos^2(\theta/2) + k_x^2\sin^2(\theta/2)\right) \\ &= k^2\left(1 - \eta^2\cos(\theta)\cos(2\phi) + \eta(1 - \cos(2\phi)\cos(\theta))\right) = k^2(\eta+1)\left(1 - \eta\cos(\theta)\cos(2\phi)\right), \end{aligned} \tag{6.3.6}$$

and so

$$\omega_k \approx k\sqrt{\eta+1}\sqrt{1-\eta\cos(\theta)\cos(2\phi)}. \tag{6.3.7}$$

Inserting these expressions in the diverging fraction of the integrand we find

$$\frac{\eta+1}{k\sqrt{1+\eta}\sqrt{1-\eta\cos(\theta)\cos(2\phi)}} + \mathcal{O}(k), \tag{6.3.8}$$

and thus we have isolated the pole. Noting that the measure of the integral removes this simple pole, we have shown that in 2 dimensions the integrand will not in fact have an infrared divergence at $k = (0, 0)$, so long as $\eta < 1$. If $\theta = 0, \pi$ then as $\eta \to 1$ the result diverges. At that point the large S expansion is invalid for any finite S, and so we cannot use the spin-wave picture at all. In other words, at the maximally frustrated point $\eta = 1$ the quantum fluctuations destroy magnetic order. But staying at $\eta < 1$, a finite S can always be chosen so as to satisfy (6.3.2).

We can obtain the expression for $k \approx (\pi, \pi)$ by the mapping $\xi_i \to -\xi_i$ in the above expression, which will yield an almost identical term in $1/k$, namely

$$\frac{\eta+1}{k\sqrt{1-\eta}\sqrt{1+\eta\cos(\theta)\cos(2\phi)}}. \tag{6.3.9}$$

Once again, the pole in k is simple, and will disappear in the integral in two-dimensions or above. In this case though, the integrand diverges as $\eta \to 1$ no matter what θ is. Finally, at the points $k = (0, \pi), (\pi, 0)$ we find that the $1/k$ terms are

$$\frac{\eta + 1}{k\sqrt{1 - \eta\cos(\theta)}\sqrt{1 + \eta\cos(2\phi)}}, \qquad \frac{\eta + 1}{k\sqrt{1 + \eta\cos(\theta)}\sqrt{1 - \eta\cos(2\phi)}}, \tag{6.3.10}$$

which both converge in 2 dimensions when integrated over k, but diverge in the integral over ϕ when $\eta = 1$.

The conclusion drawn from this analysis is that Δm_z converges for $\eta < 1$, and diverges as $\eta \to 1$. In other words, quantum fluctuations become steadily stronger as $\eta \to 1$, and eventually destroy the long-range order of the system.

6.3.2 Finite temperature correction

We now consider the finite temperature magnetization correction. Due to the Mermin-Wagner theorem, we should expect to see a divergence at $q = (0, 0)$, destroying the long-range order even for $\eta < 1$. Looking at (6.2.4) we find

$$\Delta m_z(T) = \frac{1}{2} - \frac{1}{2}\int \frac{d^2k}{(2\pi)^2}\ \coth(2J_2 S\beta\omega_k)\frac{J_n}{\omega_k}. \tag{6.3.11}$$

The second factor in the integrand has simple poles in k near the points of vanishing energy, as long as $\eta < 1$ as we saw in the zero-temperature case. Once again assuming $\eta < 1$, we expand the temperature dependent function near one of these points (by assuming $\omega_k \approx 0$) and find

$$\coth(2J_2\beta S\omega_k) = \frac{e^{\beta 2J_2 S\omega_k} + e^{-\beta 2J_2 S\omega_k}}{e^{\beta 2J_2 S\omega_k} - e^{-\beta 2J_2 S\omega_k}} \approx \frac{1}{2J_2 S\beta\omega_k} \propto \frac{T}{2J_2 S}\frac{1}{k}. \tag{6.3.12}$$

In other words, for a finite β, another simple pole is added to the simple pole from J_n/ω_k. To show that the system behaves as predicted by the Mermin-Wagner theorem, nothing more needs to be done. The second order pole leaves the integral divergent, and so no finite S can be chosen so as to satisfy (6.3.2). Nevertheless, the actual calculation becomes relevant when considering finite systems in which an infrared cutoff Λ can be made to circumvent the pole. The Brillouin zone, which is the domain of integration, is halved in both directions (from $(-\pi, \pi)$ to $(-\pi/2, \pi/2)$), and all k outside the new zone are folded into it by the identification $k + \Delta k \to k$, where Δk is one of the vectors $(\pi, \pi), (0, \pi), (\pi, 0)$. This amounts to the integral splitting into four, each defined on the reduced Brillouin zone with $k = 0$ being respectively one of the zero-energy points, $(0, 0), (\pi, \pi), (0, \pi), (\pi, 0)$. Thus we obtain the expression

$$\Delta m_z(T, \eta) = \frac{1}{2} - \frac{1}{2}\sum_{\Delta k}\int_{\Lambda<k} \frac{d^2k}{(2\pi)^2}\ \coth(2J_2\beta S\omega_{k+\Delta k})\frac{J_n(k + \Delta k)}{\omega_{k+\Delta k}}. \tag{6.3.13}$$

For later reference, the magnetization in the limit of decoupled lattices ($\eta = 0$) is

$$\Delta m_z(T, 0) = \frac{1}{2} - 2\int_{\Lambda<k} \frac{d^2k}{(2\pi)^2}\ \frac{\coth(2J_2\beta S\sqrt{1 - \xi_x^2\xi_y^2})}{\sqrt{1 - \xi_x^2\xi_y^2}}. \tag{6.3.14}$$

Like in section 5.3, we will define $J_2 S^2 = \overline{J_2}$, such that $\overline{J_2}$ is independent of S. Then

$$\begin{aligned}\Delta m_z(T,0) &= \frac{1}{2} - 2\int_{\Lambda<k} \frac{d^2k}{(2\pi)^2} \frac{\coth(2\overline{J_2}\sqrt{1-\xi_x^2\xi_y^2}/TS)}{\sqrt{1-\xi_x^2\xi_y^2}} \\ &= \frac{1}{2} - 2\int_{\Lambda<k} \frac{d^2k}{(2\pi)^2} \frac{1+2n_B(4\overline{J_2}\sqrt{1-\xi_x^2\xi_y^2}/TS)}{\sqrt{1-\xi_x^2\xi_y^2}} \\ &\approx \frac{1}{2} - 2\int_{\Lambda<k} \frac{d^2k}{(2\pi)^2} \left[\frac{1}{\sqrt{1-\xi_x^2\xi_y^2}} + \frac{TS}{2\overline{J_2}}\frac{1}{1-\xi_x^2\xi_y^2}\right],\end{aligned} \tag{6.3.15}$$

where in the last line we assumed the large S limit $\overline{J_2} \ll TS$. The temperature independent part is

$$-m_Q^0 \equiv \frac{1}{2} - 2\int \frac{d^2k}{(2\pi)^2} \frac{1}{\sqrt{1-\xi_x^2\xi_y^2}} = -0.197, \tag{6.3.16}$$

where the integration limit was extended to $\Lambda = 0$, due to the integral converging. The temperature dependent part is

$$-\frac{TS}{2\overline{J_2}} m_T^0 \equiv -\frac{TS}{2\overline{J_2}} \int_{\Lambda<k} \frac{d^2k}{(2\pi)^2} \frac{2}{1-\xi_x^2\xi_y^2}, \tag{6.3.17}$$

which does not converge if $\Lambda = 0$, and so we should characterize the divergence. We split the integral in two parts, with one such that the limit $\cos k_i \approx 1 - \frac{1}{2}k_i^2$ is valid. In that case

$$m_T^0 = \frac{1}{\pi}\int_{\Lambda}^{\tilde{\Lambda}} dk\, k\frac{1}{k^2} + \int_{\tilde{\Lambda}<k} \frac{d^2k}{(2\pi)^2} \frac{2}{1-\xi_x^2\xi_y^2} = \frac{\ln(1/\Lambda)}{\pi} + I(\tilde{\Lambda}), \tag{6.3.18}$$

where I is an irrelevant constant. Thus we find

$$\Delta m_z(T,0) = -(m_Q^0 + \frac{TS}{2\overline{J_2}} m_T^0). \tag{6.3.19}$$

This expression yields an upper bound on Λ in the finite temperature case due to the requirement $-\Delta m_z \ll S$, namely

$$\frac{T}{2\overline{J_2}} \frac{\ln(1/\Lambda)}{\pi} \ll 1 \implies \Lambda^{-1} \ll a e^{\frac{\pi 2\overline{J_2}}{T}} = \xi, \tag{6.3.20}$$

where we defined ξ and reintroduced a for comparison of units. It is noteworthy that ξ is in fact proportional to the coherence length of an antiferromagnet with only nearest neighbor interactions and interaction strength $\overline{J_2}$ [8]. Also note that the cutoff is independent of S.

On Figure 6.1 is shown the magnetization correction as a function of η calculated by numerical integration for a certain choice of parameters $\theta, \beta S$ and with a cutoff made at $\Lambda = 0.1$. An important point is that the magnetization correction is negative and only becomes more negative as η increases.

6.3.3 Small η expansion

We now calculate the integral in the expression for the magnetization correction in the limit of small sublattice coupling η. To do this we consider the integrand of $\Delta m_Z(T,\eta)$

$$\coth(2J_2\beta S\omega_k)\frac{J_n}{\omega_k} = \left(1 + 2n_B(4\overline{J_2}\omega_k)/TS\right)\frac{\eta\mathcal{E}_k + 1}{\omega_k} \approx \left(\frac{1}{\omega_k} + \frac{TS}{2\overline{J_2}}\frac{1}{\omega_k^2}\right)(\eta\mathcal{E}_k + 1), \tag{6.3.21}$$

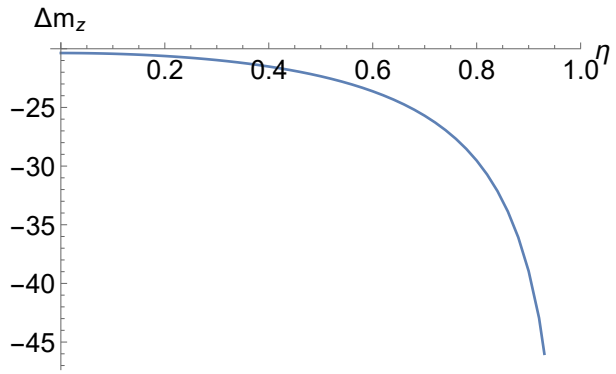


Figure 6.1: A representative example of the magnetization correction as a function of η. Parameters chosen: $\theta = 0$, $\beta S = 5$. As can be seen, the perpetually negative magnetization correction diverges as $\eta \to 1$.

where we defined $\mathcal{E}_k = \cos^2(\theta/2)\xi_x + \sin^2(\theta/2)\xi_y$ and assumed the large S limit. Define

$$\begin{aligned} a &= \cos(\theta)(\xi_x^2 - \xi_y^2) \\ b &= \cos^2(\theta/2)\xi_x\bar{\xi}_y^2 + \sin^2(\theta/2)\xi_y\bar{\xi}_x^2 \\ c &= 1 - \xi_x^2\xi_y^2, \end{aligned} \tag{6.3.22}$$

and expand the spectrum in η, keeping only up to second order

$$\begin{aligned} \frac{1}{\omega_k} &\approx \frac{1}{\sqrt{c}} - \frac{b}{c^{3/2}}\eta + \frac{3b^2 - ac}{2c^{5/2}}\eta^2, \\ \frac{1}{\omega_k^2} &\approx \frac{1}{c} - \frac{2b}{c^2}\eta + \frac{4b^2 - ac}{c^3}\eta^2. \end{aligned} \tag{6.3.23}$$

Using these expansion we may calculate the integral. To simplify the calculation we can use that some of the terms of the integrand will integrate to zero. It turns out that this is the case for all the terms which are first order in η. To see this note that b has terms linear in ξ_i. Under the summation over Δk, ξ_i may change sign (for example if $\Delta k = (\pi, 0)$, ξ_x changes sign relative to the case $\Delta k = (0, 0)$). Therefore, if b is not multiplied with a factor with the same property, it will add to zero under $\sum_{\Delta k}$. $\mathcal{E}_k$ has the same property, and

$$\begin{aligned} \sum_{\Delta k} b\mathcal{E}_k &= \sum_{\Delta k} \left[\cos^4(\theta/2)(\xi_x\bar{\xi}_y)^2 + \sin^4(\theta/2)(\xi_y\bar{\xi}_x)^2 + 2\cos^2(\theta/2)\sin^2(\theta/2)\xi_x\xi_y(\bar{\xi}_x\bar{\xi}_y)^2\right] \\ &= \sum_{\Delta k} \left[\cos^4(\theta/2)(\xi_x\bar{\xi}_y)^2 + \sin^4(\theta/2)(\xi_y\bar{\xi}_x)^2\right]. \end{aligned} \tag{6.3.24}$$

while

$$\sum_{\Delta k} b^2 = \sum_{\Delta k} \left[\cos^4(\theta/2)(\xi_x\bar{\xi}_y^2)^2 + \sin^4(\theta/2)(\xi_y\bar{\xi}_x^2)^2\right]. \tag{6.3.25}$$

Under the integration we are free to exchange x and y. This means that the two integrand terms above can further be reduced to

$$\begin{aligned} b\mathcal{E}_k &= \frac{1}{2}\left(\cos^4(\theta/2) + \sin^4(\theta/2)\right)\left((\xi_x\bar{\xi}_y^2)^2 + (\xi_y\bar{\xi}_x^2)^2\right) = \frac{1}{4}\left(1 + \cos^2\theta\right)\left((\xi_x\bar{\xi}_y)^2 + (\xi_y\bar{\xi}_x)^2\right), \\ b^2 &= \frac{1}{4}\left(1 + \cos^2\theta\right)\left((\xi_x\bar{\xi}_y^2)^2 + (\xi_y\bar{\xi}_x^2)^2\right). \end{aligned} \tag{6.3.26}$$

Next we note that a changes sign under the exchange $x \leftrightarrow y$, and so integrates to zero under the integral. To lowest non-zero order in η, all this leaves us with the integrand

$$\left(\frac{1}{\omega_k}+\frac{TS}{2\overline{J_2}}\frac{1}{\omega_k^2}\right)(\eta\mathcal{E}_k+1)\approx\left(\left[\frac{1}{\sqrt{c}}-\left(\frac{3b^2-2cb\mathcal{E}_k}{2c^{5/2}}\right)\eta^2\right]+\frac{TS}{2\overline{J_2}}\left[\frac{1}{c}-\left(\frac{4b^2-2cb\mathcal{E}_k}{c^3}\right)\eta^2\right]\right), \tag{6.3.27}$$

which is invariant under the Δk sum. Thus

$$\begin{aligned}
&\Delta m_z(T,\eta)-\Delta m_z(T,0)\\
&\qquad\approx -\eta^2(1+\cos^2\theta)\frac{1}{2}\int_{\Lambda<k}\frac{d^2k}{(2\pi)^2}\left[\frac{3[\xi_x^2\overline{\xi}_y^4+\xi_y^2\overline{\xi}_x^4]-2(1-(\xi_x\xi_y)^2)\left[\xi_x^2\overline{\xi}_y^2+\xi_y^2\overline{\xi}_x^2\right]}{2\left(1-(\xi_x\xi_y)^2\right)^{5/2}}\right.\\
&\qquad\qquad\left.+\frac{TS}{2\overline{J_2}}\frac{4\left(\xi_x^2\overline{\xi}_y^4+\xi_y^2\overline{\xi}_x^4\right)-2(1-(\xi_x\xi_y)^2)\left[\xi_x^2\overline{\xi}_y^2+\xi_y^2\overline{\xi}_x^2\right]}{\left(1-(\xi_x\xi_y)^2\right)^3}\right]\\
&\qquad\equiv -\eta^2(1+\cos^2\theta)\left(\lambda_Q+\frac{TS}{2\overline{J_2}}\lambda_T\right).
\end{aligned} \tag{6.3.28}$$

The first integral converges as $\Lambda\to 0$ and in this limit we find $\lambda_Q=0.036$. The second integral diverges as $\Lambda\to 0$, and we must characterize the divergence. For small k we may expand the integrand

$$\begin{aligned}
&\frac{1}{2}\frac{4\left(\xi_x^2\overline{\xi}_y^4+\xi_y^2\overline{\xi}_x^4\right)-2(1-(\xi_x\xi_y)^2)\left[\xi_x^2\overline{\xi}_y^2+\xi_y^2\overline{\xi}_x^2\right]}{\left(1-(\xi_x\xi_y)^2\right)^3}\approx\frac{2(k_x^4+k_y^4)-(k_x^2+k_y^2)\left[k_y^2+k_x^2\right]}{\left(k_x^2+k_y^2\right)^3}\\
&=\frac{\cos^2(2\phi)}{k^2}.
\end{aligned} \tag{6.3.29}$$

where we switched to polar coordinates from k_x, k_y. Thus

$$\lambda_T=\text{const.}+\ln(1/\Lambda)\int_0^{2\pi}\frac{d\phi}{(2\pi)^2}\cos^2(2\phi)=\text{const.}+\frac{\ln(1/\Lambda)}{4\pi}, \tag{6.3.30}$$

where the constant term is positive, but otherwise irrelevant.

