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# Spin waves in one-dimensional magnetic systems

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### **Abstract**

A magnetic material consists of a large number of coupled magnetic dipoles. Where does this coupling come from and how do differently coupled systems behave? Performing a Heitler-London calculation shows that the Coulomb interaction and the Pauli exclusion principle result in a split of energy levels which in turn causes the coupling. Which energy level is lowest will determine the type of magnetisation; ferromagnetic or antiferromagnetic. Combining exact analysis of the Ising model with mean field theory one finds that phase transitions occur in ferromagnetic systems as a function of temperature, one-dimensional systems excluded. At low temperatures a thermal fluctuation will result in a spin wave in the magnetic material. By viewing the spin wave as a perturbation of the ground state the Bloch equations are linearised and solved for one-dimensional systems. The final products are the dispersion relations that describe the motion of spin waves in differently coupled systems.

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# 1 Introduction

The refrigerator magnet is one of those seemingly ordinary and often whimsical household items which hides some beautiful quantum physics and is fun to play with. If classical electromagnetism is to be believed the fridge magnet will only stick to a fridge at temperatures near absolute zero. The permanent magnet needs quantum effects if it has any hope of holding your papers. The main tool in describing such a magnet quantum-mechanically is the Heisenberg model which describes the energy of a large amount of coupled magnetic ions on a lattice. Based on the coupling one can distinguish between ferromagnetic and antiferromagnetic materials. What determines this coupling and how do systems with different coupling behave throughout the temperature spectrum?

First of all this thesis will dig into the relevance of quantum effects when describing the coupling between magnetic moments. Secondly mean field theory and spin wave theory will be consulted in order to study the behaviour of various magnetic systems at throughout temperature spectrum. For example words will be devoted to the Ising model and its behaviour at finite temperatures which includes phase transitions. Later the emphasis will be on finding the ground states and analysing the low energy excitations known as spin waves for a variety of different systems, both ferromagnetic and antiferromagnetic.

## 2 Background

### 2.1 Electromagnetism

As mentioned in the introduction permanent magnets can not be described by classical electromagnetism. This section will show that the electromagnetic interaction between magnetic dipoles is too weak to explain experimental observations.

Magnetisation results from the alignment of magnetic moments arrayed in the material which is usually accomplished by applying an external magnetic field. After removing the magnetic field the material remains magnetised. However high temperatures cause random disturbances in the alignment of the magnetic moments, lowering the material's net magnetic moment. The Curie temperature of a magnetic material is the temperature at which the material loses its magnetic properties. This temperature ranges from  $\sim 100$  K for oxides of metals to  $\sim 1000$  K for iron. Hence the energy of the magnetic interaction should be roughly equal to the thermal energy at the Curie temperature such that the magnetic interaction can only be negated for temperatures higher than the Curie temperature.

Consider two magnetic dipoles with magnetic moments  $\vec{m}_1$  and  $\vec{m}_2$  separated by a distance  $\vec{r}_{12}$ . The magnetic field produced by the magnetic dipole moment  $\vec{m}_1$  is [1]:

$$\vec{B}_{dip}^1(\vec{r}) = \frac{\mu_0}{4\pi} \frac{1}{r^3} [3(\vec{m}_1 \cdot \hat{r})\hat{r} - \vec{m}_1] \quad (1)$$

The potential energy of the magnetic dipole moment  $\vec{m}_2$  in the magnetic field is:

$$U = -\vec{m}_2 \cdot \vec{B}_{dip}^1(\vec{r}_{12}) = \frac{\mu_0}{4\pi} \frac{1}{r_{12}^3} [\vec{m}_2 \cdot \vec{m}_1 - 3(\vec{m}_2 \cdot \hat{r}_{12})(\vec{m}_1 \cdot \hat{r}_{12})] \quad (2)$$

The absolute potential energy is at a maximum when  $\vec{r}_{12} \parallel \vec{m}_1 \parallel \vec{m}_2$ . The magnitude of the potential energy can be approximated as:

$$U = \frac{\mu_0}{2\pi} \frac{m_1 m_2}{r_{12}^3} = \frac{\mu_0}{16\pi} \frac{\mu_B^2}{a^3} \left[ \frac{m_1}{\mu_B} \frac{m_2}{\mu_B} \left( \frac{2a_0}{r_{12}} \right)^3 \right] \approx \frac{\mu_0}{16\pi} \frac{\mu_B^2}{a^3} \quad (3)$$

$$\approx 1 \text{ K}$$

in natural units ( $k_B = 1$ ), where  $\mu_B$  is the Bohr magneton and  $a$  is the Bohr radius. The magnitude of the atomic magnetic moments  $m_1, m_2$  are of the order of  $1 \mu_B$ . Additionally the distance between electrons in a magnetic material are typically of the order  $2a_0$ . Therefore the term in the square brackets is of order 1.

