Utrecht University

Faculty of Science

Quantum fluctuations in antiferromagnetic spin configurations

Bachelor Thesis

Solange Schrijnder van Velzen
Physics and Astronomy
January 2016

Supervised by R.A.Duine
Institute for Theoretical Physics
Utrecht University

Abstract

We consider fluctuations in magnetic systems around the classically-ordered ground state. We use a Holstein-Primakoff transformation to calculate the zero-point energy fluctuations in antiferromagnetic lattice configurations using the Heisenberg exchange Hamiltonian. We show that these quantum fluctuations lower the classically expected ground state. Furthermore we provide a numerical method to calculate dispersion relations for magnetic systems and specifically show that our analytical results can be produced. Also, we investigate the spin-flop transition in a one dimensional antiferromagnetic system with anisotropy. Our calculations show that the transition occurs at $B/K \approx -14$, where B is the external field and K the anisotropy constant. Furthermore, we show that quantum fluctuations decrease the energy of both the antiferromagnetic and the spin-flop state by calculating the dispersion relation. Our results imply a shift of the transition point between the two states. Our results are a first step towards incorporating the effects of quantum fluctuations in inhomogeneous antiferromagnets.

Contents

Contents **1**

1 Introduction **2**

2 Ferromagnets **4**
2.1 Semi-classical approach 4
2.2 Holstein-Primakoff Transformation 6

3 Antiferromagnets **11**
3.1 Semi-classical approach 11
3.2 Holstein-Primakoff Transformation 13

4 Numerical methods **18**
4.1 (Anti-)Ferromagnetic Heisenberg Model 19

5 Classical ground state of an antiferromagnetic Hamiltonian with Dzyaloshinskii-Moriya interactions **21**

6 Phase transition to the spin-flop state in antiferromagnets **23**
6.1 Magnon energies for the spin-flop state 25
6.2 Magnon energies for the antiferromagnetic state 27
6.3 Quantum fluctuations 28

7 Conclusion **30**

8 Appendix **31**

References **34**

1 Introduction

The magnetic behaviour of a material depends on its structure, particularly its electronic configuration. Ferromagnetic materials for example exhibit a long-range ordering which causes the unpaired electron spins to line up parallel with each other which induces a net magnetization in the material. Above a critical temperature known as the Curie temperature, ferromagnetic ordering disappears as a result of thermal agitation. Antiferromagnetic materials on the other hand have no net magnetization, since their spins align in such a way that each spin on the lattice is orientated anti-parallel to the neighbouring spin. Above the critical temperature, known as the Néel temperature, antiferromagnetic order disappears.

Excitations of the ground state of magnetic materials can be described by spin waves. Spin waves are propagating disturbances in the magnetic ordering of materials (see Figure 1). In the quantum mechanical picture the excitations can be described by a quasiparticle, a magnon, which carries a fixed amount of energy and lattice momentum. The quantum theory of spin waves enables to study physical properties of magnetic configurations at nonzero temperatures. This theory was originally introduced by F. Bloch [1] and the main assumption is that the system has an ordered ground state and the excited states are described as spin waves. It is shown that the ferromagnetic state is an eigenstate of the Heisenberg exchange Hamiltonian for positive exchange constant J, which is commonly used to describe ferromagnetic systems. On the contrary the antiferromagnetic Néel state is not an eigenstate of the Heisenberg exchange Hamiltonian for a negative exchange constant. This causes quantum fluctuations on top of the classical description of the ground state. Quantum fluctuations describe the deviation from the classical ground state due to quantum mechanical effects.

In this thesis we discuss the effect of quantum fluctuations in antiferromagnetic configurations. We incorporate Heisenberg exchange interactions, anisotropy, an external field and in some cases also the Dzyaloshinskii-Moriya coupling. The effect of quantum fluctuations in magnetic models has attracted much interest in recent years [2] [3] [4]. Experimental and theoretical studies of those systems have revealed a plethora of quantum fluctuation phenomena. In previous research quantum fluctuations in magnetic skyrmions were investigated using numerical methods [5] [6]. Skyrmions are vortex-like configurations that occur in magnetic materials. A clear analytical description of skyrmions in antiferromagnetic systems however remains an open problem. In chapter 3 we start with a description of ferromagnets, both in

a semi-classical way and a quantum mechanical way. We will see that there are no quantum fluctuations that effect the ground state of a homogeneous ferromagnet. We will also calculate the magnetization of a ferromagnetic system as a function of the temperature. In the next chapter, chapter 4, we will discuss the antiferromagnet. As for the ferromagnet, we will give a description in a semi-classical way and a quantum mechanical way and calculate the magnetization. We will show that quantum fluctuations lower the classical ground state for antiferromagnets. In chapter 5 we will discuss numerical methods to diagonalize the Hamiltonian and find the dispersion relation for magnetic configurations in general. We will provide a result for the antiferromagnet and the ferromagnet and show that this confirms our analytic calculations. In chapter 6 we investigate the phase transition from the antiferromagnetic to the spin-flop state. The pure phase transition occurs in an antiferromagnetic system without Dzyaloshinskii-Moriya interactions by increasing the strength of the external field. We explicitly calculate the dispersion relation for both states and calculate the quantum correction to the ground states.

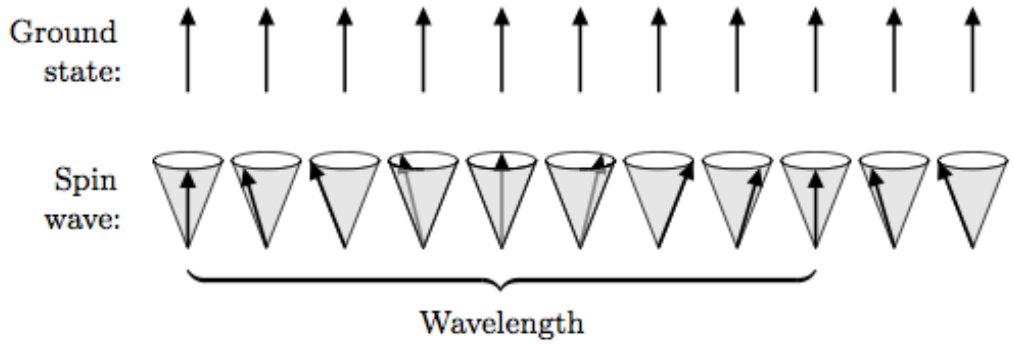


Figure 1: In the ground state of a ferromagnet, all spins point in the same direction. The lowest energy excitation is described by a single spin-wave, in which the spins precess in a conical motion. A long wavelength spin wave carries very little energy, because the difference in direction between neighbouring dipoles (spins) is small. Copyright: Addison-Wesley 2000.

2 Ferromagnets

In this chapter we discuss the basics of the ferromagnet. We first perform a classical calculation using the Heisenberg-exchange Hamiltonian. Secondly, we perform a Holstein- Primakoff transformation on the same Hamiltonian to figure out whether quantum fluctuations affect the classical ground state of the ferromagnet.

The Heisenberg exchange Hamiltonian describes a system of interacting spins in a magnetic material and can be used to examine the behaviour of spin waves (magnons). The Heisenberg exchange Hamiltonian is seen in the equation below, where the sum goes over all neighbouring pairs i and j on the lattice sites, $\mathbf{S}_i$ denotes the spin operator at site i and J is the exchange coupling constant. This coupling constant will be positive in the case of ferromagnets $J = |J|$, such that the energy is minimized when all spins are pointing in the same direction.

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{1}$$

2.1 Semi-classical approach

We will start with a semi-classical approach to the ferromagnet. Semi-classical physics refers to a theory in which one part is described classically whereas the other is treated quantum-mechanically. In this specific case we use a quantum mechanical description of the spins and the classical equations of motion described by Ehrenfest's theorem, as stated in the equation below.

$$\frac{d}{dt}\langle \mathbf{S}_k \rangle = -\frac{i}{\hbar}\langle [\mathbf{S}_k, H] \rangle. \tag{2}$$

Assume a one dimensional chain of spins pointing along the z-axis, separated by a distance a. Using the Heisenberg exchange Hamiltonian from Equation 1, where we assume only nearest neighbour interactions, Ehrenfest's theorem leads to

$$\begin{aligned}\frac{d}{dt}\langle \mathbf{S}_k \rangle = J\frac{i}{\hbar}\langle [\mathbf{S}_k, \sum_i S_i^x S_{i+1}^x + S_i^x S_{i-1}^x] + [\mathbf{S}_k, \sum_i S_i^y S_{i+1}^y + S_i^y S_{i-1}^y] \\ + [\mathbf{S}_k, \sum_i S_i^z S_{i+1}^z + S_i^z S_{i-1}^z] \rangle.\end{aligned} \tag{3}$$

There is still a sum over i left to sum all pairs. In order to evaluate the equations of motion for S_k^x, S_k^y and S_k^z we use the commutation relations

given by

$$[S_i^x, S_j^y] = i\hbar S_k^z \delta_{ij}. \tag{4}$$

We now give a detailed evaluation of Equation 3 for the S_i^x component of $\mathbf{S}_i$. With the use of Equation 4 we can simplify the expression to Equation 5a, where the sum over i vanished since the spins always commute when $k \neq i$. Furthermore, we made use of the commutation relations to simplify the expression to Equation 5b.

$$\frac{d}{dt}\langle S_i^x \rangle = J\frac{i}{\hbar}\langle [S_i^x, S_i^y S_{i-1}^y] + [S_i^x, S_i^y S_{i+1}^y] + [S_i^x, S_i^z S_{i-1}^z] + [S_i^x, S_i^z S_{i+1}^z] \rangle, \tag{5a}$$

$$\frac{d}{dt}\langle S_i^x \rangle = J\langle -S_i^z(S_{i-1}^y + S_{i+1}^y) + S_i^y(S_{i-1}^z + S_{i+1}^z) \rangle. \tag{5b}$$

The same can be done for the S_i^y and S_i^z components of $\mathbf{S}_i$, but they can also be found using a cyclic permutation on Equation 5b. The equations of motion for all three components of $\mathbf{S}_i$ are

$$\begin{aligned}
\frac{d}{dt}S_i^x &= -JS_i^z(S_{i-1}^y + S_{i+1}^y) + JS_i^y(S_{i-1}^z + S_{i+1}^z), \\
\frac{d}{dt}S_i^y &= -JS_i^x(S_{i-1}^z + S_{i+1}^z) + JS_i^z(S_{i-1}^x + S_{i+1}^x), \\
\frac{d}{dt}S_i^z &= -JS_i^y(S_{i-1}^x + S_{i+1}^x) + JS_i^x(S_{i-1}^y + S_{i+1}^y).
\end{aligned} \tag{6}$$