We have now found the contributions to the magnetization correction $\Delta m_z(T,\eta)$ to smallest non-zero order in η. The η dependent part is

$$\Delta m_z(T,\eta)-\Delta m_z(T,0)\approx -(1+\cos^2\theta)\eta^2\left[\lambda_Q+\frac{TS}{2\overline{J_2}}\lambda_T\right]. \tag{6.3.31}$$

This function depends non-trivially on θ and T. We note that the function is only valid in the large S or high temperature limit, where bosonic statistics are approximately those of distinguishable classical particles.

6.3.4 Conclusion

Defining the Holstein-Primakoff bosons on a single lattice we have found expressions for the general (θ dependent) magnonic correlation functions, $\langle b_k^\dagger b_k\rangle$ and $\langle b_{-k}^\dagger b_k^\dagger\rangle$. Using these we found the magnetization correction $\Delta m_z(\eta,\theta)$. As expected, this diverges for non-zero temperature in correspondence with the Mermin-Wagner theorem, since $\Delta m_z \ll S$ if the system is to remain ordered. To circumvent the theorem, an infrared cutoff Λ was introduced which is to be used

in finite sized systems. Using such a cutoff, the magnetization correction was found to lowest order in η and only the temperature dependent term diverges as $\Lambda \to 0$. The magnetization correction is important for two reasons. First it shows explicitly that long range magnetic order breaks down for the J_1-J_2 square lattice. The main point though, is that it shows the existence of a non-zero magnon density in the system even at zero temperature. Using this as inspiration we make a mean-field approximation of the magnonic interaction term in chapter 7, and see how this affects the spectrum of the magnons.

Chapter 7

Magnon interactions and an effective field theory

7.1 Interaction terms in the one sublattice picture

In this section the next order in the $1/S$ expansion of H is found. These are terms are bi-quadratic in H.P. bosons and can be thought of as interactions between magnons. As we shall see, the form of the interaction terms are quite general, with several anomalous terms (terms with a non-equal number of creation and annihilation operators), which makes it difficult to incorporate them in the theory. What we will do is assume mean fields equal to those obtained from zero-temperature linear spin-wave theory, and it turns out that this amounts to a renormalization of S.

In the one sublattice picture, the next order in the $1/S$ expansion of the spin operators give the terms

$$\begin{aligned}
\mathcal{O}\left((1/S)^0\right)(\tilde{S}_i^x\tilde{S}_j^x) &= -\frac{1}{8}\left[\left(b_i^\dagger b_i b_i + b_i^\dagger b_i^\dagger b_i\right)\left(b_j + b_j^\dagger\right) + \left(b_i + b_i^\dagger\right)\left(b_j^\dagger b_j b_j + b_j^\dagger b_j^\dagger b_j\right)\right] \\
\mathcal{O}\left((1/S)^0\right)(\tilde{S}_i^y\tilde{S}_j^y) &= \frac{1}{8}\left[\left(b_i^\dagger b_i b_i - b_i^\dagger b_i^\dagger b_i\right)\left(b_j - b_j^\dagger\right) + \left(b_i - b_i^\dagger\right)\left(b_j^\dagger b_j b_j - b_j^\dagger b_j^\dagger b_j\right)\right] \\
\mathcal{O}\left((1/S)^0\right)(\tilde{S}_i^z\tilde{S}_j^z) &= b_i^\dagger b_i b_j^\dagger b_j,
\end{aligned} \tag{7.1.1}$$

where i, j are indices denoting the site of the spins.

7.1.1 Expression for the interaction terms

Once again, the N.N. term of the Hamiltonian is found to be

$$\begin{aligned}
W_1 = -\frac{J_1}{2}\sum_{\langle i,j\rangle}\Bigg[&\frac{\left(b_i^\dagger b_i b_i + b_i^\dagger b_i^\dagger b_i\right)\left(b_j + b_j^\dagger\right)}{4} \\
&- \cos(\theta_i-\theta_j)\frac{\left(b_i^\dagger b_i b_i - b_i^\dagger b_i^\dagger b_i\right)\left(b_j - b_j^\dagger\right)}{4} - \cos(\theta_i-\theta_j) b_i^\dagger b_i b_j^\dagger b_j\Bigg] \\
= -\frac{J_1}{4}\sum_{i,\delta}\Bigg[&\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right)\left(b_i^\dagger b_i^\dagger b_i b_j + b_i^\dagger b_i b_i b_j^\dagger\right) \\
&+ \sin^2\left(\frac{\theta+\phi(\delta)}{2}\right)\left(b_i^\dagger b_i b_i b_j + b_i^\dagger b_i^\dagger b_i b_j^\dagger\right) - 2\cos(\theta+\phi(\delta)) b_i^\dagger b_i b_j^\dagger b_j\Bigg] \\
= -\frac{J_1}{4N}\sum_{\delta,pqkl}\Bigg[&b_p^\dagger b_l e^{-il\cdot R_\delta}\left(\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right) b_q^\dagger b_k \delta_{p-l,k-q} + \sin^2\left(\frac{\theta+\phi(\delta)}{2}\right) b_q b_k \delta_{p-l,k+q}\right) \\
&+ \left(\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right) b_k^\dagger b_q \delta_{p-l,k-q} + \sin^2\left(\frac{\theta+\phi(\delta)}{2}\right) b_k^\dagger b_q^\dagger \delta_{p-l,k+q}\right) b_l^\dagger b_p e^{il\cdot R_\delta} \\
&- 2\cos(\theta+\phi(\delta)) e^{i(k-l)\cdot R_\delta} b_p^\dagger b_q b_k^\dagger b_l \delta_{p-q,l-k}\Bigg],
\end{aligned} \tag{7.1.2}$$

where in the last step the expression was Fourier transformed and subsequently the summation over i performed. Finally, doing the sum over δ and renaming the momentum indices we find

$$\begin{aligned}
W_1 = -\frac{J_1}{2N}\sum_{pqk}\Bigg[&\cos(p_x) b_{p+q}^\dagger b_p\left(\cos^2\left(\frac{\theta}{2}\right) b_k^\dagger b_{k+q} + \sin^2\left(\frac{\theta}{2}\right) b_{-k} b_{k+q}\right) + \text{h.c.} \\
&+ \cos(p_y) b_{p+q}^\dagger b_p\left(\sin^2\left(\frac{\theta}{2}\right) b_k^\dagger b_{k+q} + \cos^2\left(\frac{\theta}{2}\right) b_{-k} b_{k+q}\right) + \text{h.c.} \\
&- 2\cos(\theta)\left(\cos(q_x) - \cos(q_y)\right) b_{p+q}^\dagger b_p b_k^\dagger b_{k+q}\Bigg] \\
= -\frac{J_1}{2N}\sum_{pqk}\Big[&\mathcal{E}_p\ b_{p+q}^\dagger b_p b_k^\dagger b_{k+q} + \overline{\mathcal{E}}_p\ b_{p+q}^\dagger b_p b_{-k} b_{k+q} + \text{h.c.} \\
&-2\cos(\theta)\left(\cos(q_x) - \cos(q_y)\right) b_{p+q}^\dagger b_p b_k^\dagger b_{k+q}\Big],
\end{aligned} \tag{7.1.3}$$

where to ease notation we defined

$$\begin{aligned}
\mathcal{E}_p(\theta) &= \cos(p_x)\cos^2\left(\frac{\theta}{2}\right) + \cos(p_y)\sin^2\left(\frac{\theta}{2}\right), \\
\overline{\mathcal{E}}_p(\theta) &= \cos(p_x)\sin^2\left(\frac{\theta}{2}\right) + \cos(p_y)\cos^2\left(\frac{\theta}{2}\right).
\end{aligned} \tag{7.1.4}$$

Next is the N.N.N. interaction term, which is

$$\begin{aligned} W_2 &= -\frac{J_2}{2}\sum_{\langle\langle i,j\rangle\rangle}\left[\frac{\left(b_i^\dagger b_i b_i + b_i^\dagger b_i^\dagger b_i\right)\left(b_j + b_j^\dagger\right)}{4} + \frac{\left(b_i^\dagger b_i b_i - b_i^\dagger b_i^\dagger b_i\right)\left(b_j - b_j^\dagger\right)}{4} + b_i^\dagger b_i b_j^\dagger b_j\right] \\ &= -\frac{J_2}{2}\sum_{\langle\langle i,j\rangle\rangle}\left[\frac{b_i^\dagger b_i b_i b_j + b_i^\dagger b_i^\dagger b_i b_j^\dagger}{2} + b_i^\dagger b_i b_j^\dagger b_j\right] \\ &= -\frac{J_2}{4N}\sum_{pkq}\Big[4\cos(p_x)\cos(p_y)\left(b_{p+q}^\dagger b_p b_{-k} b_{k+q} + b_{k+q}^\dagger b_{-k}^\dagger b_p^\dagger b_{p+q}\right) \\ &\qquad +8\cos(q_x)\cos(q_y) b_{p+q}^\dagger b_p b_k^\dagger b_{k+q}\Big]. \end{aligned} \tag{7.1.5}$$

7.1.2 Mean field approximation of W_1 and W_2

At this point we will make a mean field approximation of W_1 and W_2 inspired by the magnon expectation values (6.2.4) and (6.2.5). We make the approximations

$$b_{p+q}^\dagger b_p b_k^\dagger b_{k+q} \approx \delta_{q0}\left[b_p^\dagger b_p \langle b_k^\dagger b_k\rangle + b_k^\dagger b_k \langle b_p^\dagger b_p\rangle\right] + C_1, \tag{7.1.6}$$

$$b_{p+q}^\dagger b_p b_{-k} b_{k+q} \approx \delta_{kp}\left[b_{-p} b_p \langle b_{p+q}^\dagger b_{p+q}\rangle + b_{p+q}^\dagger b_{p+q} \langle b_p b_{-p}\rangle\right] + C_2, \tag{7.1.7}$$

where we will not be concerned with the constants C_1, C_2. Note that due to $\delta_{q,0}$ in the first equation, the third term in W_1 will always be zero when making this kind of mean-field. Inserting the two other terms in W_1 we find

$$\begin{aligned} W_1^{MF} &= -\frac{J_1}{2N}\sum_{pk}\Big[2\mathcal{E}_p(\theta)\langle b_k^\dagger b_k\rangle b_p^\dagger b_p + \overline{\mathcal{E}}_p(\theta)\left(\langle b_k^\dagger b_k\rangle b_{-p} b_p + \langle b_k^\dagger b_k\rangle b_p^\dagger b_{-p}^\dagger\right) \\ &\qquad + 2\mathcal{E}_p(\theta)\langle b_p^\dagger b_p\rangle b_k^\dagger b_k + \overline{\mathcal{E}}_p(\theta)\left(\langle b_{-p} b_p\rangle b_k^\dagger b_k + \langle b_p^\dagger b_{-p}^\dagger\rangle b_k^\dagger b_k\right)\Big] \\ &= e_1^{cl} + \frac{J_1 S_c}{2}\sum_p\left[\mathcal{E}_p(\theta)\left(b_p^\dagger b_p + b_{-p} b_{-p}^\dagger\right) + \overline{\mathcal{E}}_p(\theta)\left(b_{-p} b_p + b_p^\dagger b_{-p}^\dagger\right)\right] \\ &\qquad - 4J_2\eta\Delta_1\sum_k b_k^\dagger b_k, \end{aligned} \tag{7.1.8}$$

where $S_c = -\frac{\sum_k \langle b_k^\dagger b_k\rangle}{N}$, $e_1^{cl} \propto \sum_p \mathcal{E}_p(\theta) = 0$ and

$$\Delta_1 = \frac{1}{4N}\sum_p 2\mathcal{E}_p(\theta)\langle b_p^\dagger b_p\rangle + \overline{\mathcal{E}}_p(\theta)\langle b_{-p} b_p + b_p^\dagger b_{-p}^\dagger\rangle. \tag{7.1.9}$$

The factor S_c is nothing but the lowest order magnetization correction, Δm_z, as seen in section 6.3. For W_2 we find that the mean field approximation yields

$$\begin{aligned} W_2^{MF} &= -\frac{J_2}{4N}\sum_{pk}\Big[4\cos(p_x)\cos(p_y)\left(b_{-p} b_p + b_p^\dagger b_{-p}^\dagger\right)\langle b_k^\dagger b_k\rangle + 8\langle b_k^\dagger b_k\rangle b_p^\dagger b_p \\ &\qquad + 4\cos(p_x)\cos(p_y) b_k^\dagger b_k\langle b_{-p} b_p + b_p^\dagger b_{-p}^\dagger\rangle + 8\langle b_p^\dagger b_p\rangle b_k^\dagger b_k\Big] \\ &= e_2^{cl} + \frac{J_2 S_c}{4}\sum_p\left[4\cos(p_x)\cos(p_y)\left(b_p b_{-p} + b_{-p}^\dagger b_p^\dagger\right) + 4\left(b_p^\dagger b_p + b_{-p} b_{-p}^\dagger\right)\right] \\ &\qquad - 4J_2\Delta_2\sum_k b_k^\dagger b_k, \end{aligned} \tag{7.1.10}$$

with $e_2^{cl} = J_2 N S_c = J_2 N \Delta m_z(T,\eta)$ and

$$\Delta_2 = \frac{1}{4N}\sum_p \cos(p_x)\cos(p_y)\left\langle b_{-p}b_p + b_p^\dagger b_{-p}^\dagger\right\rangle + 2\left\langle b_p^\dagger b_p\right\rangle. \tag{7.1.11}$$