The energy of the electromagnetic interaction between atoms is roughly 1 K for all materials. In comparison the thermal energy is  $3/2 T$  per molecule at temperature  $T$ . This means that at 1 K the thermal energy would be high enough to break the magnetic interaction in practically all materials. However in reality this does not hold. As an example, the Curie temperature for iron is 1042 K [3, p.731]. This means the energy required to break the magnetic interaction is many orders of magnitude higher than the found interaction energy. This suggests the presence of an interaction that is stronger than the one described by classical electromagnetism. The next section will be devoted to deriving this interaction using quantum mechanics, specifically the Pauli exclusion principle.

## 2.2 Magnetism

If electromagnetism is not responsible for the behaviour of magnets, then what is? It turns out that magnetism is a result of the Pauli exclusion principle. The total wave function of the quantum system must be antisymmetric under the exchange of two fermions. This leads to a splitting of energy levels provided there is Coulomb interaction. The ground state is dependent on the type of material and so distinguishes between ferro- and antiferromagnetic materials.

The most common derivation of this result is the Heitler and London calculation [3, p.798]. In this derivation a neutral atom involved in magnetic interaction is pictured as a nucleus of nuclear charge  $+Ze$  together with a single electron at the outermost orbit (charge  $-e$ ). The other  $Z - 1$  electrons screen the nuclear charge perfectly from the outermost electron resulting in an effective nuclear charge of  $+e$ .

In a more realistic scenario the effective nuclear charge would be higher, especially if the atom has more than one electron in its highest orbit. Also there would be electron-electron repulsion which changes the wave function of the outermost electron. Despite the approximation the calculation is useful to gain qualitative insight.

The time-independent Schrödinger equation for one such atom at  $\vec{R}_i$  is:

$$\hat{H}_i \phi_i(\vec{r}_i) = \left[ -\frac{\hbar^2}{2m} \nabla_i^2 - \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\vec{r}_i - \vec{R}_i|} \right] \phi_i(\vec{r}_i) = E \phi_i(\vec{r}_i) \quad (4)$$

where  $\phi_i(\vec{r}_i)$  is the wave function of the outermost electron. Now consider two such atoms separated by a distance  $\vec{R}_{12} = \vec{R}_1 - \vec{R}_2$ . The Hamiltonian for two of these

atoms at a finite distance  $\vec{R}_{12}$  is:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{|\vec{r}_1 - \vec{r}_2|} + \frac{1}{|\vec{R}_{12}|} - \frac{1}{|\vec{r}_1 - \vec{R}_2|} - \frac{1}{|\vec{r}_2 - \vec{R}_1|} \right) \quad (5)$$

Besides the terms for the individual atomic contributions, interaction terms are added. The first term represents the electron-electron repulsion, the second term describes nuclei repulsion and the final two terms each cover the interaction of either electron with the other nucleus. Because the individual atoms are considered to be identical, the Hamiltonian is invariant under exchange of electrons. The total wave function is the product of the spin- and spatial wave function.

$$\Psi(\vec{r}_1, \vec{r}_2, \sigma_1, \sigma_2) = \phi(\vec{r}_1, \vec{r}_2)\chi(\sigma_1, \sigma_2) \quad (6)$$

According to the Pauli exclusion principle the total wave function should be antisymmetric under the exchange of electrons i.e.  $\Psi(\vec{r}_1, \vec{r}_2, \sigma_1, \sigma_2) = -\Psi(\vec{r}_2, \vec{r}_1, \sigma_2, \sigma_1)$ . Because the Hamiltonian does not explicitly depend on spin all the spin operators commute with the Hamiltonian. This means that the eigenfunctions of  $\hat{S}^2$  and  $\hat{S}^z$  span the spin space of the Hamiltonian:

$$\chi_{0,0} = \frac{1}{\sqrt{2}}(\chi_\uparrow(\sigma_1)\chi_\downarrow(\sigma_2) - \chi_\downarrow(\sigma_1)\chi_\uparrow(\sigma_2)) \quad S = 0, S_z = 0 \quad (7a)$$

This function is the only odd state i.e. the spin singlet.