These relations can be generalized to $\frac{d}{dt}\mathbf{S}_i^x = J\mathbf{S}_i \times (\mathbf{S}_{i-1} + \mathbf{S}_{i+1})$. Considering small deviations for $\mathbf{S}$ with reverence to the z-axis, such that $S^z = \hbar S$ and $S^x, S^y \ll S^z$, the equations of motion in Equation 6 reduce to:

$$\begin{aligned}
\frac{d}{dt}S_i^x &\approx JS(\hbar - S_{i-1}^y - S_{i+1}^y + 2S_i^y), \\
\frac{d}{dt}S_i^y &\approx JS(\hbar - 2S_i^x + S_{i-1}^x + S_{i+1}^x), \\
\frac{d}{dt}S_i^z &\approx 0.
\end{aligned} \tag{7}$$

An educated guess can now be taken by $S_j^x = Ae^{i\mathbf{k}\cdot\mathbf{R}_j - i\omega t}$ and $S_j^y = Be^{i\mathbf{k}\cdot\mathbf{R}_j - i\omega t}$, where a is the distance between the lattice points and $\mathbf{R}_j = \mathrm{j}\cdot a\hat{x}$ indicates the position in our one dimensional model. Plugging in these equations as an ansatz yields the following result:

$$\begin{aligned}
i\omega A + 2SJ\hbar B\,(1 - \cos(k_x a)) &= 0, \\
-i\omega B + 2SJ\hbar A\,(1 - \cos(k_x a)) &= 0.
\end{aligned} \tag{8}$$

Finding the dispersion relation from this set of equations can be done by using the matrix notation given by

$$\begin{bmatrix} i\omega & 2SJ\hbar(1-\cos(k_x a)) \\ 2SJ\hbar(1-\cos(k_x a)) & -i\omega \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = 0. \tag{9}$$

Calculating the zero points of the determinant will give the dispersion relation of a one dimensional ferromagnet. This results in $\omega_k = 2SJ\hbar(1 - cos(k_x a))$. Extracting the eigenvectors of this matrix will provide us the states a one dimensional ferromagnet can occupy. The two resulting eigenvectors are given by

$$v_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 1 \end{bmatrix}, \qquad v_2 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{10}$$

Eigenvector v_2 describes the static state where all the sites have their spin pointing along the positive z-axes. For eigenvector v_1 we find an eigenstate with magnons. Using v_1 for A and B in the used ansatz, the real part of this eigenstate for $a = 0$ gives

$$\begin{aligned} S_j^x &\propto \sin \omega t, \\ S_j^y &\propto \cos \omega t. \end{aligned} \tag{11}$$

This describes a precessing spin around the z-axis. If you now include all the sites you see that each site picks up an extra phase shift of $k_x a$. In fact you now have a spin wave, or magnon (see Figure 1). For $k \ll 1$, the dispersion reduces to $\omega_k \approx SJ\hbar(k_x a)^2$. As a magnon with wavevector k costs an energy $\hbar\omega_k > 0$ we conclude that the ground state of a one dimensional ferromagnet has no magnons.

2.2 Holstein-Primakoff Transformation

We will now include quantum mechanical effects in our calculations. To study the behaviour of magnons in our ferromagnetic system using spin-theory we would like to make them explicitly appear in the Hamiltonian. This can be done by using the Holstein-Primakoff transformation [7], which is a mapping from angular momentum operators to bosonic creation and annihilation operators [8]. Explicitly, the rising and lowering operators of $\mathbf{S}$ can be written in terms of creation and annihilation operators:

$$
\begin{aligned}
S_i^+ =& \hbar\sqrt{2S - a_i^\dagger a_i}\, a_i \simeq \sqrt{2S}\,\hbar a_i, \\
S_i^- =& \hbar a_i^\dagger \sqrt{2S - a_i^\dagger a_i} \simeq \sqrt{2S}\,\hbar a_i^\dagger, \\
S_i^z =& \hbar S - \hbar a_i^\dagger a_i,
\end{aligned} \tag{12}
$$

where $a_i^\dagger$ and a_i obey the commutation relation $[a_i, a_j^\dagger] = \delta_{ij}$. The operator $\hat{n}_i = a_i^\dagger a_i$ counts the number of bosons placed at site i and is therefore often called the number operator for site i. The boson number must satisfy the constraint $\langle \hat{n}_i \rangle \leq 2S$, since otherwise the expression in the square root would become negative and hence imaginary. Also, we performed a Taylor expansion on S_i^+ and S_i^- in powers of $1/S$ to simplify the expression. Keep in mind that by doing so we removed the critical information that a state with more than $2S$ magnons per lattice site would be non-physical. Furthermore, our final expansion is only accurate in the limit where S is large. In order to introduce these Holstein-Primakoff transformations we write the Hamiltonian in Equation 1 in terms of the rising and lowering operators of S. Also, since we only consider nearest neighbour interactions, we write $j = i + \delta$, where δ is a vector connecting nearest neighbour sites. To avoid double counting, we choose to run δ over only half the nearest neighbour vectors. As a model of our system we use hypercubic lattices. This means that in one dimension $\delta = +\hat{x}$, in two dimensions $\delta = +\hat{x}, +\hat{y}$ and in three dimensions $\delta = +\hat{x}, +\hat{y}, +\hat{z}$. These modifications result in the following Hamiltonian:

$$
H = -J \sum_i \sum_\delta S_i^z S_{i+\delta}^z + \frac{1}{2} S_i^+ S_{i+\delta}^+ + \frac{1}{2} S_i^- S_{i+\delta}^-. \tag{13}
$$

Consider first the fully ferromagnetic state, on which we act with the operator $\mathbf{S}$ to flip a single spin. The term $S_i^z S_{i+\delta}^z$ leaves the reversed spin at the same place and only gives an energy cost to reverse it. The terms $S_i^+ S_{i+\delta}^+ + S_i^- S_{i+\delta}^-$ will move the reversed spin to another site, such that it will create a spin wave with a certain dispersion. Now we perform the Holstein-Primakoff transformation, as described in Equation 12, to study the Heisenberg ferromagnet and its excitations. We only include terms up to quadratic order, as can be seen in Equation 14. Terms in the Hamiltonian which are higher order contain four or more boson operators and therefore represent interactions between bosons. However, since these are suppressed by at least by a factor $1/S$ compared to the non-interacting terms, their effects are small. Certainly at large S or when the boson number is small they can either be neglected to a first approximation or be treated as weak perturbations on

the non-interacting theory. After the Holstein-Primakoff transformation we find that

$$H = -J\hbar^2 \sum_i \sum_\delta S^2 - S a_i^\dagger a_i - S a_{i+\delta}^\dagger a_{i+\delta} + S a_{i+\delta}^\dagger a_i + S a_i^\dagger a_{i+\delta}. \tag{14}$$

To diagonalize this Hamiltonian we introduce Fourier-transformed boson operators by

$$\begin{aligned} a_i =& \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r_i}}\, a_{\mathbf{k}}, \\ a_i^\dagger =& \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r_i}}\, a_{\mathbf{k}}^\dagger. \end{aligned} \tag{15}$$

An important property of this transformation is that it is canonical. This means that it preserves the commutation relations. The operators $a_{\mathbf{k}}$ will obey the same kind of commutation relations as the original boson operators: $[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k},\mathbf{k}'}$. Before we insert the transformed operators we note that $-J\sum_i \sum_\delta \hbar^2 S^2$ is the same as $-JN\frac{z}{2}\hbar^2 S^2$, where z is the number of nearest neighbours. In our formulation $z = 2d$, where d denotes the dimension of the system. To calculate the rest of the sum we start by looking at the term $\sum_i \sum_\delta a_i^\dagger a_{i+\delta}$.

$$\begin{aligned} \sum_i \sum_\delta a_i^\dagger a_{i+\delta} =& \frac{1}{N} \sum_i \sum_\delta \sum_{\mathbf{kk'}} e^{-i\mathbf{k}\cdot\mathbf{r_i}} a_{\mathbf{k}}^\dagger e^{i\mathbf{k'}\cdot(\mathbf{r_i}+\delta)} a_{\mathbf{k'}}, \\ =& \frac{1}{N} \sum_{\mathbf{kk'}} \sum_\delta \sum_i e^{-i(\mathbf{k}-\mathbf{k'})\cdot\mathbf{r_i}} e^{i\mathbf{k'}\cdot\delta} a_{\mathbf{k}}^\dagger a_{\mathbf{k'}}, \\ =& \frac{1}{N} \sum_{\mathbf{kk'}} \sum_\delta N\delta_{\mathbf{kk'}} e^{i\mathbf{k'}\cdot\delta} a_{\mathbf{k}}^\dagger a_{\mathbf{k'}}, \\ =& \sum_{\mathbf{k}} \sum_\delta e^{i\mathbf{k}\cdot\delta} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}. \end{aligned} \tag{16}$$

In the third line of this calculation we used that $\sum_i e^{-i(\mathbf{k}-\mathbf{k'})\cdot\mathbf{r_i}} = N\delta_{\mathbf{kk'}}$. In a similar way we calculate the other terms. In the appendix the results of the operator multiplications are shown. By insirting the results of those multiplications the Hamiltonian in Equation 14 transforms to

$$H = -J\hbar^2 S^2 N\frac{z}{2} + J\hbar^2 Sz \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \big[1 - \gamma_{\mathbf{k}}\big], \tag{17}$$

where $\gamma_{\mathbf{k}} = \frac{2}{z}\sum_\delta \cos(\mathbf{k}\cdot\delta)$. In one dimension this means that $\gamma_k = \cos(k_x a)$, where a is again the spacing between lattice points. Finally, we can write

the Hamiltonian for ferromagnets in the compact diagonalized form:

$$H = E_0 + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}, \tag{18}$$

where $\omega_{\mathbf{k}} = SJ\hbar z(1-\gamma_{\mathbf{k}})$ and $E_0 = -J\hbar^2 S^2 N\frac{z}{2}$. In one dimension we find that $\omega_k = 2SJ(1-\cos(k_x a))$. This is the same dispersion relation as the one resulted from our semi-classical approach. Equation 18 tells us that we can describe our system as a sum of independent harmonic oscillators, each with its own wavevector $\mathbf{k}$. The quanta of the harmonic oscillator are called magnons. They are just quantized spin wave excitations with energy $\hbar\omega_{\mathbf{k}}$. As a magnon with wavevector $\mathbf{k}$ costs an energy $\hbar\omega_{\mathbf{k}}$, the minimized energy (the ground state) has no magnons. The ground state energy is therefore simply the situation where all spins point in the same direction with projection $\hbar S$ along the $z-$axis.