Now using

$$2J_1\mathcal{E}_p(\theta) + 4J_2 = J_n, \qquad 2J_1\overline{\mathcal{E}}_p(\theta) + 4J_2\cos(p_x)\cos(p_y) = J_{an}, \tag{7.1.12}$$

we obtain

$$W^{MF} = e_0^{cl} - 4J_2\Delta\sum_p b_p^\dagger b_p + \frac{S_c}{4}\sum_p\left(b_p^\dagger b_p + b_{-p}b_{-p}^\dagger\right)J_n + \left(b_p b_{-p} + b_{-p}^\dagger b_p^\dagger\right)J_{an}, \tag{7.1.13}$$

where $e_0^{cl} \equiv e_1^{cl} + e_2^{cl}$ and $\Delta = \eta\Delta_1 + \Delta_2$. Thus the mean field approximation yields one term with a form identical to the original magnon Hamiltonian and another proportional to Δ. The first term simply renormalizes the spin, $S \to S + \frac{1}{2}S_c = S + \frac{1}{2}\Delta m_z(T,\eta)$. The other term, proportional to Δ is identical to a chemical potential. The complete Hamiltonian is then

$$H = E_0^{cl} + e_0^{cl} + \frac{S+\frac{1}{2}S_c}{2}\sum_p\left(b_p^\dagger b_p + b_{-p}b_{-p}^\dagger\right)\left(J_n - \frac{8J_2\Delta}{S+\frac{1}{2}S_c}\right) + \left(b_p b_{-p} + b_{-p}^\dagger b_p^\dagger\right)J_{an}, \tag{7.1.14}$$

Which diagonalizes to

$$H = E_0^{cl} + e_0^{cl} + 4J_2(S+\frac{1}{2}S_c)\sum_p \omega_p\left(\beta_p^\dagger\beta_p + \frac{1}{2}\right), \tag{7.1.15}$$

and

$$\omega_p = \sqrt{1 - \xi_x^2\xi_y^2 + \eta^2\cos(\theta)(\xi_x^2 - \xi_y^2) + 2\eta\left(\cos^2\left(\frac{\theta}{2}\right)\xi_x\overline{\xi}_y^2 + \sin^2\left(\frac{\theta}{2}\right)\xi_y\overline{\xi}_x^2\right) + \left(\frac{\Delta}{S}\right)^2} - \frac{\Delta J_n}{4J_2 S}. \tag{7.1.16}$$

This spectrum is problematic for the following reason. For simplicity let $S \gg \Delta$, such that we can ignore the term $(\Delta/S)^2$. Since the terms not proportional to Δ cancel at certain points in the Brillouin zone (at $p = (0,0),(0,\pi),(\pi,0),(\pi,\pi)$), and since J_n is positive in the whole Brillouin zone, the spectrum will become imaginary in the vicinity of these points. This does not make sense, and is a sign that terms in the Hamiltonian with p near these points cannot be canonically diagonalized, since the Hamiltonian, which is hermitian, must have real eigenvalues (see discussion at the end of section 5.2.2). The terms with p sufficiently far away from these points, e.g. where

$$\frac{\Delta J_n}{4J_2 S} \ll 1 - \xi_x^2\xi_y^2 + \eta^2\cos(\theta)(\xi_x^2 - \xi_y^2) + 2\eta\left(\cos^2\left(\frac{\theta}{2}\right)\xi_x\overline{\xi}_y^2 + \sin^2\left(\frac{\theta}{2}\right)\xi_y\overline{\xi}_x^2\right), \tag{7.1.17}$$

are still canonically diagonalizable. In other words, only above an infrared cutoff can we still diagonalize the Hamiltonian in terms of Bogoliubov excitations. Despite this we can make the cutoff arbitrarily small by increasing S, except in the case where $\eta = 1$[1]. From now on, whenever an infrared cutoff is made, we will assume

$$\omega_p = \sqrt{1 - \xi_x^2\xi_y^2 + \eta^2\cos(\theta)(\xi_x^2 - \xi_y^2) + 2\eta\left(\cos^2\left(\frac{\theta}{2}\right)\xi_x\overline{\xi}_y^2 + \sin^2\left(\frac{\theta}{2}\right)\xi_y\overline{\xi}_x^2\right)} \tag{7.1.18}$$

.

[1] At this point whole lines in the Brillouin zone fulfill $1 - \xi_x^2\xi_y^2 + \eta^2\cos(\theta)(\xi_x^2 - \xi_y^2) + 2\eta\left(\cos^2\left(\frac{\theta}{2}\right)\xi_x\overline{\xi}_y^2 + \sin^2\left(\frac{\theta}{2}\right)\xi_y\overline{\xi}_x^2\right) = 0$

7.1.3 Mean field correction to the free energy

We will now determine whether the mean field assumptions made in section 7.1.2 will decrease or increase the free energy (5.3.7). The free energy after the renormalization of S is

$$F = E_0^{cl} + e_0^{cl} + TN\ln(2) + T\sum_q \ln\left(\sinh\left(\frac{2J_2[S+\frac{1}{2}\Delta m_z(T,\eta)]\omega_q}{T}\right)\right). \tag{7.1.19}$$

Assuming $-\Delta m_z(T,\eta) \ll S$ (an assumption that can generally only be valid on a finite lattice, as seen in 6.3.2) we can expand the free energy

$$F = F_0 + NJ_2\Delta m_z(T,\eta) + TN\frac{\Delta m_z(T,\eta)}{2S}\sum_{\Delta q}\int_{\Lambda<q}\frac{d^2q}{(2\pi)^2}x\coth(x), \tag{7.1.20}$$

where $x = 2J_2\beta S\omega_{q+\Delta q}$. The integral

$$\int_{\Lambda<q}\frac{d^2q}{(2\pi)^2}x\coth(x) \tag{7.1.21}$$

is manifestly positive since x is positive over the whole integration domain. Therefore the sign of the free energy correction

$$F - F_0 = N\left[2J_2S + \sum_{\Delta q}\int_{\Lambda<q}\frac{d^2q}{(2\pi)^2}x\coth(x)\right]\frac{\Delta m_z(T,\eta)}{2S}, \tag{7.1.22}$$

depends solely on the sign of the magnetization correction, Δm_z. As seen in section 6.3.2, to lowest non-zero order in η, Δm_z is negative and so in the limit $\eta^2 \ll 1$, the free energy is lowered by the magnetization correction and the mean field theory is justified. We end by noting that the self-consistency equation of the magnetization correction is

$$\Delta m_z(T,\eta) = \frac{1}{2} - \frac{1}{2}\sum_{\Delta k}\int_{\Lambda<k}\frac{d^2k}{(2\pi)^2}\coth(2J_2\beta[S+\frac{1}{2}\Delta m_z(T,\eta)]\omega_{k+\Delta k})\frac{J_n(k+\Delta k)}{\omega_{k+\Delta k}}. \tag{7.1.23}$$

7.2 Effective field theory

In this section we will reformulate the Hamiltonian of the J_1-J_2 model in terms of new variables that we call Néel fields, and in terms of these fields we go to the continuum limit of the model. Due to the Mermin-Wagner theorem, the magnetic correlation length, ξ is finite, and so the new Néel fields are uncorrelated at length scales greater than ξ. If an intermediate length scale $1/\Lambda$ such that $\xi \ll \Lambda \ll a^{-1}$ exists, then regions of size Λ^{-1} are approximately magnetically ordered[2]. We can define spin waves within these regions and they contribute an effective term to the action due to their effect on the free energy. Following [1] this contribution will be found in the limit of $\eta^2 \ll 1$. Then by incorporating the magnon interactions through the mean field approximation of section 7.1.2 we derive a correction to the strength of the effective term in the action and see how this affects the critical temperature predicted by Chandra, Coleman and Larking [1]. The CCL critical temperature disagrees with Monte Carlo simulations made by Weber et al. [5], and the working hypothesis in this section is that the magnon interactions will lessen this disagreement.

[2]Where the magnetic order is the ground state of the classical J_1-J_2 model.

7.2.1 J_1-J_2 model in continuum limit

We will first reformulate the Hamiltonian of the J_1-J_2 model. The Hamiltonian is

$$H = \frac{S^2}{2}\sum_{i.e_1} J_1 \mathbf{\Omega}_i \cdot \mathbf{\Omega}_{i+e_1} + \frac{S^2}{2}\sum_{i,e_2} J_2 \mathbf{\Omega}_i \cdot \mathbf{\Omega}_{i+e_2}, \tag{7.2.1}$$

where e_1 couples spins on different sublattices, while e_2 couples spins on the same sublattice. The reformulation essentially amounts to defining the vectors

$$\begin{aligned} \mathbf{n}_1(r_i) &= (-1)^{i_x+i_y}\mathbf{\Omega}(r_i), \quad r_i \in \text{sublattice 1}, \\ \mathbf{n}_2(r_i) &= (-1)^{i_x+i_y}\mathbf{\Omega}(r_i), \quad r_i \in \text{sublattice 2}, \end{aligned} \tag{7.2.2}$$

and writing the Hamiltonian in terms of $\mathbf{n}_i$. The rationale behind this is that $\mathbf{n}_i$ does not change sign between nearest neighbors on the same sublattice *in the magnetically ordered state*. We have not assumed that it is the case that the spins order. It is merely a notational rewriting which proves useful. We will call $\mathbf{n}_i(r_i)$ Néel fields even though they are strictly only Néel vectors when the system orders.

The interaction between spins on the same sublattice in the original Hamiltonian is equivalent to a coupling of the Néel field at different points. Making an expansion around the point r_i on sublattice l we find

$$\begin{aligned} \mathbf{\Omega}(r_i)\cdot\mathbf{\Omega}(r_{i+e_2}) &= -\mathbf{n}_l(r_i)\cdot\mathbf{n}_l(r_{i+e_2}) = \frac{1}{2}\left[\mathbf{n}_l(r_i) - \mathbf{n}_l(r_i+ae_2)\right]^2 - 1 \\ &\approx \frac{1}{2}\left[\mathbf{n}_l(r_i) - \mathbf{n}_l(r_i) + (\partial_\mu \mathbf{n}_l)ae_2^\mu\right]^2 - 1 = \frac{a^2}{2}(\partial_\mu\mathbf{n}_l)(\partial_\nu\mathbf{n}_l)e_2^\nu e_2^\mu - 1 \end{aligned} \tag{7.2.3}$$

where in the first line we used that $\mathbf{\Omega}^2 = 1$ and where $e_2 = \pm(1,1), \pm(1,-1)$. Also, a is the lattice constant which is later taken to zero (the continuum limit). The greek letters denote the lattice indices x, y and the summation over them is done implicitly when they are repeated. When doing the summation over e_2 we find

$$\sum_{e_2} e_2^\mu e_2^\nu = 4\delta_{\mu\nu}. \tag{7.2.4}$$

Next is the interaction between spins on different sublattices. To rewrite this we will consider the sum of four terms which are identical under the summation over lattice sites

$$\begin{aligned} &\mathbf{n}_1(r_i+ae_1)\cdot(\mathbf{n}_2(r_i) - \mathbf{n}_2(r_i+a(e_1+\hat{e}_1))) - \mathbf{n}_1(r_i+a\hat{e}_1)\cdot(\mathbf{n}_2(r_i) - \mathbf{n}_2(r_i+a(e_1+\hat{e}_1))) \\ &\approx \left[\mathbf{n}_1(r_i+ae_1) - \mathbf{n}_1(r_i+a\hat{e}_1)\right](\partial_\mu\mathbf{n}_2(r_i))a(e_1^\mu + \hat{e}_1^\mu) \\ &\approx a^2(\partial_\mu\mathbf{n}_1(r_i+ae_1))(\partial_\nu\mathbf{n}_2(r_i))(e_1^\nu - \hat{e}_1^\nu)(e_1^\mu+\hat{e}_1^\mu), \end{aligned} \tag{7.2.5}$$

where $e_1, \hat{e}_1 \in \{\pm(1,0), \pm(0,1)\}$ and $\hat{e}_1 \cdot e_1 = 0$. The summation over $\hat{e}_1$ is

$$\sum_{\hat{e}_1}(e_1^\nu - \hat{e}_1^\nu)(e_1^\mu+\hat{e}_1^\mu) = \sum_{\hat{e}_1}(e_1^\nu e_1^\mu - \hat{e}_1^\nu\hat{e}_1^\mu), \tag{7.2.6}$$

and recalling that there is a relative sign between $\mathbf{n}_1(r_i+ae_1)$ with $e_1 = \pm(1,0)$ and $\mathbf{n}_1(r_i+ae_1)$ with $e_1 = \pm(0,1)$ we find

$$\begin{aligned} &\sum_{e_1,\hat{e}_1}(\partial_\mu\mathbf{n}_1(r_i+ae_1))(\partial_\nu\mathbf{n}_2(r_i))(e_1^\nu - \hat{e}_1^\nu)(e_1^\mu+\hat{e}_1^\mu) \\ &= 4\left[(\partial_x\mathbf{n}_1)(r_i+ae_1)(\partial_x\mathbf{n}_2(r_i)) - (\partial_y\mathbf{n}_1(r_i+ae_1))(\partial_y\mathbf{n}_2(r_i))\right], \end{aligned} \tag{7.2.7}$$

Thus the final expression of the Hamiltonian becomes

$$\begin{aligned} H &= a^2 S^2 \sum_{i,l} J_2 (\partial_\mu \mathbf{n}_l)^2 + a^2 S^2 \sum_i J_1 \left[(\partial_x \mathbf{n}_1)(\partial_x \mathbf{n}_2) - (\partial_y \mathbf{n}_1)(\partial_y \mathbf{n}_2) \right] \\ &= \frac{1}{2g'} \int d^2x \sum_l (\partial \mathbf{n}_l)^2 + 2\eta \left[(\partial_x \mathbf{n}_1)(\partial_x \mathbf{n}_2) - (\partial_y \mathbf{n}_1)(\partial_y \mathbf{n}_2) \right], \end{aligned} \tag{7.2.8}$$

where the continuum limit of $a \to 0$ turns the sums into integrals, and where $g' \equiv \frac{1}{2J_2 S^2}$. This whole procedure could have just as well have been done in the coherent state path integral, and assuming that static (τ-independent) fields dominate the partition function (an assumption which is only valid for large values of T or S[8]), we would have obtained

$$Z = \int \mathcal{D}\mathbf{n}\ e^{-S}, \tag{7.2.9}$$

with the action

$$S = \frac{1}{2g} \int d^2x \sum_l (\partial \mathbf{n}_l)^2 + 2\eta \left[(\partial_x \mathbf{n}_1)(\partial_x \mathbf{n}_2) - (\partial_y \mathbf{n}_1)(\partial_y \mathbf{n}_2) \right], \tag{7.2.10}$$

and $g \equiv \frac{T}{2J_2 S^2}$.

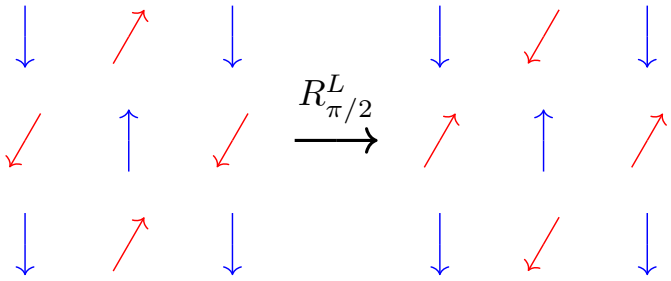


Figure 7.1: Effect of a global rotation $R^L_{\pi/2}$ in the lattice plane. If we choose a convention such that the Neel vectors for each sublattice is the one defined on the middle stripe we see that the Néel vector of one of the sublattices changes sign under the transformation.