$$\chi_{1,0} = \frac{1}{\sqrt{2}}(\chi_\uparrow(\sigma_1)\chi_\downarrow(\sigma_2) + \chi_\downarrow(\sigma_1)\chi_\uparrow(\sigma_2)) \quad S = 1, S_z = 0 \quad (7b)$$

$$\chi_{1,1} = \chi_\uparrow(\sigma_1)\chi_\uparrow(\sigma_2) \quad S = 1, S_z = 1 \quad (7c)$$

$$\chi_{1,-1} = \chi_\downarrow(\sigma_1)\chi_\downarrow(\sigma_2) \quad S = 1, S_z = -1 \quad (7d)$$

These functions are even and form the spin triplet. The spin wave functions of the Hamiltonian are either odd or even and must be paired with an even or odd spatial wave function to create an odd total wave function. Therefore the spatial wave functions are:

$$\phi_s = \frac{1}{\sqrt{2 + 2l^2}}(\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) + \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)) \quad (8a)$$

$$\phi_t = \frac{1}{\sqrt{2 - 2l^2}}(\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) - \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)) \quad (8b)$$

where the following shorthand was used for normalisation:

$$l \equiv \left| \int d\vec{r} \phi_1^*(\vec{r})\phi_2(\vec{r}) \right| \quad (8c)$$

There are four different total wave functions. The singlet wave function  $\Psi_s = \phi_s\chi_{0,0}$  which is the product of the even spatial wave function and the spin singlet. The three triplet wave functions  $\Psi_t = \phi_t\chi_{1,m}$  which are the product of the odd spatial wave function and one of the spin wave functions from the spin triplet. Because the Hamiltonian does not depend on spin the triplet wave functions all have the same energy ( $E_t$ ). Consequently there are two energy levels,  $E_s$  and  $E_t$ , which may or may not be degenerate. Whether the lowest energy level is  $E_s$  or  $E_t$  will determine if the material is ferromagnetic or antiferromagnetic.

### 2.3 Hydrogen (H<sub>2</sub>)

The Heitler and London calculation requires some major approximation for most materials as discussed in the previous section. In the case of hydrogen, where only one electron is present, none of the approximations apply. As hypothesised in section 2.1 the interaction responsible for magnetism should be stronger than the one described by electromagnetism. The difference between the energy levels determines the strength of the interaction and is referred to as the energy splitting. This section will focus on completing the Heitler and London calculation for hydrogen. The end result will be a numerical value for the energy splitting in the case of hydrogen. Let  $E$  be the energy of an isolated hydrogen atom then the Schrödinger equation for the individual atom becomes:

$$\hat{H}_i \phi_i(\vec{r}_i) = \left[ -\frac{\hbar^2}{2m} \nabla_i^2 - \frac{e^2}{\pi \epsilon_0 |\vec{r}_i - \vec{R}_i|} \right] \phi_i(\vec{r}_i) = E \phi_i(\vec{r}_i) \quad (9)$$

The total Hamiltonian in equation (5) now describes two hydrogen atoms separated by a distance  $R_{12}$ . Since the total Hamiltonian that does not depend on spin, the energy levels become:

$$E_s = \langle \phi_s | \hat{H} | \phi_s \rangle, \quad E_t = \langle \phi_t | \hat{H} | \phi_t \rangle \quad (10)$$

The two hydrogen atoms are identical so the Hamiltonian is invariant under the exchange of electrons. Using this short-hand for the Coulomb interaction:

$$U(\vec{r}_1, \vec{r}_2) = \frac{e^2}{4\pi\epsilon_0} \left( \frac{1}{|\vec{r}_1 - \vec{r}_2|} + \frac{1}{|\vec{R}_{12}|} - \frac{1}{|\vec{r}_1 - \vec{R}_2|} - \frac{1}{|\vec{r}_2 - \vec{R}_1|} \right) \quad (11)$$

one can calculate the following expressions:

$$\begin{aligned} \langle \phi_1(\vec{r}_1) \phi_2(\vec{r}_2) | \hat{H} | \phi_1(\vec{r}_1) \phi_2(\vec{r}_2) \rangle &= \int d\vec{r}_1 d\vec{r}_2 \phi_1^*(\vec{r}_1) \phi_2^*(\vec{r}_2) \hat{H} \phi_1(\vec{r}_1) \phi_2(\vec{r}_2) \\ &= \langle \phi_1(\vec{r}_2) \phi_2(\vec{r}_1) | \hat{H} | \phi_1(\vec{r}_2) \phi_2(\vec{r}_1) \rangle = \int d\vec{r}_1 d\vec{r}_2 \phi_1^*(\vec{r}_2) \phi_2^*(\vec{r}_1) \hat{H} \phi_1(\vec{r}_2) \phi_2(\vec{r}_1) \quad (12) \\ &= 2E + \int d\vec{r}_1 d\vec{r}_2 U(\vec{r}_1, \vec{r}_2) |\phi_1(\vec{r}_1)|^2 |\phi_2(\vec{r}_2)|^2 \\ &= 2E + I_1 \end{aligned}$$