Increasing the temperature of the system will lead to magnons, originating as thermally excited states of the ground state. When we ignore the ground state energy we can derive a distribution function for magnons by using the methods of statistical physics. We will first turn to the partition function for magnons, which is given by

$$Z = \prod_{\mathbf{k}} Z_{\mathbf{k}} = \prod_{\mathbf{k}} \frac{1}{1-e^{-\beta\hbar\omega_{\mathbf{k}}}}.$$

We can calculate the total energy E of the system by

$$E = -\frac{\partial}{\partial\beta}\ln Z = \sum_{\mathbf{k}} \frac{\hbar\omega_{\mathbf{k}}}{e^{\beta\hbar\omega_{\mathbf{k}}}-1} \equiv \sum_{\mathbf{k}} n_{\mathbf{k}}\hbar\omega_{\mathbf{k}},$$

where n_k is the well known Bose Einstein distribution, which describes the statistical behaviour of bosons. Note that the chemical potential of magnons is zero so that the Bose-Einstein distribution reduces to a Planck distribution function, like for photons. If there are a few magnons in the system, such that they won't interact, we can describe them as bosons. We will now look at the magnetization. The magnetization is given by $\mathbf{M} = \sum_i \mathbf{S}_i$ and is a natural parameter to describe the magnetic ordering of a system. The larger M, the stronger the ferromagnetic order. The total number of magnons at temperature T is given by [8]

$$n = \frac{1}{(2\pi)^3}\int d^3\mathbf{k} n_{\mathbf{k}} = \frac{N}{4\pi^2}\left(\frac{T}{2SJ}\right)^{\frac{3}{2}}\int_0^\infty \frac{\sqrt{x}dx}{e^x-1}.$$

Each magnon will reduce the magnetization. The magnetization will thus be dependent on temperature:

$$M(T) = M(0)[1 - const. \left(\frac{T}{2SJ}\right)^{\frac{3}{2}}].$$

We are now finished with our investigation of the ferromagnet.

3 Antiferromagnets

In this chapter we will discuss the antiferromagnet. The classical ground state of an antiferromagnet exist of neighbouring spins pointing in opposite directions: $|\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\rangle$. This can be interpreted as two sublattices, such that sites on one sublattice have as their nearest neighbours only sites from the other. We choose our labelling such that sites in sublattice A have spins pointing up and sites in the other sublattice, B, have spin down. The antiferromagnetic case corresponds to a $J < 0$ in Equation 1. So we will use the Hamiltonian described by

$$H = J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{19}$$

where J is taken to be positive such that the energy of the system is minimized when the sites in sublattice A have spin up and the sites in sublattice B have spin down.

In the following paragraphs we shall first discuss the classical features of the antiferromagnet and afterwards discuss the effects of the quantum fluctuations by performing a Holstein-Primakoff transformation to include quantum effects in our calculations.

3.1 Semi-classical approach

We start with a semi-classical approach to the antiferromagnet. The change of the spin operator in time can be summarized in the following equation:

$$\frac{\partial \mathbf{S}_j}{\partial t} = -\mathbf{S}_j \times \frac{\partial H}{\partial \mathbf{S}_j}, \tag{20}$$

If we rewrite the Hamiltonian in Equation 19 in terms of sublattice A and B and rewrite the sum over i and j we find

$$H = \frac{J}{2} \sum_{j \in A} \mathbf{S}_j^A \cdot [\mathbf{S}_{j+1}^B + \mathbf{S}_{j-1}^B] + \frac{J}{2} \sum_{j \in B} \mathbf{S}_j^B \cdot [\mathbf{S}_{j+1}^A + \mathbf{S}_{j-1}^A].$$

We now use Equation 20 to describe the evolution of the system in time, which results in

$$\begin{aligned} \frac{\partial \mathbf{S}_j^A}{\partial t} &= -J\mathbf{S}_j^A \times [\mathbf{S}_{j-1}^B + \mathbf{S}_{j+1}^B], \\ \frac{\partial \mathbf{S}_j^B}{\partial t} &= -J\mathbf{S}_j^B \times [\mathbf{S}_{j-1}^A + \mathbf{S}_{j+1}^A]. \end{aligned} \tag{21}$$

Using small deviations for S with respect to the z-axis, the spins in sublattice A and B can be described by

$$\mathbf{S}_i^A = \begin{bmatrix} \delta S_i^{A,x} \\ \delta S_i^{A,y} \\ \hbar S \end{bmatrix}, \qquad \mathbf{S}_i^B = \begin{bmatrix} -\delta S_i^{B,x} \\ -\delta S_i^{B,y} \\ -\hbar S \end{bmatrix}. \tag{22}$$

We now can construct equations of motion using Equation 21 considering small deviations described by Equation 22.

$$\begin{aligned} \delta \dot{S}_j^{A,x} &= -JS\hbar \left(-2\delta S_j^{A,y} + \delta S_{j-1}^{B,y} + \delta S_{j+1}^{B,y} \right), \\ \delta \dot{S}_j^{A,y} &= -JS\hbar \left(2\delta S_j^{A,x} - \delta S_{j-1}^{B,x} - \delta S_{j+1}^{B,x} \right), \\ -\delta \dot{S}_j^{B,x} &= -JS\hbar \left(-2\delta S_j^{B,y} + \delta S_{j-1}^{A,y} + \delta S_{j+1}^{A,y} \right), \\ -\delta \dot{S}_j^{B,y} &= -JS\hbar \left(2\delta S_j^{B,x} - \delta S_{j-1}^{A,x} - \delta S_{j+1}^{A,x} \right). \end{aligned} \tag{23}$$

Using the ansatz described by $S_j^{A,x} = A_x e^{i\mathbf{k}\cdot\mathbf{R}_j - i\omega t}$, $S_j^{A,y} = A_y e^{i\mathbf{k}\cdot\mathbf{R}_j - i\omega t}$, $S_j^{B,x} = B_x e^{i\mathbf{k}\cdot\mathbf{R}_j - i\omega t}$ and $S_j^{B,y} = B_y e^{i\mathbf{k}\cdot\mathbf{R}_j - i\omega t}$, we write the equations of motion in matrixform. In this formulation a is the distance between the lattice points and $\mathbf{R}_j = \mathrm{j}\cdot a\hat{x}$ indicates the position in a one dimensional model.

$$\begin{bmatrix} i\omega & 2J\hbar S & 0 & 2J\hbar S\cos(k_x a) \\ -2J\hbar S & i\omega & -2J\hbar S\cos(k_x a) & 0 \\ 0 & 2J\hbar S\cos(k_x a) & -i\omega & 2J\hbar S \\ -2J\hbar S\cos(k_x a) & 0 & -2J\hbar S & -i\omega \end{bmatrix} \begin{bmatrix} A_x \\ A_y \\ B_x \\ B_y \end{bmatrix} = 0. \tag{24}$$

Diagonalizing this matrix we find that $\omega_k = 2J\hbar S\sin(k_x a)$, which for small values of k_x gives a linear dependence. There are four eigenvectors associated with this Hamiltonian, which for $k = 0$ are given by

$$v_1 = \frac{1}{2}\begin{bmatrix} -i \\ -1 \\ i \\ 1 \end{bmatrix}, \quad v_2 = \frac{1}{2}\begin{bmatrix} i \\ 1 \\ i \\ 1 \end{bmatrix}, \quad v_3 = \frac{1}{2}\begin{bmatrix} -i \\ 1 \\ -i \\ 1 \end{bmatrix}, \quad v_4 = \frac{1}{2}\begin{bmatrix} i \\ -1 \\ -i \\ 1 \end{bmatrix}. \tag{25}$$

With the use of the ansatz we we find the eigenstates of the system. We look at the real part with $a = 0$. The result for v_1 is given in Equation 26. This can be interpreted as a precession in sublattice A and a precession in sublattice B. Those precessions both go clockwise and have the same phase.

Note that the spins in sublattice A point in the positive z-direction and the spins in sublattice B in the negative z-direction.

$$\begin{aligned} \delta S_x^A &= -\frac{1}{2}\sin\omega t, & -\delta S_x^B &= \frac{1}{2}\sin\omega t, \\ \delta S_y^A &= -\frac{1}{2}\cos\omega t. & -\delta S_y^B &= \frac{1}{2}\cos\omega t. \end{aligned} \tag{26}$$

Interpreting the results for the other eigenvectors we find that v_2 describes a state where the precessions in sublattice A and B have a phase difference of π, but they both spin clockwise. The real part of v_3 describes a state where both precessions go anticlockwise but have a phaseshift of π. The real part of v_4 describes a state where the precessions both go anticlockwise and have no phase shift.

3.2 Holstein-Primakoff Transformation

We will now include quantum mechanical effects in our calculations. As the ground state for classical spins is described by the Néel state, one might naively guess that the ground state for the quantum case is analogous. It turns out that the Néel-state is actually not the ground state, and is in fact not even an eigenstate for the antiferromagnetic Heisenberg model. Quantum fluctuations play an important role in the antiferromagnetic case, as they change the ground state (and therefore its energy) away from the classical result.

To illustrate this effect we will again use a Holstein-Primakoff transformation to make the magnons appear specifically in our Hamiltonian, described by Equation 19. On the A sublattice, where the sites all have spin pointing upward, we use the standard expressions in Equation 27. In the limit of large S we may approximate them.

$$\begin{aligned} S_i^{+A} &= \hbar\sqrt{2S}\left(1 - \frac{a_i^\dagger a_i}{2S}\right) a_i \simeq \sqrt{2S}\hbar a_i, \\ S_i^{-A} &= \hbar\sqrt{2S}a_i^\dagger\left(1 - \frac{a_i^\dagger a_i}{2S}\right) \simeq \sqrt{2S}\hbar a_i^\dagger, \\ S_i^{zA} &= \hbar S - \hbar a_i^\dagger a_i. \end{aligned} \tag{27}$$

The sites in sublattice B have spin pointing down, so we must modify the Holstein-Primakoff expressions accordingly to reflect this. The modifications

correspond to replacing $S^z \to -S^z$ and $S^+ \leftrightarrow S^-$:

$$\begin{aligned} S_j^{+B} &= \hbar\sqrt{2S} b_j^\dagger \left(1 - \frac{b_j^\dagger b_j}{2S}\right) \simeq \sqrt{2S}\hbar b_j^\dagger, \\ S_j^{-B} &= \hbar\sqrt{2S} \left(1 - \frac{b_j^\dagger b_j}{2S}\right) b_j \simeq \sqrt{2S}\hbar b_j, \\ S_j^{zB} &= -\hbar S + \hbar b_j^\dagger b_j. \end{aligned} \tag{28}$$

Since we can split our system in sublattice A and B, we write the Hamiltonian given by Equation 19 in terms of A and B. Also we will replace the sum over nearest neighbours i and j by a sum over i and δ, as we did in the Holstein-Primakoff transformation for ferromagnets. The Hamiltonian in terms of the lowering and rising operators of $\mathbf{S}$ that reflects our modifications is given by Equation 29

$$\begin{aligned} H = J \sum_{i\in A} \sum_{\delta} \frac{1}{2} S_i^{+A} S_{i+\delta}^{-B} + \frac{1}{2} S_i^{-A} S_{i+\delta}^{+B} + S_i^{zA} S_{i+\delta}^{zB} \\ + J \sum_{j\in B} \sum_{\delta} \frac{1}{2} S_j^{+B} S_{j+\delta}^{-A} + \frac{1}{2} S_j^{-B} S_{j+\delta}^{+A} + S_j^{zB} S_{j+\delta}^{zA}. \end{aligned} \tag{29}$$