Naively the second term of this action does not seem to be invariant under all lattice symmetry operations (e.g. $\pi/2$-rotations), but under a $\pi/2$-rotation about a spin on sublattice 1 (for example) and the operation $\mathbf{n}_2 \to -\mathbf{n}_2$ the action is invariant[1]. In other words, a $\pi/2$ rotation about a spin on one sublattice changes the sign of the Néel vector on the other, and the action is invariant under rotations when taking this into account. The fact that it is the partial derivative in the y direction that has a negative sign in the action is a consequence of which spin on each of the two sublattices one has chosen to align the Néel vector with.

7.2.2 Magnonic correction to the action

In the thermodynamic limit there will be no true long range magnetic order of the spins in the system. Therefore a finite coherence length, ξ exists. Assuming that an intermediate length scale Λ^{-1} exists such that

$$a \ll \Lambda^{-1} \ll \xi, \tag{7.2.11}$$

a region of size Λ^{-1} will be approximately magnetically ordered like the classical J_1-J_2 lattice for $\eta < 1$. Within these regions magnons contribute a term to the free energy

$$F_0 = E_0 + N \sum_{\Delta q} \int_{\Lambda < k} \frac{d^2 q}{(2\pi)^2} T \ln \left(\sinh \left(2J_2 \beta S \omega_{q+\Delta q} \right) \right) \tag{7.2.12}$$

where the infrared cutoff Λ naturally appears due to the finiteness of the region of order. Assuming now that $\eta \ll 1$ we can expand the integrand in powers of η. The first order term in η is zero, but the second order term has a non-zero component

$$\delta F_0(\eta) = F_0(\eta) - F_0(0) = -NE_1(T)\left[1 + \cos^2\theta\right], \tag{7.2.13}$$

where $E_1(T) = \frac{J_1^2 S^2}{2J_2}\left[\gamma_Q \frac{1}{2S} + \gamma_T \frac{T}{2J_2 S^2}\right]$ and

$$\gamma_{Q,T} = \int \frac{d^2q}{(2\pi)^2} \frac{(\xi_x\bar{\xi}_y^2)^2 + (\xi_y\bar{\xi}_x^2)^2}{4(1-(\xi_x\xi_y)^2)^{\alpha_{Q,T}}}, \tag{7.2.14}$$

where $\alpha_Q = 3/2$ and $\alpha_T = 2$ such that $\gamma_T = 0.159$ and $\gamma_Q = 0.130$. Note that the integration limits were extended to $\Lambda = 0$. This is merely due to the fact that these particular integrals do not diverge in this limit, and so we formally extend the limit. It does not mean that the magnetically orderd region has been extended to infinity, and it would be invalid if the extension changed the qualitative nature of $\gamma_{Q,T}$ e.g. by changing the sign. Now the angle θ is the angle between the Néel vectors of the two sublattices. By reexponentiating this free energy correction, and using the fact that $\cos\theta = \mathbf{n}_1 \cdot \mathbf{n}_2$ we obtain a correction to the action

$$S' = -\frac{NE_1(T)}{Ta^2}\int d^2x (\mathbf{n}_1 \cdot \mathbf{n}_2)^2. \tag{7.2.15}$$

This term which emerges as an effective correction due to the existence of spin-waves in the ordered regions prefers to either align or anti-align the Néel vectors of the system. The aligned or anti-aligned states are now the ground states of the system, and if the barrier between these states becomes big enough the system effectively undergoes spontaneous symmetry breaking[1].

We will mention something which the original article by CCL writes which we disagree with. It is not a mistake but a misprint, and is mentioned here only to avoid confusion if one compares these results with those of the original article. The integrals for $\gamma_{Q,T}$ yield almost the same results as CCL write except for a factor of $1/4$ which they do not have[3]. But when doing the integration suggested by the CCL the result in fact diverges, which we interpret to there being a misprint in the article.

Finally one more comment on the article. It seems the barrier height in the article is proportional to $\xi(T)^2$, the magnetic correlation length, and not Λ^{-2}. Since N is proportional to the area of the domain of magnetic order, $N \sim \Lambda^{-2}$, and it should be Λ^{-2} that is included in the barrier height. It could be that this is simply a way of proceeding with the calculation, since CCL have an expression for $\xi(T)$. It could be argued, that if $\xi(T)$ is very large, $\Lambda^{-1} \sim \sqrt{\xi}$ could serve as an intermediate length scale. In that case one could proceed in the article without many changes. We have not otherwise solved this apparent discrepancy and will from now on treat $\Lambda^{-1} \sim \xi$.

[3]This factor also appears in the calculation made by Weber et al.[5].

7.2.3 Nematic moments

With the term (7.2.15), the action of the system affords the following interpretation of the physical system. The Néel fields couple through $(\mathbf{n}_1 \cdot \mathbf{n}_2)^2$, and minimize the action by aligning or anti-aligning. The nematic moment at each point in the system is defined as $\mathbf{n}_1 \cdot \mathbf{n}_2 = \cos(\theta)$, which ranges between ± 1. For a small barrier size the moment can change in both sign and strength without decreasing the action, but when the barrier becomes of the order of the temperature, that is when $W(T) = E(T)N/a^2 \sim T$, the moments start to stabilize. As the barrier increases, it becomes increasingly more difficult to have other nematicity than ± 1 at each point in the system. The nematic moments couple through the rest of the action, 7.2.10, and it is possible for a nematic phase transition to occur. On the illustration of Figure 7.2 the nematicity is represented by lines where horizontal/vertical lines represent nematicity ± 1 while lines tilted in between have a value between ± 1.

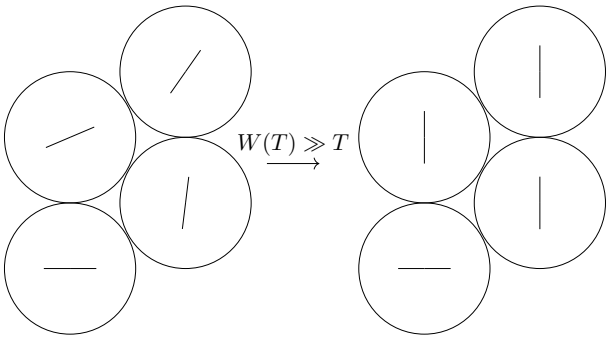


Figure 7.2: The nematic moments of the system become stable at the values ± 1 when $W(T) \gg T$. The moments can now substantiate non-zero average nematicity of the system.

7.2.4 Free energy correction in small η limit

We will now derive the magnon correction term while incorporating interactions through the mean field theory of section 7.1.3. As seen in that section the free energy in the renormalized theory is

$$F(T,\eta) = E_0 + N2J_2S_0\frac{\Delta m_z(T,\eta)}{2S_0} + T\sum_q \ln\left(\sinh\left(2J_2\frac{S\omega_q}{T}\right)\right). \tag{7.2.16}$$

where $S = S_0 + \frac{1}{2}\Delta m_z(T,\eta)$ and S_0 is the non-renormalized spin. Going to the large T limit

$$F(T,\eta) \approx E_0 + N2J_2S_0\frac{\Delta m_z(T,\eta)}{2S_0} + 2J_2S\sum_q \omega_q + T\sum_q \ln(\omega_q) + T\sum_q \ln(4J_2S/T), \tag{7.2.17}$$

and finally expanding in η assuming $\eta^2 \ll 1$

$$F(T,\eta) \approx F(T,0) - N2J_2S_0^2\eta^2(1+\cos^2\theta)\left[\frac{1}{2}\left(\lambda_Q\frac{1}{S_0} + \lambda_T\frac{T}{2J_2S_0^2}\right)\left(\frac{1}{S_0} + \kappa_Q\frac{1}{S_0} + \kappa_T\frac{T}{2J_2S_0^2}\right) - \left(\gamma_Q\frac{S_0+\Delta m_z(T,0)}{2S_0^2} + \gamma_T\frac{T}{2J_2S_0^2}\right)\right] \tag{7.2.18}$$

where

$$F(T,0) = E_0 + N2J_2S_0\frac{\Delta m_z(T,0)}{2S_0} + NT\sum_{\Delta q}\int_{\Lambda<q}\frac{d^2q}{(2\pi)^2}\ln\left(\sinh\left(2J_2\beta S_0\sqrt{1-(\xi_x\xi_y)^2}\right)\right), \tag{7.2.19}$$

is the η-independent free energy and where $\kappa_Q = 4\int \frac{d^2q}{(2\pi)^2}\sqrt{1-(\xi_x\xi_y)^2} = 0.842$ and $\kappa_T = 4\int \frac{d^2q}{(2\pi)^2} = 1$. Thus the free energy with renormalized S and $\overline{J_i} = J_i S_0^2$ is

$$F(T,\eta) = F(T,0) - NE(T)(1+\cos^2\theta) \tag{7.2.20}$$

with

$$\begin{aligned} E(T) = \frac{\overline{J_1}^2}{2\overline{J_2}}\Bigg(&\gamma_Q \frac{S_0 + \Delta m_z(T,0)}{2S_0^2} + \gamma_T \frac{T}{2\overline{J_2}} \\ &+ \frac{1}{2}\left(\lambda_Q \frac{1}{S_0} + \lambda_T \frac{T}{2\overline{J_2}}\right)\left[(1+\kappa_Q)\frac{1}{S_0} + \kappa_T \frac{T}{2\overline{J_2}}\right]\Bigg), \end{aligned} \tag{7.2.21}$$

and the parameters are listed in Figure 7.3.

γ_Q	0.130
γ_T	0.159
λ_Q	0.036
λ_T	$\frac{\ln(1/\Lambda)}{4\pi}$
κ_Q	0.842
κ_T	1

Figure 7.3: Numerical parameters of the magnonic free energy correction.

7.2.5 Critical temperature of the nematic phase transition

According to CCL, an Ising phase transition to a phase with non-zero average nematicity $\sigma = \mathbf{n}_1 \cdot \mathbf{n}_2$ occurs at the critical temperature $T_c = \frac{8\pi\overline{J_2}}{z_0 \ln(T_c/E(T_c))}$, with $z_0 = 2\eta/\left(\arcsin(\eta) + \eta\sqrt{1-\eta^2}\right)$. The assumption is that the the phase transition will occur when the barrier height, $W(T) = \frac{NE(T)}{a^2}$ is of the order of the temperature, $W(T_c) \sim T_c$. In [1], they give an estimate of the magnetic correlation length $\xi \sim ae^{2\pi/(gz_0)}$. Making the assumption that the domains of approximate magnetic order are of size ξ leads to $N \sim \xi^2$ and the barrier height

$$W(T) \sim E(T)e^{4\pi/(gz_0)}. \tag{7.2.22}$$

Thus at the critical temperature estimated by CCL

$$e^{8\pi\overline{J_2}/(z_0T_c)} = T_c/E(T_c) \implies T_c = \frac{8\pi\overline{J_2}}{z_0 \ln\left(T_c/E(T_c)\right)}. \tag{7.2.23}$$

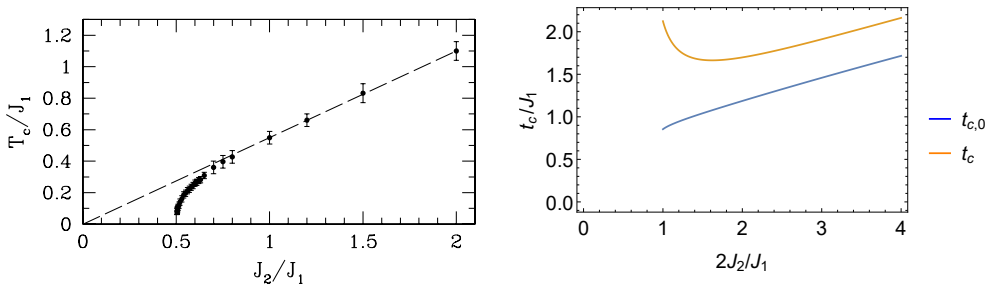
Inserting the cutoff $\Lambda = e^{-\frac{4\pi\overline{J_2}z_0}{T}}$, and using Eq. (7.2.21) in the large S_0 limit we find

$$E(T)/T \approx \eta^2\left(\gamma_T + \frac{1}{2}\frac{\eta}{\arcsin(\eta) + \eta\sqrt{1-\eta^2}}\kappa_T\right), \tag{7.2.24}$$

and thus

$$t_c/\overline{J_1} = \frac{\eta^{-1}}{z_0 \ln\left(\eta^{-2}\left[\gamma_T + \frac{1}{2}\frac{\eta}{\arcsin(\eta)+\eta\sqrt{1-\eta^2}}\kappa_T\right]^{-1}\right)}, \tag{7.2.25}$$

where $t_c \equiv T_c/4\pi$. On Figure 7.4b is shown the critical temperature before and after the mean



(a) (b)

Figure 7.4: Left: Monte Carlo results of the critical temperature of the nematic phase transition. For large J_2, the critical temperature scales linearly with J_2 but drops to zero with infinite slope as we approach the critical point $2J_2/J_1 = 1$. Figure taken from the paper by Weber et al.[5]. Right: The regular CCL result for the critical temperature $t_{c,0}$ and the mean-field corrected critical temperature t_c. The mean field correction does not seem to better the discrepancy between CCL and Monte Carlo calculations, but in fact makes the low J_2 critical temperature behavior further deviate from Monte Carlo.

field correction and (for reference) the numerically calculated critical temperature made in [5]. It is clear that the mean-field assumption, made to lessen the gap of the low J_2 behavior of the critical temperature between CCL and Monte Carlo, actually worsens it. The hypothesis that the incorporation of the magnonic interactions through the mean field approximation of section 7.1.3 yields a more accurate critical temperature is thus wrong.

It is not clear why incorporating interactions through our choice of mean field worsened the critical temperature prediction. One could argue that the critical temperature calculated by CCL is not valid as we approach $\eta \to 1$ because the magnon correction to the action was found in the small η limit and only the lowest order contribution in an η expansion was found. Since all corrections to the field theory made from the mean-field theory have also only been found in the small η, the compounding of different terms that are all invalid in the regime of interest could be the reason why the new result is worse than the old. In fact, as we have seen, the magnetization correction diverges in the limit $\eta \to 1$, while this is not the case when only taking into account the lowest order terms in η. It seems at least plausible that this diverging of the magnetization correction is what destroys the nematic ordering in the system. At this point this is of course only speculation, but it might be a relevant starting point in future research.
It is also possible that CCL made a wrong estimate of the critical temperature. As we have seen they estimate that the phase transition occurs when the nematic barrier height, $W(T)$, is of the order of the temperature, but this need not be the case. In appendix B we show how one can arrive at a field theory of not only the Néel fields but of a nematic field σ through a Hubbard-Stratonovich transformation of the coupling term $(\mathbf{n}_1 \cdot \mathbf{n}_2)^2$ as was also done by Tsvelik [11]. An equation for the critical temperature is found. Unfortunately the calculation has not been finished but this could also be ground for future work.