$$\begin{aligned} \langle \phi_1(\vec{r}_2) \phi_2(\vec{r}_1) | \hat{H} | \phi_1(\vec{r}_1) \phi_2(\vec{r}_2) \rangle &= \int d\vec{r}_1 d\vec{r}_2 \phi_1^*(\vec{r}_2) \phi_2^*(\vec{r}_1) \hat{H} \phi_1(\vec{r}_1) \phi_2(\vec{r}_2) \\ &= \langle \phi_1(\vec{r}_1) \phi_2(\vec{r}_2) | \hat{H} | \phi_1(\vec{r}_2) \phi_2(\vec{r}_1) \rangle = \int d\vec{r}_1 d\vec{r}_2 \phi_1^*(\vec{r}_1) \phi_2^*(\vec{r}_2) \hat{H} \phi_1(\vec{r}_2) \phi_2(\vec{r}_1) \quad (13) \\ &= 2E + \int d\vec{r}_1 d\vec{r}_2 U(\vec{r}_2, \vec{r}_1) \phi_1^*(\vec{r}_1) \phi_2^*(\vec{r}_2) \phi_1(\vec{r}_2) \phi_2(\vec{r}_1) \\ &= 2E + I_2 \end{aligned}$$

The integrals  $I_1$  and  $I_2$  represent the interaction between the atoms and depend only on the distance between the atoms  $R_{12}$ . Notice that these interactions do not exist

without the Coulomb interaction i.e. if  $U(\vec{r}_1, \vec{r}_2) = 0$  then  $I_1, I_2 = 0$ .  
The energy levels in (10) become:

$$E_s = \langle \phi_s | \hat{H} | \phi_s \rangle = 2 \frac{2E + I_1 + 2l^2E + I_2}{2 + 2l^2} = 2E + \frac{I_1 + I_2}{1 + l^2} \quad (14a)$$

$$E_t = \langle \phi_t | \hat{H} | \phi_t \rangle = 2 \frac{2E + I_1 - 2l^2E - I_2}{2 - 2l^2} = 2E + \frac{I_1 - I_2}{1 - l^2} \quad (14b)$$

So the energy splitting will be:

$$J \equiv E_s - E_t = \frac{2I_2 - 2l^2I_1}{1 - l^4} \quad (15)$$

This also shows that if there is no Coulomb interaction ( $U(\vec{r}_1, \vec{r}_2) = 0$ ) there will be no energy splitting.

The ground state spatial wave function of an isolated hydrogen atom is known to be:

$$\phi_i(\vec{r}_i) = \frac{1}{\sqrt{\pi a_0^3}} e^{-|\vec{r}_i - \vec{R}_i|/a_0} \quad (16)$$

with eigenenergy  $E = -13.6 \text{ eV} \approx 1.6 \cdot 10^5 \text{ K}$ . The energy splitting can be calculated numerically and depends only on the distance  $R_{12}$ . The graph in figure 1 shows the value of the energy splitting for hydrogen for different values of  $R_{12}$ . The energy splitting is negative, so the singlet state is the ground state. Therefore a hydrogen molecule is an example of an antiferromagnet, the spins of the two electrons are oppositely aligned.

The typical distance between two hydrogen atoms in a hydrogen molecule is  $1.4 a_0$ . At this distance the energy splitting is  $J \approx -6.6 \cdot 10^4 \text{ K}$ . The coupling is four orders of magnitude stronger than the coupling described by electromagnetism making it a more plausible explanation for magnetic behaviour. In comparison the energy splitting of iron is roughly  $J \approx 175 \text{ K}$  which is two orders of magnitude smaller than that of hydrogen. So does the Heitler and London calculation overestimate the coupling if done for iron instead of hydrogen? Not necessarily, the difference between hydrogen and iron can be explained by outlining the following discrepancies. First of all the Heitler-London calculation works less well in the case of iron since more approximations are required. A big factor in the approximations are the electron screening effects. For instance, iron naturally has two electrons in its outermost shell while only one is considered in the calculation. Consequently the other electron does not screen the nucleus as much as it would when in a lower shell. Additionally the calculation assumes that all electrons in lower shells screen the nucleus perfectly, i.e. each electron reduces the effective nuclear charge by  $e$ . In reality they do not. Together these effects contribute to a higher effective nuclear charge and thus a stronger coupling. Secondly the typical atom spacing between iron atoms is roughly  $5.4 a_0$  [10] which is larger than it is between hydrogen atoms ( $1.4 a_0$ ) thus based on this one would expect a much lower energy splitting. At the end of the day the two effects should amount to a energy splitting of roughly  $175 \text{ K}$ , however a complete calculation is beyond the scope of this thesis.