In this definition the sum over i and j runs over the lattice sites belonging to sublattices A and B respectively. Inserting the Holstein-Primakoff transformations described by Equation 27 and Equation 28 and considering only terms up to quadratic order in operator products, our Hamiltonian transforms to

$$\begin{aligned} H = J\hbar^2 \sum_{i\in A} \sum_{\delta} S(a_i b_{i+\delta} + a_i^\dagger b_{i+\delta}^\dagger) - S^2 + S(a_i^\dagger a_i + b_{i+\delta}^\dagger b_{i+\delta}) \\ + J\hbar^2 \sum_{j\in B} \sum_{\delta} S(b_j a_{j+\delta} + b_j^\dagger a_{j+\delta}^\dagger) - S^2 + S(b_j^\dagger b_j + a_{j+\delta}^\dagger a_{j+\delta}). \end{aligned} \tag{30}$$

We will now Fourier transform the operators in order to diagonalize the Hamiltonian. We will choose the vectors $\mathbf{k}$ to lie in the Brillouin zone associated with each sublattice. The Brillouin zone is identical for sublattice A and B. Therefore $\frac{-\pi}{2} < \mathbf{k} < \frac{\pi}{2}$ and the Fourier transformed operators are given by

$$a_j = \frac{1}{\sqrt{N_a}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} a_{\mathbf{k}}, \qquad b_i = \frac{1}{\sqrt{N_b}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} b_{\mathbf{k}}. \tag{31}$$

Including our transformed operators in the term $\sum_\delta a_i b_{i+\delta}$ we find

$$\begin{aligned}\sum_i \sum_\delta a_i b_{i+\delta} &= \frac{1}{NaNb} \sum_i \sum_\delta \sum_{\mathbf{k},\mathbf{k'}} e^{i(\mathbf{k}+\mathbf{k'})\cdot \mathbf{r}_i} e^{i\mathbf{k'}\delta} a_{\mathbf{k}} b_{\mathbf{k'}}, \\ &= \sum_\delta \sum_{\mathbf{k},\mathbf{k'}} \delta_{\mathbf{k}\text{-}\mathbf{k'}} e^{i\mathbf{k'}\delta} a_{\mathbf{k}} b_{\mathbf{k'}}, \\ &= \sum_\delta \sum_{\mathbf{k}} e^{-i\mathbf{k}\delta} a_{\mathbf{k}} b_{\text{-}\mathbf{k}}. \end{aligned} \tag{32}$$

The same can be done for the other components in the Hamiltonian. The results of these operator multiplications are given in the appendix. The Hamiltonian in terms of these transformed operators, as seen below, is not diagonal.

$$H = -J\hbar^2 N \frac{z}{2} S^2 + J\hbar^2 Sz \sum_{\mathbf{k}} \left[a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}}\right] + J\hbar^2 Sz \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \left[a_{\mathbf{k}} b_{-\mathbf{k}} + a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger\right], \tag{33}$$

with $\gamma_{\mathbf{k}} = \frac{2}{z} \sum_\delta \cos(\mathbf{k}\cdot\delta)$. In contrast to the ferromagnetic case, performing a fourier transform does not diagonalize the Hamiltonian. To diagonalize the Hamiltonian we will now introduce Bogoliubov transformations [9]. The basic idea of the Bogoliubov transformations is introducing a new set of operators α and β such that the Hamiltonian has only terms proportional to $\alpha^\dagger\alpha$ and $\beta^\dagger\beta$ [10]. The operators α and β are defined in Equation 34, where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are assumed to be real functions of vector $\mathbf{k}$.

$$\begin{aligned}\alpha_{\mathbf{k}} &= u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger, \\ \beta_{\mathbf{k}} &= u_{\mathbf{k}} b_{\mathbf{k}} - v_{\mathbf{k}} a_{-\mathbf{k}}^\dagger. \end{aligned} \tag{34}$$

The transformations are canonical, in the sense that the new operators will obey the Bose commutation rules. From this we conclude that, since $[\alpha_{\mathbf{k}}, \alpha_{\mathbf{k'}}^\dagger] = [\beta_{\mathbf{k}}, \beta_{\mathbf{k'}}^\dagger] = \delta_{\mathbf{k},\mathbf{k'}}$, it follows that $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$. This will be automatically satisfied when $u_{\mathbf{k}} = \cosh\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \sinh\theta_{\mathbf{k}}$. The requirement $[\alpha_{\mathbf{k}}, \beta_{\mathbf{k'}}^\dagger] = 0$ gives another condition, namely $u_{\mathbf{k}} v_{-\mathbf{k}} = u_{-\mathbf{k}} v_{\mathbf{k}}$. This is solved by setting $u_{\mathbf{k}} = u_{-\mathbf{k}}$ and $v_{-\mathbf{k}} = v_{\mathbf{k}}$. These conditions are assumed to hold in the inverse transformations, given by Equation 35.

$$\begin{aligned}a_{\mathbf{k}} &= u_{\mathbf{k}} \alpha_{\mathbf{k}} + v_{\mathbf{k}} \beta_{-\mathbf{k}}^\dagger, \\ b_{\mathbf{k}} &= u_{\mathbf{k}} \beta_{\mathbf{k}} + v_{\mathbf{k}} \alpha_{-\mathbf{k}}^\dagger. \end{aligned} \tag{35}$$

If we now express the Hamiltonian from Equation 33 in terms of the α and β bosons and use the corresponding commutation relations we can rewrite

the Hamiltonian to

$$H = H_0 + J\hbar^2 Sz \sum_{\mathbf{k}} \big[[u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 + 2\gamma_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}](\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}) + 2(v_{\mathbf{k}}^2 + \gamma_k v_{\mathbf{k}} u_{\mathbf{k}}) + [\gamma_{\mathbf{k}}(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) + 2u_{\mathbf{k}} v_{\mathbf{k}}](\beta_{-\mathbf{k}} \alpha_{\mathbf{k}} + \beta_{-\mathbf{k}}^\dagger \alpha_{\mathbf{k}}^\dagger) \big], \tag{36}$$

where $H_0 = -J\hbar^2 N \frac{z}{2} S^2$. Now we choose $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ such that the terms involving $\beta_{-\mathbf{k}} \alpha_{\mathbf{k}}$ and $\beta_{-\mathbf{k}}^\dagger \alpha_{\mathbf{k}}^\dagger$ cancel. Inserting $u_{\mathbf{k}} = \cosh\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \sinh\theta_{\mathbf{k}}$ the constraint for $\theta_{\mathbf{k}}$ is described by

$$\gamma_{\mathbf{k}} = -\tanh 2\theta_{\mathbf{k}}. \tag{37}$$

This constraint simplifies the Hamiltonian to

$$H = -NJ\hbar^2 \frac{z}{2} S^2 + J\hbar^2 SZ \sum_{\mathbf{k}} \big[u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 + 2\gamma_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \big] \big(\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} + 1 \big) + J\hbar^2 Sz \sum_{\mathbf{k}} \big(v_{\mathbf{k}}^2 - u_{\mathbf{k}}^2 \big). \tag{38}$$

After some manipulations we find the diagonal Hamiltonian given by

$$H = E_0 + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \big(\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} \big), \tag{39}$$

where $\omega_{\mathbf{k}} = J\hbar Sz\sqrt{1 - \gamma_{\mathbf{k}}^2}$ and

$$E_0 = -\frac{1}{2} NJ\hbar^2 (S^2 + S)z + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}. \tag{40}$$

In this diagonalized form of the Hamiltonian it becomes clear that the operators α and β create magnon excitations with wavevector $\mathbf{k}$ and energy $\hbar\omega_{\mathbf{k}}$. We first note that for each $\mathbf{k}$ there are two types of magnons (α and β), which are degenerate in energy. Furthermore, note that while $\mathbf{k}$ approaches zero $\omega_{\mathbf{k}} \to 0$, as in the ferromagnetic case. But unlike the ferromagnetic case, for which a quadratic dispersion was found in this limit, in the antiferromagnetic case we find a linear dispersion for small values of $\mathbf{k}$. So in a one dimensional antiferromagnet where $k_x \ll 1$ the dispersion relation is given by $\omega_k \approx J\hbar Sz|k_x|a$. The ground state energy E_0, given in Equation 40, gives the energy in the limit $T \to 0$. The term $-\frac{1}{2} NJ\hbar^2 S^2 z$ is just the ground state energy of a classical antiferromagnet with nearest-neighbour interactions between the spins. The other terms represent the quantum corrections to the classical ground state energy. The contribution of the quantum corrections is

thus described by $E_{qc} = -\frac{1}{2}NJ\hbar^2Sz + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} = JS\hbar^2 z \sum_{\mathbf{k}} \left(\sqrt{1-\gamma_{\mathbf{k}}^2} - 1\right)$. Since this is always smaller than zero we conclude that quantum fluctuations lower the energy of an antiferromagnetic system.

Looking at the magnetization of the system it is convenient to look at the sublattice magnetization. The total magnetization can not be used since it turns out to be zero in the presence of antiferromagnetic order. The correction for the sublattice magnetization to the classical result S is given by $\Delta M_A = \frac{1}{N}\sum_{\mathbf{k}} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle$. Using the Bogoliubov transformations in Equation 35 on the operators a we find

$$\Delta M_A = -\frac{1}{2} + \frac{2}{N}\sum_{\mathbf{k}} \left(n_{\mathbf{k}} + \frac{1}{2}\right) \frac{1}{\sqrt{1-\gamma_{\mathbf{k}}^2}} = -\frac{1}{2} + \frac{2}{N}\sum_{\mathbf{k}} \left(n_{\mathbf{k}} + \frac{1}{2}\right) \frac{JSz}{\omega_{\mathbf{k}}}. \tag{41}$$

In the limit that $T \to 0$ we find that $\Delta M_A \neq 0$. Even at zero temperature the magnetization of an antiferromagnet is reduced due to quantum fluctuations.

This concludes our analytical description of the ferromagnet and antiferromagnet. We now proceed numerically, such that we can consider more complicated magnetic configurations.