7.3 Conclusion

We have found the expression for the first order term in the $1/S$ expansion of the spin operators represented by H.P. operators, and thus found the corresponding term in J_1-J_2 Hamiltonian. These were two-particle terms (with four bosonic operators), and a mean field approximation of them, inspired by the non-zero single-particle magnonic correlation functions, turned out to lower the free energy of the system, at least to smallest order in η. Crucially we limited the

system to a finite sized one, so as to circumvent the Mermin-Wagner theorem. The effect of the mean field approximation was primarily a renormalization of S to $S + \Delta m_z/2$, but it also produced a term which made the spectrum imaginary at certain points in the Brillouin zone. This term turns out to be insignificant in finite sized systems with a sufficiently large S.

Following [1] with the renormalized parameters, an effective action for Néel fields $\mathbf{n}_i$ in an infinite system was found. The critical assumption made was for the existence of an intermediate length scale Λ^{-1}, between the correlation length of the Néel fields and the lattice constant. The magnons existing within domains of size Λ^{-1} then contribute a term $\sim (\mathbf{n}_1 \cdot \mathbf{n}_2)^2$ to the action. In such a system, a phase transition takes place with order parameter $\sigma = \mathbf{n}_1 \cdot \mathbf{n}_2$ and the critical temperature found in[1] was corrected with the renormalized parameters. This correction did not solve the discrepancy between Monte-Carlo calculations and the original CCL prediction in the low J_2 regime but actually worsened it. It would therefore seem that this is a bad mean-field choice and one could try another mean-field to see whether this will do better.

Chapter 8

Conclusion and Outlook

In this thesis we have explored the nematic phase transition in the J_1-J_2 square lattice first discussed by Chandra, Coleman and Larkin in 1990 [1]. In their paper, CCL showed that spin waves in locally magnetically ordered regions affect the effective action of the system. The underlying assumption was that a length scale Λ^{-1} which is much smaller than the magnetic correlation length, i.e. $\Lambda^{-1} \ll \xi$ exists. The effective term was interpreted in this thesis as a stabilizer of the nematic moment, σ, of the magnetically ordered domains of size Λ^{-1}. CCL argued that a phase transition would occur when $W(T)$ the barrier strength between the two possible nematic moments is of the order of the temperature.

Weber et al. confirmed numerically[5] a phase transition with properties similar to the one predicted by CCL, but showed that their calculation was wrong in the vicinity of $\eta = J_1/2J_2 = 1$. We set out to explore whether incorporating interactions between spin waves using a mean field approximation would resolve this discrepancy. Because the Hamiltonian of the J_1-J_2 square lattice is not diagonalizable in terms of quantized spin waves (also called magnons), the magnonic expectation values $\langle b_q^\dagger b_q \rangle$ and $\langle b_q^\dagger b_{-q}^\dagger \rangle$ are non-zero even at zero temperature. Expressions for these were found and used to make a mean field approximation of the interaction term between magnons which served to simply renormalize the spin S of the spins on the lattice.

The incorporation of magnon interactions by use of our mean field approximation did not solve the discrepancy between the numerical result of Weber et al. and the result of CCL but in fact made it larger. It would therefore seem that the choice of mean field was not a good one, which opens up the question of whether another choice might prove more successful. It makes sense that the mean field theory did not yield correct results very close to $\eta \sim 1$, since at this point the magnon number diverges which leads to the loss of magnetic order. The hypothesis was that the mean field theory would extend the range in which the CCL result still compares well with numerics. It is not clear why this fails, but one reason could be that since both the CCL result and the correction to it by the mean field approximation become invalid as η approaches 1, compounding them makes the result even worse. We have also suggested that the critical temperature estimate made by CCL, based on the assumption that the phase transition occurs at the temperature where the barrier strength $W(T)$ is of the order T, could be wrong. The barrier strength only indicates when nematic moments are stabilizing. A calculation similar to one made in [11] has been started, but was not finished, in appendix B. Here a new field, σ, is introduced into the theory by a Hubbard-Stratonovic transformation and the magnetic degrees of freedom integrated out. The resulting theory of σ is then analyzed to find an equation for the critical temperature. Unfortunately the necessity of introducing a constraint field, λ, to integrate out $\mathbf{n}_i$, complicates the equations. This would be an excellent point to further explore in future work.

Finally it would be interesting to study how including the τ-dependency in the field theory may affect it, as has been done by Lante and Parola in 2006[17]. The τ dynamics become relevant when both the temperature and spin of the system are small. Therefore it becomes important for the phase transition at the highly frustrated regime, $\eta = 1$, since Weber predicts that the critical temperature goes to zero at this point.

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Appendices

Appendix A

Fourier transformation convention

Throughout this thesis the Fourier transform of a function $f(x)$ with x a space coordinate is

$$f(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d^d x \; e^{-ik\cdot x} f(x), \quad f_k = \frac{1}{\sqrt{N}} \sum_i e^{-ik\cdot x_i} f_{x_i}, \tag{A.0.1}$$

with opposite convention for time coordinates

$$f(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt \; e^{i\omega t} f(t), \quad f_\omega = \frac{1}{\sqrt{N}} \sum_i e^{i\omega t} f_{t_i}. \tag{A.0.2}$$

The inverse Fourier transforms are

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d^d k \; e^{ik\cdot x} f(k), \quad f_i = \frac{1}{\sqrt{N}} \sum_k e^{ik\cdot x_i} f_k, \tag{A.0.3}$$

These conventions are also used for the Fourier transforms of operators. Frequently we will use identities of the form

$$\int_{-\infty}^{\infty} d^d x e^{i(k-k')\cdot x} = 2\pi\delta(k-k'), \quad \sum_{x_i} e^{i(k-k')\cdot x_i} = N\delta_{k,k'}. \tag{A.0.4}$$

A.1 Translation invariance

Assume a function f of two spatial coordinates which only depends on the difference between the coordinates

$$f(x_1, x_2) = f(x_1 - x_2), \tag{A.1.1}$$

then f is said to be translationally invariant. Fourier transforming each coordinate we find

$$f(x_1 - x_2) = \frac{1}{N} \sum_{k_1,k_2} e^{ik_1\cdot x_1 - ik_2\cdot x_2} f_{k_1,k_2} = \frac{1}{N} \sum_{k_1,k_2} e^{ik_1\cdot(x_1-x_2) - i(k_2-k_1)\cdot x_2} f_{k_1,k_2}. \tag{A.1.2}$$

Now for f to only depend on $x_1 - x_2$, $f_{k_1,k_2} = f_{k_1}\delta_{k_1,k_2}$, and we obtain

$$f(x_1 - x_2) = \frac{1}{N} \sum_k f_k e^{ik\cdot(x_1-x_2)}. \tag{A.1.3}$$

Appendix B

Hubbard-Stratonovich decoupling of quadratic Néel fields

We have shown that the mean-field approximation made in section 7.1.2 does not improve the critical temperature found by CCL. This was attributed to a bad choice of mean field. It could also be true that the estimate for the critical temperature, as approximately the temperature where the nematic barrier $W(T)$ is equal to the temperature, is a bad estimate. As we have argued, the barrier strength should only determine the stability of nematic moments in the system and maybe the temperature at which the moments are stable is higher than the critical temperature of the nematic phase transition.

In this section we will use a Hubbard-Stratonovich transformation to decouple the term in the action which is biquadratic in the Néel fields, an idea also utilized by [11]. Doing this we will try to give an estimate of the critical temperature.

B.1 Hubbard-Stratonovich transformation

We begin by writing the effective action of the Néel fields

$$\mathcal{S}_{\mathbf{n}} = \frac{1}{2g}\int d^2x \sum_l \partial(\mathbf{n}_l)^2 + 2\eta\left[(\partial_x\mathbf{n}_1)\cdot(\partial_x\mathbf{n}_2) - (\partial_y\mathbf{n}_1)\cdot(\partial_y\mathbf{n}_2)\right] - c\int d^2x(\mathbf{n}_1\cdot\mathbf{n}_2)^2, \tag{B.1.1}$$

where $g = \frac{T}{2\overline{J}_2}$ and $c = \frac{E(T)}{T}\frac{N}{a^2}$ and where $E(T)$ is, for now, the parameter found by CCL, not the one changed by mean-field theory. We now multiply the partition function by the unity

$$1 = \int \mathcal{D}\sigma \exp\left(-\mathcal{S}_\sigma\right), \tag{B.1.2}$$

with $\mathcal{S}_\sigma = \frac{c^{-1}}{4}\sigma(x)^2$. Note that the measure of this Gaussian integral is defined so as normalize it. The field σ is now redefined

$$\sigma \to \sigma + 2c(\mathbf{n}_1\cdot\mathbf{n}_2), \tag{B.1.3}$$

a transformation with Jacobian determinant 1. Doing this, the sum of the two actions yields

$$\begin{aligned}\mathcal{S}_{\mathbf{n}} + S_\sigma = \frac{1}{2g}\int d^2x \sum_l \partial(\mathbf{n}_l)^2 + 2\eta\left[(\partial_x\mathbf{n}_1)\cdot(\partial_x\mathbf{n}_2) - (\partial_y\mathbf{n}_1)\cdot(\partial_y\mathbf{n}_2)\right] \\ + \frac{c^{-1}}{4}\sigma(x)^2 + 4c(\mathbf{n}_1\cdot\mathbf{n}_2)\sigma.\end{aligned} \tag{B.1.4}$$

Finally the integrations over the Néel fields, which are bound to the unit sphere S^2, are relaxed to include all of $\mathbb{R}^3$ by introducing into the path integral

$$\delta(\mathbf{n}_i^2 - 1) = \int \mathcal{D}\lambda_i \exp\left(-i\lambda_i \int d^2x(\mathbf{n}_i^2 - 1)\right). \tag{B.1.5}$$

The partition function is now

$$Z = \int \mathcal{D}(\mathbf{n}_1, \mathbf{n}_2)\mathcal{D}\sigma\mathcal{D}\lambda \ \exp(-S), \tag{B.1.6}$$

where $S = S_{\mathbf{n}} + S_\sigma + S_\lambda$. We now proceed to Fourier transform the action. We will assume that the λ_i fields are constant, and then

$$\int d^2x \ i\lambda_i(\mathbf{n}_i - 1) = i\sum_q \lambda\left(|\mathbf{n}_i(q)|^2 - N\right), \tag{B.1.7}$$

where $n_i^*(q) = n_i(-q)$ due to the fields being real. Similarly

$$\int d^2x \ \frac{c^{-1}}{4}\sigma(x)^2 = \frac{c^{-1}}{4}\sum_q |\sigma_q|^2. \tag{B.1.8}$$

Finally the Fourier transforms of the terms of $\mathbf{S_n}$ are

$$\int d^2x \ \partial(\mathbf{n}_l)^2 = \sum_q q^2|\mathbf{n}_l(q)|^2, \tag{B.1.9}$$

$$\int d^2x \ 2\left[(\partial_x\mathbf{n}_1)\cdot(\partial_x\mathbf{n}_2) - (\partial_y\mathbf{n}_1)\cdot(\partial_y\mathbf{n}_2)\right] = \sum_q (q_x^2 - q_y^2)(\mathbf{n}_1^*(q)\cdot\mathbf{n}_2(q) + \mathbf{n}_1(q)\cdot\mathbf{n}_2^*(q)), \tag{B.1.10}$$

$$\int d^2x \ \sigma \ \mathbf{n}_1\cdot\mathbf{n}_2 = \frac{1}{2\sqrt{N}}\sum_{qq'}\left(\sigma_{q-q'}\mathbf{n}_1(q)\cdot\mathbf{n}_2^*(q') + \sigma_{q-q'}^*\mathbf{n}_1^*(q')\cdot\mathbf{n}_2(q)\right). \tag{B.1.11}$$

Thus the Fourier transformed action is

$$\mathcal{S} = -i\frac{N}{2g}\lambda_i + \sum_{qq'}\frac{c^{-1}}{4}|\sigma_q|^2\delta_{qq'} + \begin{pmatrix}\mathbf{n}_1^*(q') & \mathbf{n}_2^*(q')\end{pmatrix}\mathbf{G}^{-1}(q,q')\begin{pmatrix}\mathbf{n}_1(q)\\ \mathbf{n}_2(q)\end{pmatrix}, \tag{B.1.12}$$

where

$$\mathbf{G}^{-1} = \frac{1}{2g}\begin{pmatrix}\left(q^2 + i\lambda_1\right)\delta_{qq'} & \eta(q_x^2 - q_y^2)\delta_{qq'} + g\frac{\sigma_{q-q'}}{\sqrt{N}}\\ \eta(q_x^2 - q_y^2)\delta_{qq'} + g\frac{\sigma_{q-q'}^*}{\sqrt{N}} & \left(q^2 + i\lambda_2\right)\delta_{qq'},\end{pmatrix}. \tag{B.1.13}$$

and λ_i have been rescaled to absorb $2g$. At this point the action is quadratic in the Néel fields and can therefore be integrated out. The action that follows is

$$\mathcal{S} = -i\frac{N}{2g}\lambda_i + \frac{c^{-1}}{4}\sum_{qq'}|\sigma_q|^2\delta_{qq'} + \mathrm{Tr}\ln\left(\mathbf{G}^{-1}(\sigma,\lambda)\right). \tag{B.1.14}$$

B.2 Saddle-point equations

The next step is to find the saddle-point equations of eq. (B.1.13). In the limit of large $\mathcal{N}$ (with $\mathcal{N}$ being the number of vector components of the Néel fields), the fields satisfying these equations are the dominant contribution to the partition function[11]. We will assume that also the nematic field, σ, is homogeneous and that $\lambda_1 = \lambda_2 = \lambda$. Then

$$\frac{\delta S}{\delta \lambda} = 0 \implies i\frac{N}{g} = i\mathrm{Tr}\left[\mathbf{G}\frac{\delta \mathbf{G}^{-1}}{\delta \lambda}\right] = i\frac{1}{2g}\mathrm{Tr}\left[\mathbf{G}\right]. \tag{B.2.1}$$

To proceed we note that per the usual inversion of 2×2 matrices

$$\mathbf{G} = \frac{2g}{(q^2+i\lambda)^2 - \left[\eta(q_x^2-q_y^2) + g\frac{\sigma_0}{\sqrt{N}}\right]^2}\begin{pmatrix} q^2+i\lambda & -\eta(q_x^2-q_y^2) - g\frac{\sigma_0}{\sqrt{N}} \\ -\eta(q_x^2-q_y^2) - g\frac{\sigma_0}{\sqrt{N}} & q^2+i\lambda, \end{pmatrix} \tag{B.2.2}$$

and thus the saddle point equation is

$$\begin{aligned} 1 &= \frac{2g}{N}\sum_q \frac{q^2+i\lambda}{(q^2+i\lambda)^2 - \left[\eta(q_x^2-q_y^2)+g\sigma_0\right]^2} \\ &= 2g\int \frac{d^2q}{(2\pi)^2}\frac{q^2+i\lambda}{(q^2+i\lambda)^2 - \left[\eta(q_x^2-q_y^2)+g\sigma_0\right]^2}, \end{aligned} \tag{B.2.3}$$

where the nematic field was scaled by $1/\sqrt{N}$. Similarly one can show that the other saddle point equation yields

$$\frac{c^{-1}}{4}\sigma_0 = 2g\int \frac{d^2q}{(2\pi)^2}\frac{\eta(q_x^2-q_y^2)+g\sigma_0}{(q^2+i\lambda)^2 - \left[\eta(q_x^2-q_y^2)+g\sigma_0\right]^2}. \tag{B.2.4}$$