4 Numerical methods

In this chapter we construct a method to numerically calculate the energymodes of any magnetic configuration. Specifically we will calculate the dispersion for antiferromagnets and ferromagnets and compare this with our analytic description in chapter 3 and 4. We would like to modify the Hamiltonian such that we obtain a matrixform. Let us assume a two dimensional lattice n x m, where we label the site at the bottom left corner with 1. Now we count the cells in the positive x-direction on each row, such that the site in the upper right corner will be labeled nm. The matrixform of the Hamiltonian can now be written as [11]

$$H = \begin{pmatrix} a^\dagger a \end{pmatrix} H_m \begin{pmatrix} a \\ a^\dagger \end{pmatrix} - \frac{1}{2} Tr[H_m], \tag{42}$$

where $\begin{pmatrix} a^\dagger a \end{pmatrix} = \begin{pmatrix} a_1^\dagger, a_2^\dagger, ..., a_N^\dagger, a_1, a_2, ..., a_N \end{pmatrix}$ and $H_m = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$, with A and B matrices. In order to obtain only physical modes/magnons, H_m is constrained to be positive-definite. The bosonic operators a can be transformed using a para-unitary $2N \times 2N$ matrix T, such that the matrix H_m will be diagonalized according to the following scheme [9]:

$$\begin{pmatrix} a^\dagger a \end{pmatrix} H_m \begin{pmatrix} a \\ a^\dagger \end{pmatrix} = \begin{pmatrix} a^\dagger a \end{pmatrix} T^\dagger (T^\dagger)^{-1} H_m T^{-1} T \begin{pmatrix} a \\ a^\dagger \end{pmatrix} = \begin{pmatrix} \gamma^\dagger \gamma \end{pmatrix} D \begin{pmatrix} \gamma \\ \gamma^\dagger \end{pmatrix}, \tag{43}$$

where $D = (T^\dagger)^{-1} H_m T^{-1} = \frac{1}{2}\hbar \text{ diag}(\omega_1, \omega_2, ..., \omega_N, \omega_1, \omega_2, ..., \omega_N)$ with all ω_i positive. This transformation is similar to the Bogoliubov transformations discussed previously, but is now performed in real space, rather than in momentum space after a Fourier transform. This more general form is needed in case there is no translation invariance such that a Fourier description will not useful. By doing so we defined a new basis as shown in Equation 44. The para-unitary property of T ensures that the operators γ are bosonic creation/annihilation and therefore satisfy $[\gamma, \gamma^\dagger] = \delta_{ij}$.

$$\begin{pmatrix} \gamma \\ \gamma^\dagger \end{pmatrix} = T \begin{pmatrix} a \\ a^\dagger \end{pmatrix}, \qquad \begin{pmatrix} \gamma^\dagger \gamma \end{pmatrix} = \begin{pmatrix} a^\dagger a \end{pmatrix} T^\dagger. \tag{44}$$

We are now interested in finding T^{-1}. Since T is para-unitary it must satisfy $T^\dagger \phi = \phi T$, where ϕ is the para-unit matrix given by ϕ =diag$(1, 1, ..., -1, -1)$. Also, we know D from Equation 43. Therefore we can conclude that

$$D = \texttt{diag}(\lambda_1, \lambda_2, ..., \lambda_N, -\lambda_{N1}, -\lambda_{N+2}, ..., -\lambda_{2N}) = \phi\, \Lambda, \tag{45}$$

where $\lambda_i = \frac{1}{2}\hbar\omega_i$ for i from 1 to N and $\lambda_i = -\frac{1}{2}\hbar\omega_i$ for i from $N+1$ to $2N$. Also, Λ is introduced as a list of λ_i to simplify the notation. Multiplying both sides of Equation 45 with ϕT^{-1} gives $\phi D T^{-1} = \Lambda T^{-1}$. From which can easily be seen that each column of T^{-1} satisfies

$$(\phi D - \lambda_p)\omega_p = 0, \tag{46}$$

where ω_p denotes the column p of T^{-1}. The para-unitary matrix T^{-1} can now be obtained by finding the eigenvectors ω_p of the matrix ϕD and use them to create $T^{-1} = (\omega_1, \omega_2, ..., \omega_{2N})$. In summary we find that our transformation matrix is given by

$$T^{-1} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}, \tag{47}$$

where we define $U = \begin{pmatrix} u_1 & u_2 & u_3 & ... & u_N \end{pmatrix}$ and $V = \begin{pmatrix} v_1 & v_2 & v_3 & ... & v_N \end{pmatrix}$, with u_p and v_p column vectors. Those can be found by calculating $\omega_p = \begin{pmatrix} u_p & v_p \end{pmatrix}'$, where the prime indicates that it is a column vector.

4.1 (Anti-)Ferromagnetic Heisenberg Model

To show that this method actually works, we calculate the spin wave spectrum for a one dimensional ferromagnet and antiferromagnet consisting of 64 spins. We use the Heisenberg model in Equation 1 for ferromagnets and in Equation 19 for antiferromagnets. We will diagonalize those Hamiltonians using the matrix form explained in this chapter and also in ref [5].

We first perform the calculations on a ferromagnet and find that in the classical limit the energy spectrum gives a sinusoidal shape, as shown in Figure 2. This is in accordance with our analytical dispersion relation calculated in chapter 3. Every mode is associated with a wave vector k, but every spin wave going in the opposite direction has the same energy due to symmetries of the model, such that the values of ω_k appear twice. The total energy of this spectrum is 128. The contribution $\frac{1}{2}\sum_k \omega_k$ is therefore the same as the classical ground state energy, $JS\hbar N\frac{z}{2}$ with $J = 1$, $S = 1$, $\hbar = 1$, $N = 64$ and $z = 2$. So we can again conclude that the ground state remains unchanged due to quantum fluctuations in the ferromagnet.

In the antiferromagnetic case we find the results shown in Figure 2. The quadruple effect appears as result of degenerate eigenmodes, described in Equation 25. The dispersion relation analytically calculated in chapter 4 produces the same energy spectrum as the numerical results. The classical ground state energy is the same as for the ferromagnet. The total energy of

the antiferromagnetic dispersion relation gives 81.4. We therefore conclude that the quantum fluctuations lower the ground state energy of the one dimensional antiferromagnet by $Eqc = -JS\hbar\frac{z}{2} + \frac{1}{2}\sum_k \omega_k$, which for $J = 1$, $S = 1$ and $\hbar = 1$ gives $Eqc = -23.3$.

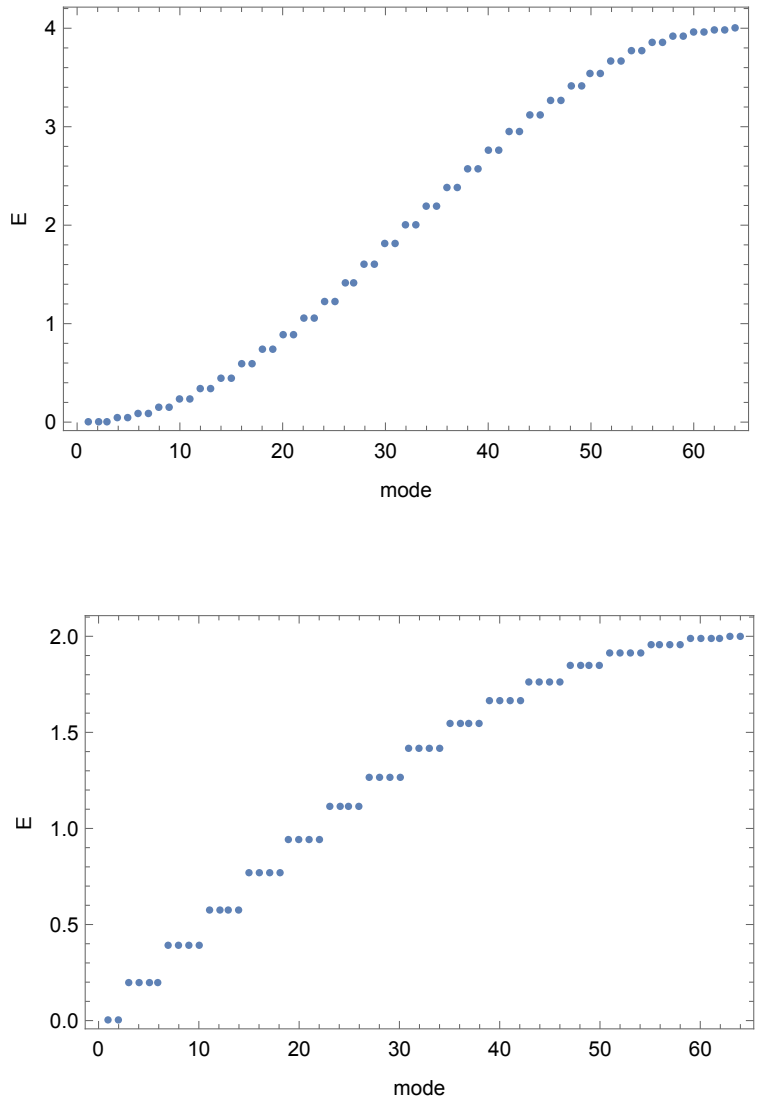


Figure 2: Energy spectrum for a one dimensional ferromagnet (top) and antiferromagnet (bottom) consisting of 64 spins. We used $S = 1$, $J = 1$, $\hbar = 1$ and $a = 1$. The energy eigenvalues are plotted by ordering the energies from small to large.

5 Classical ground state of an antiferromagnetic Hamiltonian with Dzyaloshinskii-Moriya interactions

In the previous chapters we calculated the dispersion relations for ferro- and antiferromagnets by assuming only the coupling of nearest neighbours. To gain a more realistic result we also have to include the influence of an external field, anisotropy and Dzyaloshinskii-Moriya interactions in our Hamiltonian. In this chapter we will discuss the effects of Dzyaloshinskii-Moriya coupling in an antiferromagnet. This coupling is also known as the antisymmetric exchange and describes a contribution to the total magnetic exchange interaction between neighbouring spins that occurs when inversion symmetry is broken. We will see that whirling types of magnetization in chiral magnets [1] are induced by the Dzyaloshinskii-Moriya interaction. An example of such a whirling magnetic configuration is a skyrmion. The skyrmion is a vortex-like configuration and was originally introduced in particle physics by T.H.R. Skyrme in 1962 [12]. Although they were predecited they were discovered experimentally just recently [13] [14]. Skyrmions are potentially good for data storage, because of their topological stability and easy manipulation with very low electrical currents [15] [5]. Therefore skyrmions are an active field of research.

We start with a ferromagnetic Hamiltonian, containing only the Heisenberg exchange coupling and Dzyaloshinskii-Moriya interaction given by

$$H = \frac{J}{2}\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \mathbf{S}_i \cdot \mathbf{S}_{i-1} - \frac{D}{2}\sum_i (\mathbf{S}_i \times \mathbf{S}_{i+1})^y - (\mathbf{S}_{i+1} \times \mathbf{S}_i)^y, \quad (48)$$

where J is the Heisenberg exchange coupling constant and D is the Dzyaloshinskii-Moriya interaction constant. For simplicity we use natural units during the calculations. After expanding the Fourier transform of the Hamiltonian for small q and using the continuum limit the Hamiltonian is given by

$$H = C - \frac{J}{2a}\int \mathbf{S}(x) \cdot \frac{d^2\mathbf{S}(x)}{dx^2}dx + \frac{D}{a}\int \mathbf{S}(x) \times \frac{d\mathbf{S}(x)}{dx}dx. \quad (49)$$

By minimizing the variation of the Hamiltonian we find that the corresponding Euler equations are solved by

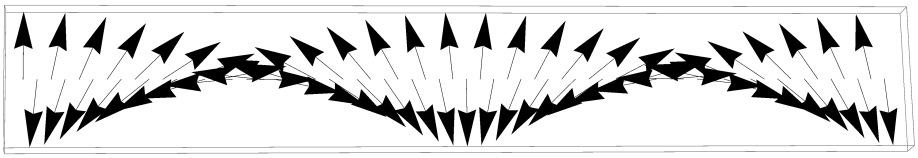
$$\mathbf{S} = \begin{bmatrix} S\sin(\frac{D}{J}x) \\ 0 \\ S\cos(\frac{D}{J}x) \end{bmatrix}. \quad (50)$$

[1] Chirality is a form of asymmetry of the system. If the atomic structure of a magnet lacks inversion symmetry we call them chiral magnets.

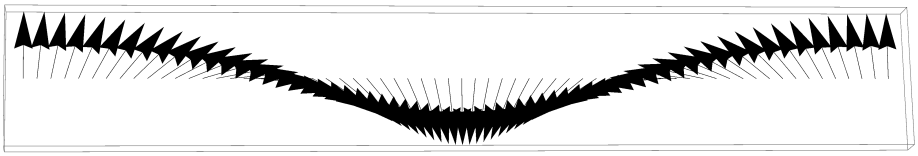
To find the ground state of the antiferromagnet we use a staggered notation of the antiferromagnetic spin, given by $\mathbf{S}_i^{stag} = \mathbf{S}_i(-1)^i$. In this way we can use the ferromagnetic Hamiltonian. By minimizing the ferromagnetic Hamiltonian for all three components of the spin we find three constrains:

$$\begin{aligned} S_{i+1}^y &= S_{i-1}^y, \\ J(S_{i+1}^x + S_{i-1}^x) &= D(S_{i-1}^z - S_{i+1}^z), \\ J(S_{i+1}^z + S_{i-1}^z) &= D(S_{i+1}^x - S_{i-1}^x). \end{aligned} \tag{51}$$

From the continuous result given by Equation 50 we derive an educated guess for this discrete case: $\mathbf{S}_i = S(-1)^i\big[\sin(aqi), 0, \cos(aqi)\big]$, where the constraint for aq is given by Equation 51 and will therefore be $aq = \arctan\frac{D}{J}$. We see that $\mathbf{S}_i$ makes a precession with period $p = 2\pi/\arctan\frac{D}{J}$. For 64 spins, $J = 1$, $S = 1$, $a = 1$ and choosing D such that there is exactly one period, the configuration for the staggered ground state of an antiferromagnet is shown in Figure 3b. The ground state of an antiferromagnet can now easily be obtained and is shown in Figure 3a.



(a)



(b)

Figure 3: (a) Ground state of a one dimensional antiferromagnetic configuration where $D = 0.09849$, $J = 1$ and $S = 1$. The ground state is described by one magnon. (b) As for (a) but staggered.

6 Phase transition to the spin-flop state in antiferromagnets

We thoroughly treated the quantum effects in the ferro- and antiferromegnet considering only Heisenberg exchange interactions. Also, we constructed a numerical method to calculate the dispersion relations in magnetic configurations. In this chapter we will use this knowledge to calculate the effect of quantum fluctuations in the transition between an antifromagnetic Néel state and a spin-flop state. In Figure 4 a classical picture of both spin-states is shown. We first examine the classical interpretation of the transition in two dimensions. The Hamiltonian used contains exchange coupling, anisotropy, magnetization and Dzyaloshinskii-Moriya interaction. The phase transition from an antiferromagnetic state to a spin-flop state occurs when the Dzyaloshinskii-Moriya interaction is zero [16]. In our calculations we used natural units and the effective energy in Equation 52 for simplicity. An effective Hamiltonian is a Hamiltonian that acts in a reduced space and only describes a part of the eigenvalue spectrum. The anisotropy factor K in the Hamiltonian will make sure that our system has an 'easy-axis' along which it would like to magnetize either up or down, which in our case will be the z-axis. The strength of the external field B, oriented in the z-direction, eventually forces the antiferromagnetic state to change to the spin-flop state. The transition-value for B is found at the crossing of the minimized energy for both phases at $D = 0$.

$$H_{eff} = J\mathbf{S}_{ij} \cdot (\mathbf{S}_{ij+x} + \mathbf{S}_{ij+y}) + K(\mathbf{S}_{ij}^z)^2 - B\mathbf{S}_{ij}^z \tag{52}$$

In a pure antiferromagnetic state we describe the spin by $\mathbf{S}_{ij}^{AF}$ given in Equation 53. This gives an effective energy, $H_{eff}^{AFM} = -2J+K$. The external field has no influence on the effective energy as it remains constant by increasing B. In the pure spin-flop state $\mathbf{S}_{ij}^{SF}$ from Equation 53 can be used to describe the spinstates. After minimizing the effective energy in Equation 52 as function of θ, we find $H_{eff}^{SF} = -2J - \frac{B^2}{4(4J+K)}$.

$$\mathbf{S}_{ij}^{AF} = \begin{pmatrix} 0 \\ 0 \\ (-1)^{i+j} \end{pmatrix} \qquad \mathbf{S}_{ij}^{SF} = \begin{pmatrix} (-1)^{i+j}\cos[\phi]\sin[\theta] \\ (-1)^{i+j}\sin[\phi]\sin[\theta] \\ \cos[\theta] \end{pmatrix} \tag{53}$$

The minimized energy in the antiferromagnetic state is independent of the strength of the external field B. However, the minimized energy in the

spin-flop state has a quadratic dependence on B. In Figure 5 the minimized energy for both phases is plotted. Increasing B causes the spin-flop state to eventually become the favoured state of the system and therefore a phase transition will occur at $B \approx 0.796$. The same calculations can be done in one dimension, which results in a transition at $B \approx 0.56$.

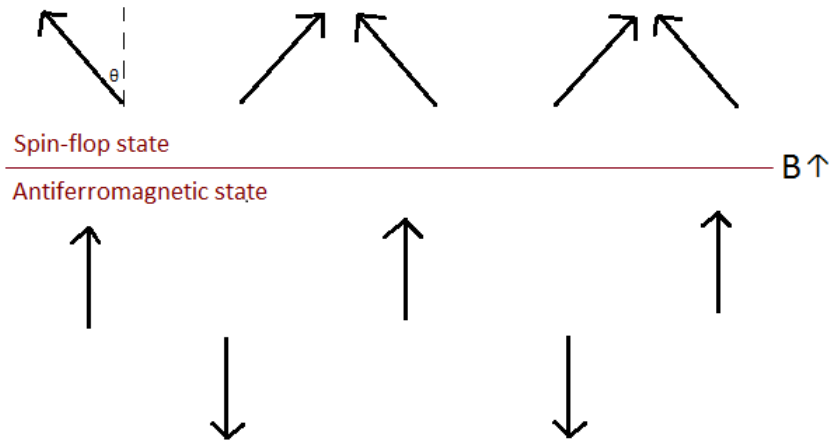


Figure 4: Classical picture of the spin-flop and antiferromagnetic state.

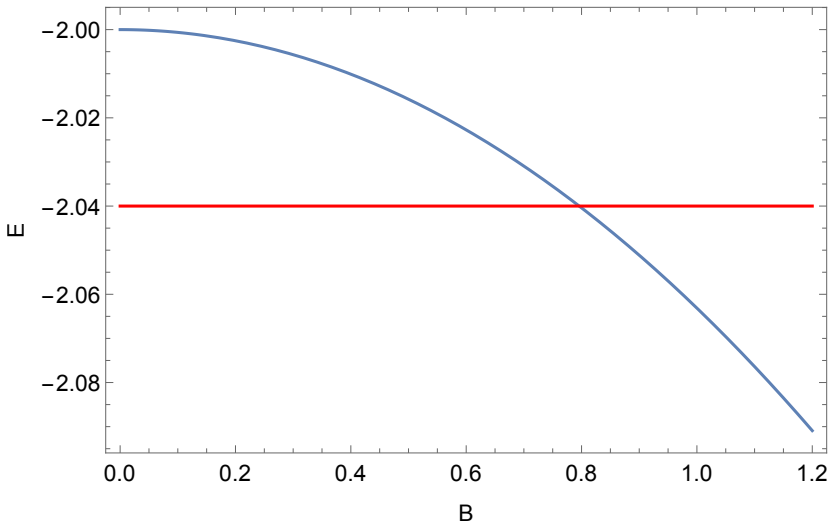


Figure 5: Effective energy of the antiferromagnetic state (red) and the spin-flop state (blue) in two dimensions. The crossing happens at $B \approx 0.796$. Here we used $J = 1$, $S = 1$ and $K = -0.04$.

6.1 Magnon energies for the spin-flop state

Increasing B will cause the antiferromagnetic state to eventually change to the spin-flop state. It is therefore interesting to calculate the dispersion relation of the spin-flop state such that the effect of quantum fluctuations on the ground state can be obtained. In the next section we will also calculate the dispersion relation of the antiferromagnetic state such that we can investigate the effects of quantum fluctuations on the transition between the two states. As before, a Holstein-Primakoff transformation can be used to calculate the energy spectrum. The Holstein-Primakoff representation of the spin operator given by Equation 12 discriminates only in one direction. Therefore, in the case of non-collinear classical ground states such as the spin-flop state, it is convenient to define a rotated local coordinate system as follows [11]:

$$\begin{aligned}
\hat{e}_1^i &= \cos\theta_i \cos\phi_i \, \hat{x} + \cos\theta_i \sin\phi_i \, \hat{y} - \sin\theta_i \, \hat{z} \\
\hat{e}_2^i &= \hat{e}_3^i \times \hat{e}_1^i \\
\hat{e}_3^i &= \sin\theta_i \cos\phi_i \, \hat{x} + \sin\theta_i \sin\phi_i \, \hat{y} + \cos\theta_i \, \hat{z},
\end{aligned} \tag{54}$$

or, in more compact form:

$$\hat{e}_a^i = (R_{a,b}^i)^{-1} \, \hat{r}^b, \tag{55}$$

where θ_i and ϕ_i are the angles that characterize the spin direction of the classical ground state at site i, $R_{a,b}^i$ is a rotation matrix and $\hat{r}^b$ are the Cartesian axis. The Hamiltonian that includes nearest neighbour interactions, external field and anisotropy can now be expressed in this frame:

$$\begin{aligned}
H = J \sum_{<ij>} (\mathbf{S}_i \cdot \hat{e}_\alpha^i)(\mathbf{S}_j \cdot \hat{e}_\beta^j) R_{\alpha,\gamma}^i R_{\beta,\gamma}^j - B \sum_i (\mathbf{S}_i \cdot \hat{e}_\alpha^i) R_{\alpha,3}^i \\
+ K \sum_i (\mathbf{S}_i \cdot \hat{e}_\alpha^i)(\mathbf{S}_i \cdot \hat{e}_\beta^i) R_{\alpha,3}^i R_{3,\beta}^i,
\end{aligned} \tag{56}$$

where we included that $\mathbf{B} = B\hat{z}$ and chose $\hat{z}$ as the anisotropic easy axis. We choose $\hat{e}_3^i$ along the spindirection at every site i such that we can easily use a Holstein-Primakoff transformation for the small fluctuations around the spin direction. In the specific case of a spin-flop state this results in $\phi_i = \pi i$ and $\theta_i = \arccos[\frac{B}{2(zJ+K)}]$, where z is the number of neighbours. The value of ϕ_i is chosen such that each neighbouring spin has opposite sign in the direction of the chain, as can be seen in Figure 4. The constant value of θ_i can be found by minimizing the energy as function of θ_i, as we did in the previous section for Equation 52. Implementing those values of ϕ_i and θ_i in Equation 54, a rotation matrix $R_{a,b}^i$ can be constructed from Equation 55.