The sum of these equations is

$$1 + \frac{c^{-1}\sigma_0}{4} = 2g\int \frac{d^2q}{(2\pi)^2}\frac{1}{q^2+i\lambda - \left[\eta(q_x^2-q_y^2)+g\sigma_0\right]}, \tag{B.2.5}$$

and the difference is

$$1 - \frac{c^{-1}\sigma_0}{4} = 2g\int \frac{d^2q}{(2\pi)^2}\frac{1}{q^2+i\lambda + \left[\eta(q_x^2-q_y^2)+g\sigma_0\right]}. \tag{B.2.6}$$

This is the equation we will use to find the critical temperature. Assume that the nematic field is non-zero below some critical temperature T_c. The critical temperature can then be determined by the condition $\sigma_0(T_c) = 0$. This yields the equation

$$1 = 2g_c\int \frac{d^2q}{(2\pi)^2}\frac{1}{q^2+i\lambda - \left[\eta(q_x^2-q_y^2)\right]} = 2g_c\int \frac{dq}{(2\pi)^2}\, q\int_0^{2\pi} d\theta \frac{1}{q^2+i\lambda+\eta q^2\cos(2\theta)}, \tag{B.2.7}$$

Where $g_c = T_c/(2\overline{J_2})$. Using the equation

$$\int d\theta \frac{1}{a+b\cos(\theta)} = \frac{2\arctan\left[\frac{a-b}{\sqrt{a^2-b^2}}\tan(\theta/2)\right]}{\sqrt{a^2-b^2}}, \tag{B.2.8}$$

we find

$$2\int_0^{\pi} d\theta \frac{1}{q^2+i\lambda+\eta q^2\cos(\theta)} = \frac{2\pi}{\sqrt{(q^2+i\lambda)^2-\eta^2q^4}}. \tag{B.2.9}$$

Thus we are left with the equation

$$1 = 2g_c\int \frac{dq}{2\pi}\frac{q}{\sqrt{(q^2+i\lambda)^2-\eta^2q^4}}. \tag{B.2.10}$$

Appendix C

Correlation functions in the magnetically ordered state

C.1 Spin-spin correlation function

To consider the spin-spin correlation functions we first review some general theory. We will define the imaginary-time correlation functions as

$$\tilde{R}^{\alpha\alpha'}_{ii'}(\tau,\tau') = \frac{1}{Z}\left\langle e^{-\beta H_0} T_\tau [S^\alpha_i(\tau) S^{\alpha'}_{i'}(\tau')]\right\rangle , \tag{C.1.1}$$

where

$$S^\alpha_i(\tau) = e^{H_0\tau} S^\alpha_i e^{-H_0\tau}, \tag{C.1.2}$$

and H_0 is the Hamiltonian in Eq. (5.2.26), and in the end relate these to the retarded correlation functions through analytical continuation. In general the interesting object is the dynamical structure factor

$$S^{\alpha\alpha'}(q,\omega) = \frac{1}{2\pi N}\sum_{ii'}\int_{-\infty}^{\infty} e^{-iq\cdot(R_i-R_j)+i\omega t} S^{\alpha\alpha'}_{ii'}(t), \tag{C.1.3}$$

with $S^{\alpha\alpha'}_{ii'}(t-t') = \langle S^\alpha_i(t) S^{\alpha'}_{i'}(t')\rangle$, since this can be related to measurable quantities in neutron diffraction experiments[8]. The structure factor only depends on q,ω due to the assumption of spatial and temporal homogeneity.
The general expression of the dynamical structure factor is in fact too general. We are interested in the same-time correlation functions, or the static structure factor, with $\alpha = \alpha'$

$$S(q) = \frac{1}{N}\sum_{ij}\langle S^\alpha_i S^\alpha_j\rangle = \langle S^\alpha_q S^\alpha_{-q}\rangle . \tag{C.1.4}$$

since no time-dependent external field affects the system. By finding this quantity the magnetic correlation length could be found.

C.2 Zero temperature correlations - four sublattices

Equipped with the ground state of the spin lattice, namely the state annihilated by all Bogoliubov annihilation operators (see equation 5.2.26), we may evaluate spin-spin correlation functions. First

$$\mathbf{S}_{i,a}\cdot\mathbf{S}_{j,b} = S^x_{i,a}S^x_{j,b} + \cos\theta_{(i,a),(j,b)}\left(S^y_{i,a}S^y_{j,b} + S^z_{i,a}S^z_{j,b}\right) + \sin\theta_{(i,a),(j,b)}\left(S^y_{i,a}S^z_{j,b} - S^z_{i,a}S^y_{j,b}\right). \tag{C.2.1}$$

The vacuum fluctuations pick $\theta = 0, \pi$ so let us assume $\theta = 0$. A completely equivalent calculation may be done for $\theta = \pi$. We expand the spin-operators to smallest non-classical order in S. Using the vacuum state of Bogoliubov bosons

$$\begin{aligned}\langle \mathbf{S}_{i,a} \cdot \mathbf{S}_{j,b} \rangle =& \frac{S(1+(-1)^{\lambda_{a,b}})}{2} \langle b^\dagger_{i,a} b_{j,b} + b^\dagger_{j,b} b_{i,a} \rangle + \frac{S(1-(-1)^{\lambda_{a,b}})}{2} \langle b_{i,a} b_{j,b} + b^\dagger_{j,b} b^\dagger_{i,a} \rangle \\ &+ (-1)^{\lambda_{a,b}} \left(S^2 - S \langle b^\dagger_{i,a} b_{i,a} + b^\dagger_{j,b} b_{j,b} \rangle \right) \\ &\approx \frac{S(1+(-1)^{\lambda_{a,b}})}{2} \langle b^\dagger_{i,a} b_{j,b} + b^\dagger_{j,b} b_{i,a} \rangle + \frac{S(1-(-1)^{\lambda_{a,b}})}{2} \langle b_{i,a} b_{j,b} + b^\dagger_{j,b} b^\dagger_{i,a} \rangle + (-1)^{\lambda_{a,b}} S^2,\end{aligned} \tag{C.2.2}$$

where $\lambda_{a,b}$ is two if a, b are in the same row within the unit cell or are equal and is one if a, b and in the same column but are unequal, and where we disregarded the contribution from the same site expectation value, assuming this to much smaller than S. The next step is to Fourier transform this expression, which will yield terms like

$$\langle b^\dagger_{i,a} b_{j,b} \rangle = \frac{1}{N} \sum_{qQ} \langle b^\dagger_{q,a} b_{q+Q,b} \rangle \, e^{iq \cdot (R_{i,a} - R_{j,b})} e^{iQ \cdot R_{j,b}}, \tag{C.2.3}$$

and now

$$\begin{aligned}\langle b^\dagger_{q,a} b_{q+Q,b} \rangle &= \sum_{cd} \langle \boldsymbol{\beta}^\dagger_{q,c} \mathcal{B}^\dagger_{ca}(q) \mathcal{B}_{bd}(q+Q) \boldsymbol{\beta}_{q+Q,d} \rangle = \sum_{cd} \mathcal{B}^\dagger_{ca}(q) \mathcal{B}_{bd}(q+Q) \langle \boldsymbol{\beta}^\dagger_{q,c} \boldsymbol{\beta}_{q+Q,d} \rangle \\ &= \sum_{c=5}^{8} \mathcal{B}_{bc}(q) \mathcal{B}^\dagger_{ca}(q) \delta_{Q,0} = (\mathcal{V}_q \mathcal{V}_q^\dagger)^*_{ba} \delta_{Q,0},\end{aligned} \tag{C.2.4}$$

where in the first equality we simply transformed from H.P.- to Bogoliubov bosons, in the third equality we used that $\langle \boldsymbol{\beta}^\dagger_{q,c} \boldsymbol{\beta}_{q+Q,d} \rangle = \begin{cases} \delta_{cd} \delta_{Q,0} \text{ if } c \geq 5 \\ 0 \text{ if } c < 5 \end{cases}$, in the fourth equality used that

$$\mathcal{B}(q) = \mathcal{G}\mathcal{A}\mathcal{G} = \begin{pmatrix} \mathcal{U}_q & -\mathcal{V}^*_q \\ -\mathcal{V}_q & \mathcal{U}^*_q \end{pmatrix}, \tag{C.2.5}$$

and finally used that $\mathcal{V}_q = \mathcal{V}_{-q}$. Similarly

$$\langle b_{i,a} b_{j,b} \rangle = \frac{1}{N} \sum_{qQ} \langle b_{q,a} b_{-q+Q,b} \rangle \, e^{-iq \cdot (R_{i,a} - R_{j,b})} e^{-iQ \cdot R_{j,b}}, \tag{C.2.6}$$

and

$$\begin{aligned}\langle b_{q,a} b_{-q+Q,b} \rangle &= \sum_{cd} \langle \boldsymbol{\beta}^\dagger_{-q,c} \mathcal{B}^\dagger_{c,a+4}(-q) \mathcal{B}_{bd}(-q+Q) \boldsymbol{\beta}_{-q+Q,d} \rangle \\ &= \sum_{cd} \mathcal{B}^\dagger_{c,a+4}(-q) \mathcal{B}_{bd}(-q+Q) \langle \boldsymbol{\beta}^\dagger_{-q,c} \boldsymbol{\beta}_{-q+Q,d} \rangle \\ &= \sum_{c=5}^{8} \mathcal{B}_{bc}(q) \mathcal{B}^\dagger_{c,a+4}(q) \delta_{Q,0} = (-\mathcal{V}_q \mathcal{U}_q^\dagger)^*_{ba} \delta_{Q,0}.\end{aligned} \tag{C.2.7}$$

Thus we find

$$\delta \langle \mathbf{S}_{i,a} \cdot \mathbf{S}_{j,b} \rangle = \frac{1}{N} \sum_q S \left(1 + (-1)^{\lambda_{ab}} \right) \Re \left(\left(\mathcal{V}_q \mathcal{V}_q^\dagger \right)_{ba} e^{-iq \cdot R} \right) + S \left(1 - (-1)^{\lambda_{ab}} \right) \Re \left(\left(-\mathcal{V}_q \mathcal{U}_q^\dagger \right)_{ba} e^{iq \cdot R} \right), \tag{C.2.8}$$

with $\delta\langle \mathbf{S}_{i,a}\cdot\mathbf{S}_{j,b}\rangle = \langle \mathbf{S}_{i,a}\cdot\mathbf{S}_{j,b}\rangle - (-1)^{\lambda_{ab}}S^2$, representing the modification to the correlations due to spin-waves. R is the relative distance between spins.
Next we consider the Fourier transformed spin-spin correlation function

$$\langle \mathbf{S}_{i,a}\cdot\mathbf{S}_{j,b}\rangle = \frac{1}{N}\sum_{qQ}\langle \mathbf{S}_{q,a}\cdot\mathbf{S}_{-q+Q,b}\rangle\, e^{iq\cdot(R_{i,a}-R_{j,b})}e^{iQ\cdot R_{j,b}}. \tag{C.2.9}$$

Since the system is translationally invariant, it is reasonable to assume that the spin-spin correlation function only depends on relative distance. Thus we argue $Q=0$ is the only contribution in the Q-sum, such that

$$\langle \mathbf{S}_{i,a}\cdot\mathbf{S}_{j,b}\rangle = \frac{1}{N}\sum_{q}\langle \mathbf{S}_{q,a}\cdot\mathbf{S}_{-q,b}\rangle\, e^{iq\cdot R}, \tag{C.2.10}$$

yielding

$$\langle \mathbf{S}_{q,a}\cdot\mathbf{S}_{-q,b}\rangle = \frac{1}{N}e^{iq\cdot\phi}\sum_{i,j}\langle \mathbf{S}_{i,a}\cdot\mathbf{S}_{j,b}\rangle\, e^{-iq\cdot R} = \sum_{R}\langle \mathbf{S}_{i,a}\cdot\mathbf{S}_{j,b}\rangle\, e^{-iq\cdot R}, \tag{C.2.11}$$

where R is the distance between i and j in the superlattice, and where we introduced a phase factor, stemming from the difference of position inside the magnetic unit cell. For example if had we looked at $a=1, b=2$

$$\langle \mathbf{S}_{q,1}\cdot\mathbf{S}_{-q,2}\rangle = e^{iq_y}\sum_{R}\langle \mathbf{S}_{i,a}\cdot\mathbf{S}_{j,b}\rangle\, e^{-iq\cdot R}. \tag{C.2.12}$$

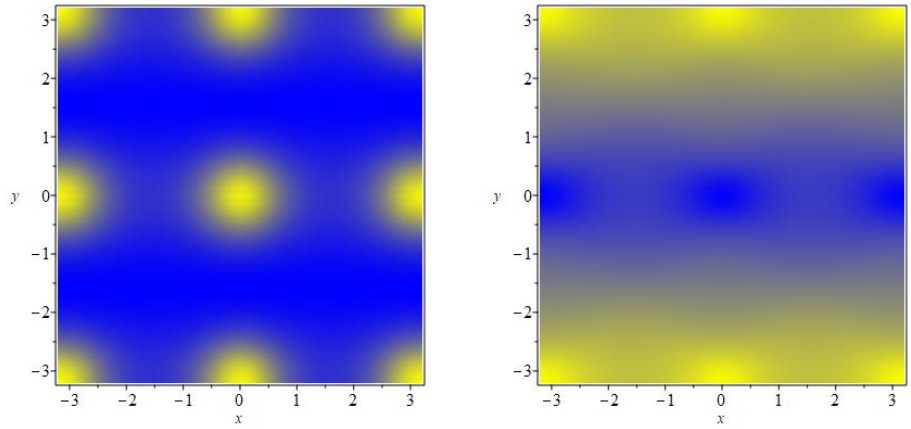
In this example, since $R = 2\,(i_x - j_x, i_y - j_y)$, the periodicity of q from the phase factor in the sum is π in both directions, but the periodicity from the phase factor outside of the sum is 2π in the y-direction. Thus, from this correlation function, we would expect a periodicity of 2π in the y-direction and one of π in the x-direction.
The lowest order correction to the correlation function is then

$$\delta\langle \mathbf{S}_{q,a}\cdot\mathbf{S}_{-q,b}\rangle = S\left[\left(1+(-1)^{\lambda_{ab}}\right)\Re\left(\left(\mathcal{V}_q\mathcal{V}_q^\dagger\right)_{ba}\right) + \left(1-(-1)^{\lambda_{ab}}\right)\Re\left(\left(-\mathcal{V}_q\mathcal{U}_q^\dagger\right)_{ba}\right)\right]. \tag{C.2.13}$$

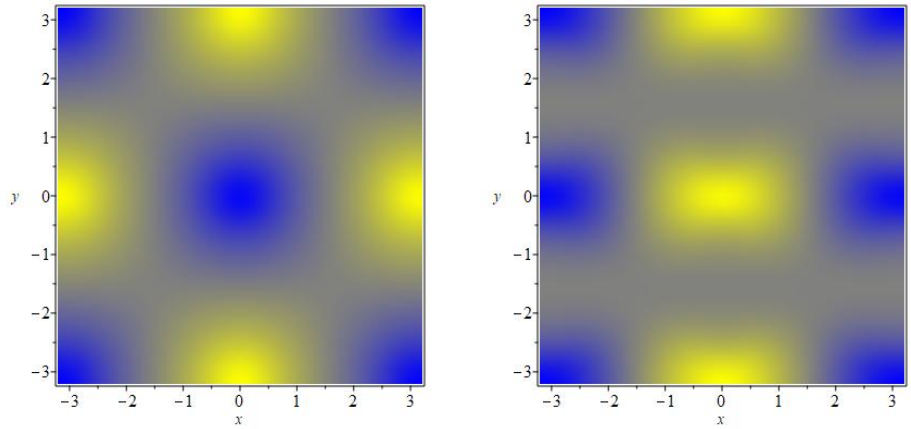
Let us consider the correlation between a spin on sublattice 1 and one on each sublattice. From the explicit forms shown in Eqs. (5.4.28) and (5.4.30), we find

$$\begin{aligned}
\frac{\delta\langle \mathbf{S}_{q,1}\cdot\mathbf{S}_{-q,1}\rangle}{4S} &= (M_2^+)^2 + (M_2^-)^2 = \frac{(T_{av}+T_2)^2}{4\omega^+(\omega^+ + M_3^+)} + \frac{(T_{av}-T_2)^2}{4\omega^-(\omega^- + M_3^-)},\\
\frac{\delta\langle \mathbf{S}_{q,1}\cdot\mathbf{S}_{-q,2}\rangle}{4S} &= -M_2^+(M_3^+ + \omega^+) - M_2^-(M_3^- + \omega^-) = -\left(\frac{(T_{av}+T_2)}{4\omega^+} + \frac{(T_{av}-T_2)}{4\omega^-}\right),\\
\frac{\delta\langle \mathbf{S}_{q,1}\cdot\mathbf{S}_{-q,3}\rangle}{4S} &= -M_2^+(M_3^+ + \omega^+) + M_2^-(M_3^- + \omega^-) = -\left(\frac{(T_{av}+T_2)}{4\omega^+} - \frac{(T_{av}-T_2)}{4\omega^-}\right),\\
\frac{\delta\langle \mathbf{S}_{q,1}\cdot\mathbf{S}_{-q,4}\rangle}{4S} &= \left((M_2^+)^2 - (M_2^-)^2\right) = \frac{(T_{av}+T_2)^2}{4\omega^+(\omega^+ + M_3^+)} - \frac{(T_{av}-T_2)^2}{4\omega^-(\omega^- + M_3^-)}.
\end{aligned} \tag{C.2.14}$$

Illustrations of these correlation functions are shown in Fig. C.1, but these are only suggestive, as the actual expressions diverge around the points $q = (0,0), (0,\pi), (\pi,0), (\pi,\pi)$.