The exact form $R^i_{a,b}$ for the spin-flop state can be found in Equation 62 in the appendix. To diagonalize the resulting Hamiltonian we use the Holstein-Primakoff transformation described by the combined use of Equation 12 and the following expressions[11]:

$$\begin{aligned} S_i^{\pm} &= \mathbf{S}_i \cdot \hat{e}_1^i \pm i\mathbf{S}_i \cdot \hat{e}_2^i, \\ S - a_i^\dagger a_i &= \mathbf{S}_i \cdot \hat{e}_3^i. \end{aligned} \tag{57}$$

We will proceed in one dimension, so $z = 1$. By keeping only terms up to the second order in bosonic operators α, $\alpha^\dagger$ we find the Hamiltonian below. In this formulation $E_0 = -J - \frac{B^2}{4(2J+K)}$, $x = \frac{B}{2(2J+K)}$ and $y = \sqrt{1-x^2}$.

$$\begin{aligned} H = E_0 &+ \sum_i S(Bx + 2J(1-2x^2) - 2Kx^2 - y^2K(-1)^i)\, a_i^\dagger a_i \\ &+ JSy^2 \sum_i a_i^\dagger a_{i+1}^\dagger + a_i a_{i+1} - x^2 JS \sum_i a_i^\dagger a_{i+1} + a_i a_{i+1}^\dagger \\ &- \frac{y^2 KS}{2} \sum_i a_i a_i + a_i^\dagger a_i^\dagger. \end{aligned} \tag{58}$$

Now we are able to write the Hamiltonian in the matrix form explained in Equation 42. We then use the diagonalization techniques described in chapter 4 to find the excitation energies for the spin-flop state. In Figure 6 the results for a one dimensional chain of spins are shown.

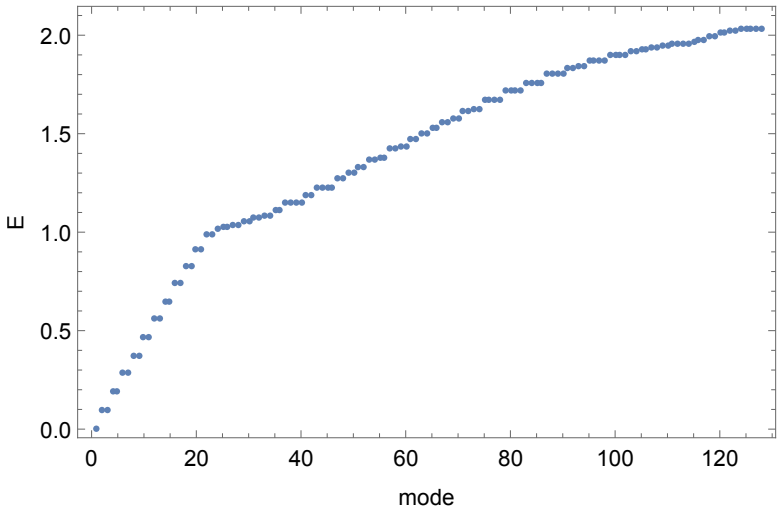


Figure 6: Energy spectrum for the spin-flop state considering a one dimensional system consisting of 128 spins. In this graph $S = 1$, $J = 1$, $B = 1$ and $K = -0.04$.

6.2 Magnon energies for the antiferromagnetic state

Since we are interested in the effects of quantum fluctuations on the transition between the antiferromagnetic and the spin-flop state we will now calculate the energy spectrum for the antiferromagnet. We use the Hamiltonian in Equation 56 as we did for the spin-flop state. We again choose $\hat{e}_3^i$ along the spindirection at every site i such that we can easily use a Holstein-Primakoff transformation for the small fluctuations around the spin direction. The rotation matrix for the antiferromagnet can be constructed from the combined use of Equation 54 and Equation 55 with $\theta_i = \pi i$ and $\phi_i = 0$. The exact form $R^i_{a,b}$ for the antiferromagnetic state is given in Equation 63 in the appendix. The resulting Hamiltonian can now be transformed using Equation 12 and Equation 57. Here we show the one dimensional form:

$$H = E_0 + \sum_i (2JS - 2KS + B(-1)^i)\, a_i^\dagger a_i - JS \sum_i (a_i a_{i+1} + a_i^\dagger a_{i+1}^\dagger), \quad (59)$$

where $E_0 = KS^2N - JS^2N$. The dispersion relation that results from diagonalization is shown in Figure 7.

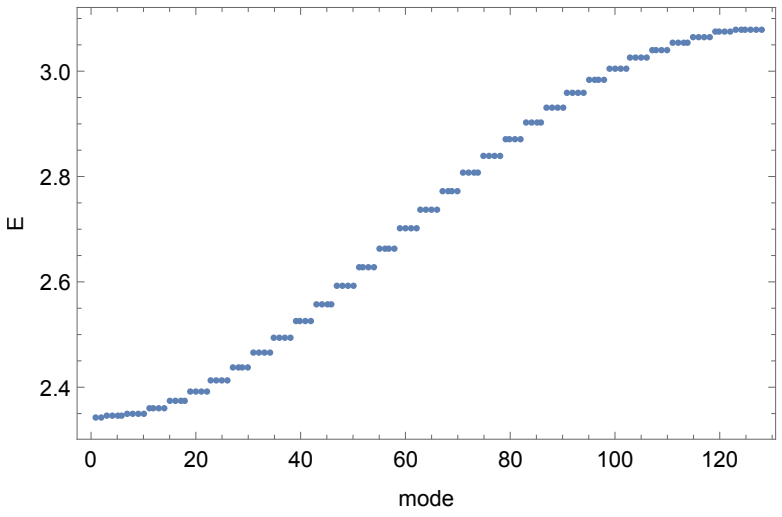


Figure 7: Energy spectrum for the antiferromagnetic state considering a one dimensional system consisting of 128 spins. In this graph $S = 1$, $J = 1$, $B = 1$ and $K = -0.04$.

6.3 Quantum fluctuations

After obtaining the dispersion relation for the antiferromagnetic and spin-flop state we are now able to calculate the influence of quantum fluctuations in the system. The contribution to the groundstate energy due to quantum fluctuations can be calculated by $\mathrm{E}qc = \frac{1}{2}\sum_k \omega_k - \frac{1}{2}\mathrm{Tr}(\mathrm{H}_m)$[11]. We will calculate the contribution due to quantum fluctuations in a one dimensional chain of 128 spins for $S = 1$, $J = 1$ and $K = -0.04$.

First we calculate the fluctuations in the spin-flop state, where the matrix H_m was constructed from Equation 58. We found that the quantum fluctuations lower the energy of the classically known ground state. Note that by changing the value of the external field the quantum fluctuations also change. We calculated the quantum fluctuations for several values of B. Unfortunately we faced the problem that the matrix H_m was not always positive definite and therefore some values for B could not be used for the calculation. Afterwards we calculate the quantum fluctuations in the antiferromagnetic state by constructing H_m from Equation 59. We found that quantum fluctuations also lower the ground state of the antiferromagnetic state.

In figure Figure 8 the effect of quantum fluctuations on the transition between the two states in one dimension is shown. The quantum fluctuations for both states decrease for increasing B. Due to the effect of quantum fluctuations the transition seems to be moved and the crossing now appears to happen around $B = 0$. These results imply that the one dimensional antiferromagnetic state would only be favoured at $B = 0$, if at all. Due to uncertainties we cannot exclude the possibility that there is no crossing at all. There could also be other physical aspects that influence the ground states, such that the classically known ground states change accordingly. More research is needed to provide the decisive answer.

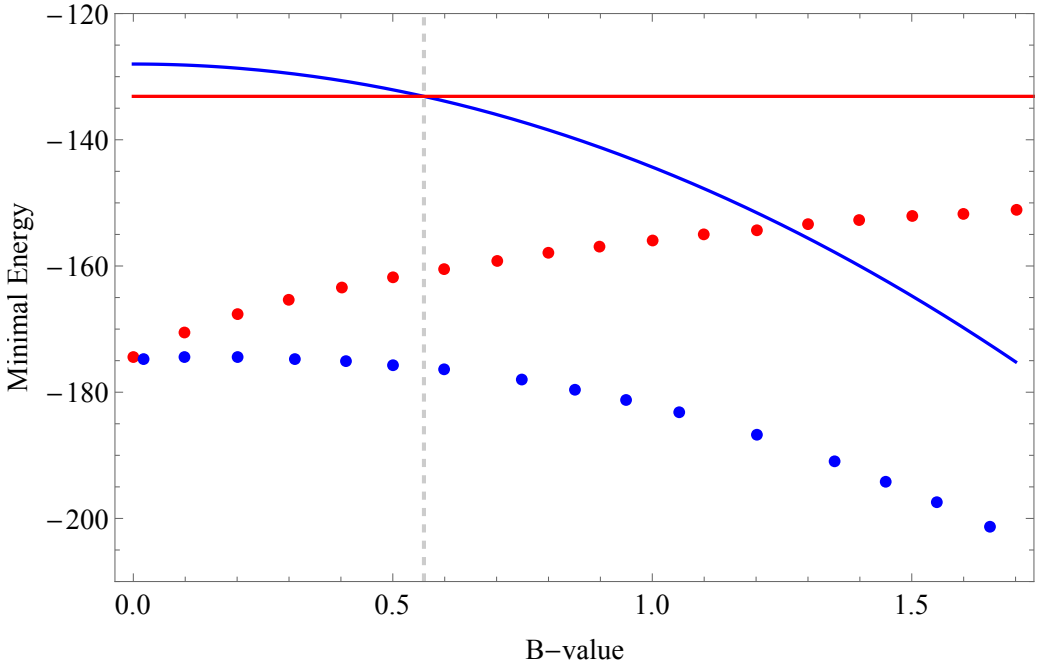


Figure 8: The solid lines represent the classical ground states of the antiferromagnetic (red) and spin-flop (blue) state. The effect of quantum fluctuations on the ground state is indicated by the dots. In this one dimensional system the classical crossing happens at $B \approx 0.56$. We used $J = S = 1$ and $K = -0.04$.

7 Conclusion

In this thesis we discussed the impact of quantum fluctuations on the classical description of magnetic configurations. We started with a general investigation of the ferro- and antiferromagnet. We found that quantum effects lower the energy of an antiferromagnet and that the energy of ferromagnet remains unchanged. Afterwards we constructed a numerical method to obtain the energy spectrum of magnetic configurations, which could be used for further research. In the end we investigated the spin-flop state. The spin-flop state appears in antiferromagnets after increasing the external field. This phase transition is classically well understood and therefore we used a numerical method to investigate the influence of quantum fluctuations on this transition. With the energy spectrum of the antiferromagnetic and the spin-flop state we calculated the quantum correction to the ground state. We found that the quantum fluctuations lower the energy of both states. Our results indicate the antiferromagnetic state is only the ground state, if at all, around $B = 0$. This could mean that in one dimension the spin-flop state is the ground state for all values of the external field except zero. Due to uncertainties our results do not give a definite answer to the question whether there is a transition point at all.

For further research it would therefore be interesting to optimize our calculations and investigate how quantum fluctuations influence the phase transition from an antiferromagnetic to a spin-flop state in one dimension. We also suggest to calculate the dispersion relations for both phases in momentum space using the Hamiltonian given in Equation 64 in the appendix and diagonalizing it with a Bogoliubov transformation. by doing so an analytical description of the quantum fluctuations could be obtained. Also, higher dimensions could be explored. In two and three dimensions our expectation is that the quantum fluctuations will lower the classical energy and the transition point will be shifted. The classical transition value in two and three dimension happens at a higher value for B than in the one dimenional case. Therefore, we expect the antiferromagnetic state to still be the groundstate for low values of B in the two and three dimensional cases. Nevertheless, we expect the transition to spin-flop state to be shifted to a lower value of B in those cases. Furthermore, other phase transitions in the antiferromagnet could be investigated using real space numerical diagonalization. For example the transition from the antiferromagnetic to spiral state, which happens at $B = 0$. Another example is the transition from the spin-flop to the spiral state, which occurs for positive anisotropy [6].

8 Appendix

Operator Multiplications

A list of operator multiplications used to express the Hamiltonian in Equation 14 in terms of $a_i^\dagger a_i$:

$$\begin{aligned}
\sum_i \sum_\delta a_i^\dagger a_i &= \frac{z}{2} \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \\
\sum_i \sum_\delta a_{i+\delta}^\dagger a_{i+\delta} &= \frac{z}{2} \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \\
\sum_i \sum_\delta a_{i+\delta}^\dagger a_i &= \sum_{\mathbf{k}} \sum_\delta e^{-i\mathbf{k}\cdot\delta} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}.
\end{aligned} \tag{60}$$

A list of operator multiplications used to express the Hamiltonian in Equation 30 in terms of $a_i^\dagger a_i$ and $b_i^\dagger b_i$:

$$\begin{aligned}
\sum_i \sum_\delta a_i^\dagger b_{i+\delta}^\dagger &= \sum_\delta \sum_{\mathbf{k}} e^{i\mathbf{k}\delta} a_{\mathbf{k}}^\dagger b_{\text{-}\mathbf{k}}^\dagger, \\
\sum_i \sum_\delta a_{i+\delta} b_i &= \sum_\delta \sum_{\mathbf{k}} e^{i\mathbf{k}\delta} a_{\mathbf{k}} b_{\text{-}\mathbf{k}}, \\
\sum_i \sum_\delta a_{i+\delta}^\dagger b_i^\dagger &= \sum_\delta \sum_{\mathbf{k}} e^{-i\mathbf{k}\delta} a_{\mathbf{k}}^\dagger b_{\text{-}\mathbf{k}}^\dagger, \\
\sum_i \sum_\delta a_{i+\delta}^\dagger a_{i+\delta} &= \sum_i \sum_\delta a_i^\dagger a_i = \frac{z}{2} \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \\
\sum_i \sum_\delta b_{i+\delta}^\dagger b_{i+\delta} &= \sum_i \sum_\delta b_i^\dagger b_i = \frac{z}{2} \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}.
\end{aligned} \tag{61}$$

Rotation Matrices

Rotation matrix $R_{a,b}^i$ for the spin-flop state is obtained when $\phi_i = \pi i$ and $\theta_i = \arccos x$:

$$R_{a,b}^i = \begin{bmatrix} x(-1)^i & 0 & y(-1)^i \\ 0 & (-1)^i & 0 \\ -y & 0 & x \end{bmatrix}, \tag{62}$$

where $x = \frac{B}{2(4J+K)}$ in 2D, $x = \frac{B}{2(2J+K)}$ in 1D and $y = \sqrt{1-x^2}$.

Rotation matrix $R^i_{a,b}$ for the antiferromagnetic state is obtained when $\theta = \pi i$ and $\phi = 0$:

$$R^i_{a,b} = \begin{bmatrix} (-1)^i & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & (-1)^i \end{bmatrix}. \tag{63}$$

Matrixform of the Hamiltonian in momentum space

Up to this point we did calculations for the spin-flop state in real space. At the end of the research program we were working on an analytical description of the wave spectrum for the spin-flop state. Implementing the rotation matrix $R^i_{a,b}$, for the spin-flop state given in Equation 62, in the Hamiltonian from Equation 56 results in the Hamiltonian in Equation 58. In this notation $x = \frac{B}{2(zJ+K)}$ with z the number of neighbours and $y = \sqrt{1-x^2}$. We performed a Fourier transformation on the Hamiltonian in the process of diagonalizing. We used the fact that $\sum_j (-1)^j = \sum_j e^{iQaj}$, where $Q = \frac{\pi}{2a}$ with a the spacing between the lattice points. The result of the transformation is given in the Hamiltonian given below, where $E_0 = -J - \frac{B^2}{4(zJ+K)}$ and z denotes the number of neighbours.

$$\begin{aligned} H = {} & E_0 + J\frac{z}{2}Sy^2 \sum_k \cos[ka](a_k a_{-k} + a_k^\dagger a_{-k}^\dagger) \\ & - J\frac{z}{2}Sx^2 \sum_k \cos[ka](a_k^\dagger a_k + a_k a_k^\dagger) \\ & + (BS\frac{x}{2} - KSx^2 - JzS(-1+2x^2)) \sum_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) \\ & - \frac{a^2}{2}KS \sum_k (a_k^\dagger a_{k-Q} + a_k a_{k+Q}^\dagger + a_k^\dagger a_{-k+Q}^\dagger + a_k a_{-k-Q}). \end{aligned} \tag{64}$$

We already tried to make a symetric and hermetian matrixform of this Hamiltonian by constructing a $8N \times 8N$ notation, by making use of cyclic boundaries, as can be seen in Equation 65. For further research a total diagonalization of this Hamiltonian using Bogoliubov transformations would provide a way to analytically calculate the dispersion relation.

$$H = E_0 + \begin{bmatrix} \chi^\dagger & \chi \end{bmatrix} \begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix} \begin{bmatrix} \chi \\ \chi^\dagger \end{bmatrix} - \frac{1}{2}\mathrm{Tr}\begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix}, \tag{65}$$

where $\chi = \begin{pmatrix} a_k^\dagger & a_{k+Q}^\dagger & a_{-k} & a_{-k-Q} \end{pmatrix}$ and

$$A = \begin{bmatrix} \frac{L}{2} & -\frac{a^2}{8}KS & 0 & -\frac{a^2}{8}KS \\ -\frac{a^2}{8}KS & 0 & 0 & 0 \\ 0 & 0 & \frac{L}{2} & 0 \\ -\frac{a^2}{8}KS & 0 & 0 & 0 \end{bmatrix},$$

$$B = \begin{bmatrix} 0 & -\frac{a^2}{8}KS & \frac{JSa^2\cos(ka)}{2} & -\frac{a^2}{8}KS \\ -\frac{a^2}{8}KS & 0 & 0 & 0 \\ \frac{JSa^2\cos(ka)}{2} & 0 & 0 & 0 \\ -\frac{a^2}{8}KS & 0 & 0 & 0 \end{bmatrix},$$

with $L = (BS\frac{x}{2} - KSx^2 - JzS(-1 + 2x^2) - JS\frac{x^2}{2}\cos(ka))$ and a the spacing between the spins.

References

[1] F. Bloch, Z. Phys. **61**, (1930) 206.

[2] Mattia Crescioli, Paolo Politi, Ruggero Vaia, *Re-entrant spin-flop transition in nanomagnets*, Phys. Rev. B **90**, 100401(R) (2014)

[3] N. B. Ivanov, J. Ummethum, J. Schnack, *Phase diagram of the alternating-spin Heisenberg chain with extra isotropic three-body exchange interactions*,Eur. Phys. J. B **87** (2014) 226

[4] C. A. Lamas, D. C. Cabra, P. Pujol, G. L. Rossini, *Diagnosing order by disorder in quantum spin systems*, Eur. Phys. J. B **88** (2015) 176

[5] P. van Dieten, *Quantum fluctuations and degeneracies of two-dimensional magnetic skyrmions*, Bachelor Thesis, Utrecht University (2015).

[6] M. Raaijmakers, *Inhomogeneous groundstates in antiferromagnets with Dzyaloshinskii- Moriya interactions*, Bachelor Thesis, Utrecht University (2015).

[7] T. Holstein and H. Primakoff, *Dependence of the Intrinsic Domain Magnetization of a Ferromagnet*, Physical Review **58**, (1940).

[8] D. I. Khomskii, *Basic Aspects of the Quantum Theory of Solids*, Cambridge University Press, New York (2010) 1973: Random House, N.Y.

[9] J. H. P. Colpa, *Diagonalization of the quadratic boson Hamiltonian*, Physica **93A**, 327-353 (1978).

[10] H.T.C. Stoof, K.B. Gubbels and D.B.M. Dickerscheid, *Ultracold quantum fields*, 207-211, Springer (2009).

[11] A. Roldán-Molina, M.J. Santander and Á.S. Núñez, J. Fernández-Rossier, *Quantum theory of spin waves in finite chiral spin chains*, Phys. Rev. B **89**, 054403 (2014).

[12] T. H. R. Skyrme, *A unified field theory of mesons and baryons*, Nucl. Phys.**31**, 556-569 (1962).

[13] S. Mühlbauer, B. Binz, F. Jonietz, C. P eiderer, A. Rosch, A. Neubauer, R. Georgii, P. Böni, *Skyrmion Lattice in a Chiral Magnet*, Science **323**, 915-919 (2009).

[14] C. Pappas, E. Lelièvre-Berna, P. Falus, P. M. Bently, E. Moskvin, S. Grigoriev, P. Fouquet, B. Farago, *Chiral Paramagnetic Skyrmion-like Phase in MnSi*, Phys. Rev. Lett. **102**, 197202 (2009).

[15] F. Jonietz, S. Mühlbauer, C. Pleiderer, A. Neubauer, W. Münzer, A. Bauer, T. Adams, R. Georgii, P. Böni, R. A. Duine, K. Evershor, M. Garst, A. Rosch, *Spin Transfer Torques in MnSi at Ultralow Current Densities*, Science **330**, 1648-1651 (2010).

[16] S. Mahdavifar, M. R. Soltani, A. A. Masoudi, *Quantum corrections of the Dzyaloshinskii-Moriya interaction on the spin-$\frac{1}{2}$ antiferromagnet-Heisenberg chain in an uniform magnetic field*, Eur. Phys. J. B **62**, 215-220 (2008).

[17] S. J. Venema,*Magnetic phase diagrams of spin systems with inversion asymmetry*, Bachelor Thesis, Utrecht University (2014).