(a) $(a,b) = (1,1)$ (b) $(a,b) = (1,2)$



(c) $(a,b) = (1,3)$ (d) $(a,b) = (1,4)$

Figure C.1: Quantum corrections to the momentum spin-spin correlation function. Parameters: $\theta = 0$, $\eta = 0.625$.

C.3 Finite temperature correlations - four sublattices

We assume now that the temperature is no longer zero. This modifies the expectation value of the Bogoliubov-operators, namely such that

$$\langle \boldsymbol{\beta}^\dagger_{q,a} \boldsymbol{\beta}_{q+Q,b} \rangle = \delta_{ab}\delta_{Q,0} \begin{cases} n_B(\omega_{a,q}) \text{ if } a \leq 4, \\ 1 + n_B(\omega_{a,q}) \text{ if } a \geq 5 \end{cases} , \tag{C.3.1}$$

where $n_B(\omega)$ is the Bose-function. Then

$$\begin{aligned} \langle b^\dagger_{q,a} b_{q+Q,b} \rangle &= \sum_{cd} \langle \boldsymbol{\beta}^\dagger_{q,c} \mathcal{B}^\dagger_{ca}(q) \mathcal{B}_{bd}(q+Q) \boldsymbol{\beta}_{q+Q,d} \rangle = \sum_{cd} \mathcal{B}^\dagger_{ca}(q) \mathcal{B}_{bd}(q+Q) \langle \boldsymbol{\beta}^\dagger_{q,c} \boldsymbol{\beta}_{q+Q,d} \rangle \\ &= \sum_{c=1}^{4} n_B(\omega_{q,c}) \mathcal{B}_{bc}(q) \mathcal{B}^\dagger_{ca}(q) \delta_{Q,0} + \sum_{c=5}^{8} \left(1 + n_B(\omega_{q,c})\right) \mathcal{B}_{bc}(q) \mathcal{B}^\dagger_{ca}(q) \delta_{Q,0} \\ &= \delta_{Q,0} \left(\mathcal{U}_q \underline{\underline{n_B}}(q) \mathcal{U}^\dagger_q + \mathcal{V}_q \left(1 + \underline{\underline{n_B}}(q)\right) \mathcal{V}^\dagger_q \right)^*_{ba}, \end{aligned} \tag{C.3.2}$$

where

$$\underline{\underline{n_B}}(q) = \begin{pmatrix} n_B(\omega_{q,1}) & 0 & 0 & 0 \\ 0 & n_B(\omega_{q,2}) & 0 & 0 \\ 0 & 0 & n_B(\omega_{q,3}) & 0 \\ 0 & 0 & 0 & n_B(\omega_{q,4}) \end{pmatrix}. \tag{C.3.3}$$

Similarly

$$\langle b_{q,a} b_{-q+Q,b} \rangle = -\delta_{Q,0} \left(\mathcal{U}_q \underline{\underline{n_B}}(q) \mathcal{V}_q^\dagger + \left(\mathcal{V}_q \left(1 + \underline{\underline{n_B}}(q) \right) \mathcal{U}_q^\dagger \right)^* \right)_{ba}. \tag{C.3.4}$$

Thus the temperature-dependent quantum correction to the structure factor is

$$\begin{aligned} \frac{\delta \langle \mathbf{S}_{q,a} \cdot \mathbf{S}_{-q,b} \rangle (T)}{S} &= \left(1 + (-1)^{\lambda_{ab}} \right) \Re \left[\left(\mathcal{U}_q \underline{\underline{n_B}}(q) \mathcal{U}_q^\dagger + \mathcal{V}_q \left(1 + \underline{\underline{n_B}}(q) \right) \mathcal{V}_q^\dagger \right)^*_{ba} \right] \\ &\quad - \left(1 - (-1)^{\lambda_{ab}} \right) \Re \left[\left(\mathcal{U}_q \underline{\underline{n_B}}(q) \mathcal{V}_q^\dagger + \left(\mathcal{V}_q \left(1 + \underline{\underline{n_B}}(q) \right) \mathcal{U}_q^\dagger \right)^* \right)_{ba} \right]. \end{aligned} \tag{C.3.5}$$

C.4 Zero-temperature correlation - single lattice

To lowest order in $1/S$ in the single lattice picture we find

$$\begin{aligned} \mathbf{S}_i \cdot \mathbf{S}_j = S^2 \cos(\theta_j - \theta_i) + S \Bigg[& \frac{1 + \cos(\theta_j - \theta_i)}{2} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) \\ & + \frac{1 - \cos(\theta_j - \theta_i)}{2} \left(b_i b_j + b_j^\dagger b_i^\dagger \right) - \cos(\theta_j - \theta_i) \left(b_i^\dagger b_i + b_j^\dagger b_j \right) \Bigg]. \end{aligned} \tag{C.4.1}$$

The first term represents the spin-spin correlation due to the assumption of magnetic order on which the H.P. operators are defined, and is not interesting. The magnonic contribution is the Fourier transform of

$$\Delta S(R_{ij}) = \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle - S(S - 2 \langle b_i^\dagger b_i \rangle) \cos(\theta_j - \theta_i), \tag{C.4.2}$$

where we included the contribution from the magnons which simply reparametrizes S. Now, consider the relation

$$\cos(\theta_j - \theta_i) = e^{iQ_1 \cdot R_{ij}} \cos^2(\theta/2) + e^{iQ_2 \cdot R_{ij}} \sin^2(\theta/2), \tag{C.4.3}$$

where $Q_1 = (0, \pi)$, $Q_2 = (\pi, 0)$. To see that this relation is true we should in principle check whether it holds for spins on all different ferromagnetic sublattices. For instance a spin with $\theta_i = 0$ and its' nearest neighbor with $\theta_j = \theta$ their relative angle is θ and $R_{ij} = R_i - R_j = (1, 0)$ (since the lattice constant is set to one). Then

$$\begin{aligned} &\cos(\theta_j - \theta_i) = \cos(\theta) \\ &e^{iQ_1 \cdot R_{ij}} \cos^2(\theta/2) + e^{iQ_2 \cdot R_{ij}} \sin^2(\theta/2) = \cos^2(\theta/2) - \sin^2(\theta/2) = \cos(\theta), \end{aligned} \tag{C.4.4}$$

and similar relations may be checked for i, j on other sites. We start by Fourier transforming $\cos(\theta_j - \theta_i) \langle b_i^\dagger b_j \rangle$

$$\begin{aligned} &\int d^2 R_{ij} \; e^{-iq \cdot R_{ij}} \left(e^{iQ_1 \cdot R_{ij}} \cos^2(\theta/2) + e^{iQ_2 \cdot R_{ij}} \sin^2(\theta/2) \right) \langle b_i^\dagger b_j \rangle \\ &= \cos^2(\theta/2) \langle b_{q-Q_1}^\dagger b_{q-Q_1} \rangle + \sin^2(\theta/2) \langle b_{q-Q_2}^\dagger b_{q-Q_2} \rangle, \end{aligned} \tag{C.4.5}$$

where we used that $\langle b_i^\dagger b_j \rangle = \int \frac{d^2 q}{(2\pi)^2} e^{iq \cdot R_{ij}} \langle b_q^\dagger b_q \rangle$, which follows from translation invariance. Similarly

$$\begin{aligned} &\int d^2 R_{ij} \; e^{-iq \cdot R_{ij}} \left(e^{iQ_1 \cdot R_{ij}} \cos^2(\theta/2) + e^{iQ_2 \cdot R_{ij}} \sin^2(\theta/2) \right) \langle b_i b_j \rangle \\ &= \cos^2(\theta/2) \langle b_{q-Q_1} b_{-q+Q_1} \rangle + \sin^2(\theta/2) \langle b_{q-Q_2} b_{-q+Q_2} \rangle. \end{aligned} \tag{C.4.6}$$

Combining these expressions we find

$$\begin{aligned}\Delta S_q/S &= \langle b_q^\dagger b_q\rangle + \cos^2(\theta/2)\,\langle b_{q-Q_1}^\dagger b_{q-Q_1}\rangle + \sin^2(\theta/2)\,\langle b_{q-Q_2}^\dagger b_{q-Q_2}\rangle \\ &+ \frac{\langle b_q b_{-q}\rangle + \langle b_{-q}^\dagger b_q^\dagger\rangle}{2} + \cos^2(\theta/2)\frac{\langle b_{q-Q_1} b_{-q+Q_1}\rangle + \langle b_{-q+Q_1}^\dagger b_{q-Q_1}^\dagger\rangle}{2} \\ &+ \sin^2(\theta/2)\frac{\langle b_{q-Q_1} b_{-q+Q_1}\rangle + \langle b_{-q+Q_1}^\dagger b_{q-Q_1}^\dagger\rangle}{2} \\ &= -1 + \frac{J_n(q)}{2\omega_q} + \cos^2(\theta/2)\frac{J_n(q-Q_1)}{2\omega_{q-Q_1}} + \sin^2(\theta/2)\frac{J_n(q-Q_2)}{2\omega_{q-Q_2}} \\ &- \left(\frac{J_{an}(q)}{2\omega_q} + \cos^2(\theta/2)\frac{J_{an}(q-Q_1)}{2\omega_{q-Q_1}} + \sin^2(\theta/2)\frac{J_{an}(q-Q_2)}{2\omega_{q-Q_2}}\right),\end{aligned} \tag{C.4.7}$$

where in the last line we used the expressions for the zero-temperature magnon expectation values (6.2.1) and (6.2.2). Thus the magnonic correction to the spin-spin correlation function in Fourier space is

$$\begin{aligned}\Delta S_q + S = \frac{S}{2}\Bigg[&\sqrt{\frac{J_n(q)-J_{an}(q)}{J_n(q)+J_{an}(q)}} + \cos^2(\theta/2)\sqrt{\frac{J_n(q-Q_1)-J_{an}(q-Q_1)}{J_n(q-Q_1)+J_{an}(q-Q_1)}} \\ &+ \sin^2(\theta/2)\sqrt{\frac{J_n(q-Q_2)-J_{an}(q-Q_2)}{J_n(q-Q_2)+J_{an}(q-Q_2)}}\Bigg].\end{aligned} \tag{C.4.8}$$

Take now the first term in (C.4.8) and expand it to first power in η. We then obtain

$$\begin{aligned}&\sqrt{\frac{J_n(q)-J_{an}(q)}{J_n(q)+J_{an}(q)}} \\ &\approx \frac{1-\xi_{q_x}\xi_{q_y} - \eta\left[(\cos^2(\theta/2)\xi_{q_x}\bar{\xi}_{q_y}^2 + \sin^2(\theta/2)\xi_{q_y}\bar{\xi}_{q_x}^2)(1+\xi_{q_x}\xi_{q_y}) + \cos\theta(\xi_{q_x}-\xi_{q_y})\right]}{\sqrt{1-\xi_{q_x}^2\xi_{q_y}^2}}.\end{aligned} \tag{C.4.9}$$

The coefficient to the zeroth power in η diverges at $q = (0,\pi), (\pi,0)$.

Appendix D

Interaction terms in the four sublattice picture

We will here write the interaction Hamiltonian in the four sublattice picture. The next order terms of the large S expansion in eqs. 5.1.10-5.1.12 are

$$\mathcal{O}((1/S)^0)(\tilde{S}_1^{i,a}\tilde{S}_1^{j,b}) = -\frac{\left(b_{i,a}^\dagger b_{i,a} b_{i,a} + b_{i,a}^\dagger b_{i,a}^\dagger b_{i,a}\right)\left(b_{j,b} + b_{j,b}^\dagger\right) + \left(b_{i,a} + b_{i,a}^\dagger\right)\left(b_{j,b}^\dagger b_{j,b} b_{j,b} + b_{j,b}^\dagger b_{j,b}^\dagger b_{j,b}\right)}{8}$$

$$\mathcal{O}((1/S)^0)(\tilde{S}_2^{i,a}\tilde{S}_2^{j,b}) = \frac{\left(b_{i,a}^\dagger b_{i,a} b_{i,a} - b_{i,a}^\dagger b_{i,a}^\dagger b_{i,a}\right)\left(b_{j,b} - b_{j,b}^\dagger\right) + \left(b_{i,a} - b_{i,a}^\dagger\right)\left(b_{j,b}^\dagger b_{j,b} b_{j,b} - b_{j,b}^\dagger b_{j,b}^\dagger b_{j,b}\right)}{8}$$

$$\mathcal{O}((1/S)^0)(\tilde{S}_3^{i,a}\tilde{S}_3^{j,b}) = b_{i,a}^\dagger b_{i,a} b_{j,b}^\dagger b_{j,b}.$$

These are all four-operator terms and mostly resemble interaction terms between the H.P. bosons, albeit with some anomalous terms containing unequal factors of creation/annihilation operators.

D.1 N.N. interaction terms

The N.N. interaction term can now be written

$$\begin{aligned}
W_1 = -\frac{J_1}{2}\sum_{\langle(i,a),(j,b)\rangle}\Bigg[&\frac{\left(b_{i,a}^\dagger b_{i,a} b_{i,a} + b_{i,a}^\dagger b_{i,a}^\dagger b_{i,a}\right)\left(b_{j,b} + b_{j,b}^\dagger\right) + \left(b_{i,a} + b_{i,a}^\dagger\right)\left(b_{j,b}^\dagger b_{j,b} b_{j,b} + b_{j,b}^\dagger b_{j,b}^\dagger b_{j,b}\right)}{8} \\
&- \cos(\theta_{j,b} - \theta_{i,a})\frac{\left(b_{i,a}^\dagger b_{i,a} b_{i,a} - b_{i,a}^\dagger b_{i,a}^\dagger b_{i,a}\right)\left(b_{j,b} - b_{j,b}^\dagger\right) + \left(b_{i,a} - b_{i,a}^\dagger\right)\left(b_{j,b}^\dagger b_{j,b} b_{j,b} - b_{j,b}^\dagger b_{j,b}^\dagger b_{j,b}\right)}{8} \\
&- \cos(\theta_{i,a} - \theta_{j,b}) b_{i,a}^\dagger b_{i,a} b_{j,b}^\dagger b_{j,b}\Bigg] \\
= -\frac{J_1}{2}\sum_{\langle(i,a),(j,b)\rangle}\Bigg[&\frac{\left(b_{i,a}^\dagger b_{i,a} b_{i,a} + b_{i,a}^\dagger b_{i,a}^\dagger b_{i,a}\right)\left(b_{j,b} + b_{j,b}^\dagger\right)}{4} \\
&- \cos(\theta_{i,a} - \theta_{j,b})\frac{\left(b_{i,a}^\dagger b_{i,a} b_{i,a} - b_{i,a}^\dagger b_{i,a}^\dagger b_{i,a}\right)\left(b_{j,b} - b_{j,b}^\dagger\right)}{4} - \cos(\theta_{i,a} - \theta_{j,b}) b_{i,a}^\dagger b_{i,a} b_{j,b}^\dagger b_{j,b}\Bigg],
\end{aligned} \tag{D.1.1}$$

where we used, that some of the terms are equal under the summation. Rearranging and using $1-\cos(x) = 2\cos(x/2)^2$ we obtain

$$W_1 = -\frac{J_1}{4}\sum_{\langle(i,a),(j,b)\rangle}\left[\cos^2\left(\frac{\theta_{i,a}-\theta_{j,b}}{2}\right)\left(b^\dagger_{i,a}b^\dagger_{i,a}b_{i,a}b_{j,b}+b^\dagger_{i,a}b_{i,a}b_{i,a}b^\dagger_{j,b}\right)\right.$$
$$\left.+\sin^2\left(\frac{\theta_{i,a}-\theta_{j,b}}{2}\right)\left(b^\dagger_{i,a}b_{i,a}b_{i,a}b_{j,b}+b^\dagger_{i,a}b^\dagger_{i,a}b_{i,a}b^\dagger_{j,b}\right)-2\cos(\theta_{i,a}-\theta_{j,b})b^\dagger_{i,a}b_{i,a}b^\dagger_{j,b}b_{j,b}\right], \tag{D.1.2}$$

which becomes

$$W_1 = -\frac{J_1}{4}\sum_{i,a,\delta}\left[\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right)\left(b^\dagger_{i,a}b^\dagger_{i,a}b_{i,a}b_{j,b}+b^\dagger_{i,a}b_{i,a}b_{i,a}b^\dagger_{j,b}\right)\right.$$
$$\left.+\sin^2\left(\frac{\theta+\phi(\delta)}{2}\right)\left(b^\dagger_{i,a}b_{i,a}b_{i,a}b_{j,b}+b^\dagger_{i,a}b^\dagger_{i,a}b_{i,a}b^\dagger_{j,b}\right)-2\cos\left(\theta+\phi(\delta)\right)b^\dagger_{i,a}b_{i,a}b^\dagger_{j,b}b_{j,b}\right], \tag{D.1.3}$$

where δ is a vector connecting (i,a) to one of its' nearest neighbors and (j,b), ϕ depend on δ. The phase ϕ is defined as in eq. (5.1.17). A Fourier transform of the separate terms yields

$$b^\dagger_{i,a}b^\dagger_{i,a}b_{i,a}b_{j,b}+b^\dagger_{i,a}b_{i,a}b_{i,a}b^\dagger_{j,b} = \frac{1}{N^2}\sum_{pqkl}\left[b^\dagger_{p,a}b^\dagger_{q,a}b_{k,a}b_{l,b}e^{i(p+q-k-l)\cdot R_{i,a}}e^{-il\cdot\delta}\right.$$
$$\left.+b^\dagger_{p,a}b_{q,a}b_{k,a}b^\dagger_{l,b}e^{i(p-q-k+l)\cdot R_{i,a}}e^{il\cdot\delta}\right] \tag{D.1.4}$$

$$b^\dagger_{i,a}b_{i,a}b_{i,a}b_{j,b}+b^\dagger_{i,a}b^\dagger_{i,a}b_{i,a}b^\dagger_{j,b} = \frac{1}{N^2}\sum_{pqkl}\left[b^\dagger_{p,a}b_{q,a}b_{k,a}b_{l,b}e^{i(p-q-k-l)\cdot R_{i,a}}e^{-il\cdot\delta}\right.$$
$$\left.+b^\dagger_{p,a}b^\dagger_{q,a}b_{k,a}b^\dagger_{l,b}e^{i(p+q-k+l)\cdot R_{i,a}}e^{il\cdot\delta}\right], \tag{D.1.5}$$

which upon an insertion into the interaction term and a subsequent summation over i yields

$$W_1 = -\frac{J_1}{4N}\sum_{\substack{a\delta\\pqkl}}\left[b^\dagger_{p,a}b_{l,b}e^{-il\cdot\delta}\left(\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right)b^\dagger_{q,a}b_{k,a}\delta_{p-l,k-q}+\sin^2\left(\frac{\theta+\phi(\delta)}{2}\right)b_{q,a}b_{k,a}\delta_{p-l,k+q}\right)\right.$$
$$+\left(\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right)b^\dagger_{k,a}b_{q,a}\delta_{p-l,k-q}+\sin^2\left(\frac{\theta+\phi(\delta)}{2}\right)b^\dagger_{k,a}b^\dagger_{q,a}\delta_{p-l,k+q}\right)b^\dagger_{l,b}b_{p,a}e^{il\cdot\delta}$$
$$\left.-2\cos\left(\theta+\phi(\delta)\right)e^{i(k-l)\cdot\delta}b^\dagger_{p,a}b_{q,a}b^\dagger_{k,b}b_{l,b}\delta_{p-q,l-k}\right], \tag{D.1.6}$$

which can be rewritten

$$W_1 = -\frac{J_1}{4N}\sum_{\substack{a\delta\\pqk}}\left[b^\dagger_{p+q,a}b_{p,b}e^{-ip\cdot\delta}\left(\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right)b^\dagger_{k,a}b_{k+q,a}+\sin^2\left(\frac{\theta+\phi(\delta)}{2}\right)b_{-k,a}b_{k+q,a}\right)\right.$$
$$+\left(\cos^2\left(\frac{\theta+\phi(\delta)}{2}\right)b^\dagger_{k+q,a}b_{k,a}+\sin^2\left(\frac{\theta+\phi(\delta)}{2}\right)b^\dagger_{k+q,a}b^\dagger_{-k,a}\right)b^\dagger_{p,b}b_{p+q,a}e^{ip\cdot\delta}$$
$$\left.-2\cos\left(\theta+\phi(\delta)\right)e^{iq\cdot\delta}b^\dagger_{p+q,a}b_{p,a}b^\dagger_{k,b}b_{k+q,b}\right]. \tag{D.1.7}$$

Finally, the sum over δ is performed,

$$W_1 = -\frac{J_1}{2N}\sum_{a,pqk}\Bigg[\cos(p_x)b^\dagger_{p+q,a}b_{p,a+\sigma(a)}\left(\cos^2\left(\frac{\theta}{2}\right)b^\dagger_{k,a}b_{k+q,a}+\sin^2\left(\frac{\theta}{2}\right)b_{-k,a}b_{k+q,a}\right)+\text{h.c.}$$
$$+\cos(p_y)b^\dagger_{p+q,a}b_{p,a-\sigma(a)}\left(\sin^2\left(\frac{\theta}{2}\right)b^\dagger_{k,a}b_{k+q,a}+\cos^2\left(\frac{\theta}{2}\right)b_{-k,a}b_{k+q,a}\right)+\text{h.c.}$$
$$-2\cos(\theta)\,b^\dagger_{p+q,a}b_{p,a}\left(\cos(q_x)b^\dagger_{k,a+\sigma(a)}b_{k+q,a+\sigma(a)}-\cos(q_y)b^\dagger_{k,a-\sigma(a)}b_{k+q,a-\sigma(a)}\right)\Bigg], \tag{D.1.8}$$

where $\sigma(a)$ is defined as in eq. (5.1.20). This is equivalent to

$$W_1 = -\frac{J_1}{2N}\sum_{a,pqk}\Bigg[\cos(p_x)\mathbf{b}^\dagger_{p+q,a}\mathbf{b}_{p,a\oplus\sigma(a)}\left(\cos^2\left(\frac{\theta}{2}\right)\mathbf{b}^\dagger_{k,a}\mathbf{b}_{k+q,a}+\sin^2\left(\frac{\theta}{2}\right)\mathcal{F}_{ab}\mathbf{b}^\dagger_{k,b}\mathbf{b}_{k+q,a}\right)+\text{h.c.}$$
$$+\cos(p_y)\mathbf{b}^\dagger_{p+q,a}\mathbf{b}_{p,a\ominus\sigma(a)}\left(\sin^2\left(\frac{\theta}{2}\right)\mathbf{b}^\dagger_{k,a}\mathbf{b}_{k+q,a}-\cos^2\left(\frac{\theta}{2}\right)\mathcal{F}_{ab}\mathbf{b}^\dagger_{k,b}\mathbf{b}_{k+q,a}\right)+\text{h.c.}$$
$$+2\cos(\theta)\,\mathbf{b}^\dagger_{p+q,a}\mathbf{b}_{p,a}\left(\cos(q_x)\mathbf{b}^\dagger_{k,a\oplus\sigma(a)}\mathbf{b}_{k+q,a\oplus\sigma(a)}-\cos(q_y)\mathbf{b}^\dagger_{k,a\ominus\sigma(a)}\mathbf{b}_{k+q,a\ominus\sigma(a)}\right)\Bigg], \tag{D.1.9}$$

where the symbol $\oplus$ ($\ominus$) refers to summation (subtraction) modulo 4, and is not to be confused with a direct sum. Formally, this may be written in the much neater form

$$W_1 = -\frac{J_1}{2N}\sum_{pqk}\mathbf{b}^\dagger_{p+q,a_1}\mathbf{b}_{p,b_1}\mathcal{W}_{1a_1,b_1,a_2,b_2}(p,q)\mathbf{b}^\dagger_{k,a_2}\mathbf{b}_{k+q,b_2}+\text{h.c.}, \tag{D.1.10}$$

where we assume implicit summation over repeated sublattice indices, and these range from 1 to 4.

D.2 N.N.N. interaction terms

For the N.N.N. interaction, the relative angle between the interacting spins is always equivalent to π. From eq. (D.1.2) we may infer

$$W_2 = -\frac{J_2}{4}\sum_{i,a,\delta}\left(b^\dagger_{i,a}b_{i,a}b_{i,a}b_{j,b}+b^\dagger_{i,a}b^\dagger_{i,a}b_{i,a}b^\dagger_{j,b}\right)+2b^\dagger_{i,a}b_{i,a}b^\dagger_{j,b}b_{j,b}, \tag{D.2.1}$$

where δ connects site (i,a) with one of it's nearest neighbors, and (j,b) depends on δ. A Fourier-transform and subsequent summation over i yields

$$W_2 = -\frac{J_2}{4N}\sum_{\substack{a,\delta\\pqkl}}\Big[\left(b^\dagger_{p,a}b_{q,a}b_{k,a}b_{l,b}e^{-il\cdot\delta}\delta_{p-l,k+q}+b^\dagger_{q,a}b^\dagger_{k,a}b_{p,a}b^\dagger_{l,b}e^{il\cdot\delta}\delta_{p-l,k+q}\right)$$
$$+2b^\dagger_{p,a}b_{q,a}b^\dagger_{k,b}b_{l,b}e^{i(k-l)\cdot\delta}\delta_{p-q,l-k}\Big], \tag{D.2.2}$$

which upon redefining indices becomes

$$W_2 = -\frac{J_2}{4N}\sum_{\substack{a,\delta\\pqk}}\Big[\left(b^\dagger_{p+q,a}b_{p,b}b_{-k,a}b_{k+q,a}e^{-ip\cdot\delta}+b^\dagger_{k+q,a}b^\dagger_{-k,a}b^\dagger_{p,b}b_{p+q,a}e^{ip\cdot\delta}\right)$$
$$+2b^\dagger_{p+q,a}b_{p,a}b^\dagger_{k,b}b_{k+q,b}e^{-iq\cdot\delta}\Big], \tag{D.2.3}$$

and finally doing the δ-sum

$$W_2 = -\frac{J_2}{4N}\sum_{a,pqk}\Big[4\cos(p_x)\cos(p_y)\left(b^\dagger_{p+q,a}b_{p,a+2}b_{-k,a}b_{k+q,a} + b^\dagger_{k+q,a}b^\dagger_{-k,a}b^\dagger_{p,a+2}b_{p+q,a}\right) \\ +8\cos(q_x)\cos(q_y)b^\dagger_{p+q,a}b_{p,a}b^\dagger_{k,a+2}b_{k+q,a+2}\Big]. \tag{D.2.4}$$

Again, this is equivalent to

$$W_2 = -\frac{J_2}{N}\sum_{pqk}\cos(p_x)\cos(p_y)\left(\mathbf{b}^\dagger_{p+q,a}\mathbf{b}_{p,a\oplus 2}\mathcal{F}_{ab}\mathbf{b}^\dagger_{k,b}\mathbf{b}_{k+q,a} + \mathbf{b}^\dagger_{k+q,a}\mathcal{F}_{ab}\mathbf{b}_{k,b}\mathbf{b}^\dagger_{p,a\oplus 2}\mathbf{b}_{p+q,a}\right) \\ +\cos(q_x)\cos(q_y)\mathbf{b}^\dagger_{p+q,a}\mathbf{b}_{p,a}\mathbf{b}^\dagger_{k,a\oplus 2}\mathbf{b}_{k+q,a\oplus 2}, \tag{D.2.5}$$

and once more, this can be formally written as

$$W_2 = -\frac{J_2}{N}\sum_{a,pqk}\mathbf{b}^\dagger_{p+q,a_1}\mathbf{b}_{p,b_1}\mathcal{W}_{2a_1,b_1,a_2,b_2}(p,q)\mathbf{b}^\dagger_{k,a_2}\mathbf{b}_{k+q,b_2} + \text{h.c.} \tag{D.2.6}$$

D.3 Full interaction term

Due to the results of the two previous subsections, we may write the interaction between Holstein-Primakoff bosons as

$$W = -\frac{1}{N}\sum_{pqk}\mathbf{b}^\dagger_{p+q,a_1}\mathbf{b}_{p,b_1}\mathcal{W}_{a_1,b_1,a_2,b_2}(p,q)\mathbf{b}^\dagger_{k,a_2}\mathbf{b}_{k+q,b_2} + \text{h.c.}, \tag{D.3.1}$$

where $\mathcal{W} = J_2\left(\eta\mathcal{W}_1 + \mathcal{W}_2\right)$. As expected, the interaction due to nearest-neighbor spins vanishes as η goes to zero, which is the limit where the system decouples into two non-interacting AFM sublattices.