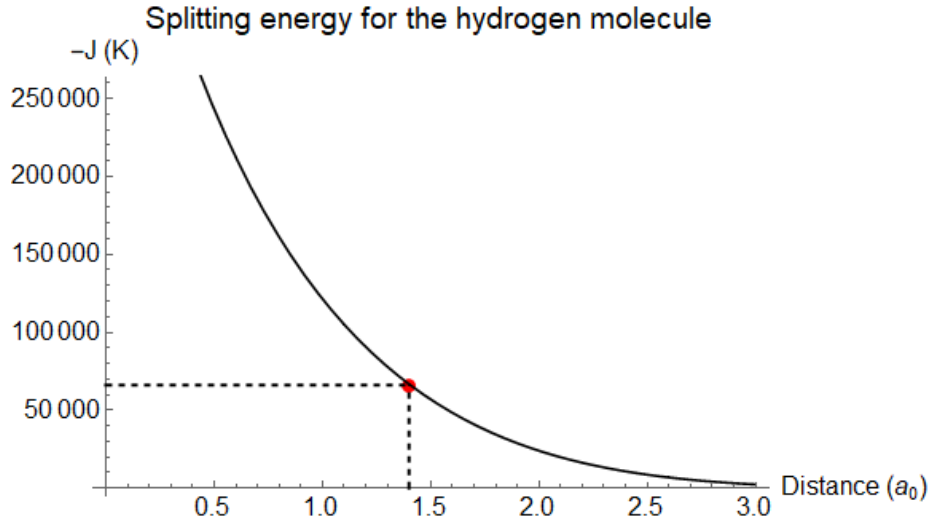


Figure 1: The energy splitting for the hydrogen molecule as a function of the distance between the hydrogen atoms. The red dot represents the point on the graph specific to hydrogen with  $R_{12} = 1.4a_0$  and  $J = -66000\text{K}$

## 2.4 Spin Hamiltonian

The Hamiltonian in equation (5) is one that acts only on the spatial degrees of freedom of the system. There exists however an equivalent expression that instead acts only on the spin degrees of freedom of the electrons. Such a Hamiltonian is referred to as a spin Hamiltonian. This section is devoted to showing that the two representations are equivalent. The spin Hamiltonian also forms the basis for the Heisenberg model which will be derived shortly after.

The spin Hamiltonian for the two atoms is of the form [3]:

$$\hat{H}_{spin} = \alpha + \beta(\hat{S}_1 \cdot \hat{S}_2) = \alpha + \frac{1}{2}\beta(\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2) \quad (17)$$

where  $\alpha$  and  $\beta$  are constants,  $\hat{S}_i$  are the spin angular momentum operators of the individual spin-1/2 systems i.e. the outermost electrons and  $\hat{S} = \hat{S}_1 + \hat{S}_2$  is the total angular momentum operator. As mentioned in section 2.2, the eigenfunctions in equation (7) form a basis of the 4-dimensional spin space of the Hamiltonian. For any of the eigenfunctions the spin operators of the individual systems satisfy  $\hat{S}_i = \frac{1}{2}(\frac{1}{2} + 1) = \frac{3}{4}$ . Therefore one can rewrite the spin Hamiltonian as:

$$\hat{H}_{spin} = \alpha + \frac{1}{2}\beta(\hat{S}^2 - \frac{3}{2}) \quad (18)$$

When the spin Hamiltonian acts on the singlet state one finds an energy of  $E_s = \alpha - \frac{3}{4}\beta$ , whereas for the triplet state  $E_t = \alpha + \frac{1}{4}\beta$ . The goal is to choose  $\alpha$  and  $\beta$  such that the spin Hamiltonian gives identical results as the Hamiltonian in equation

(5). With a simple calculation one finds:

$$\hat{H}_{spin} = \frac{3E_t - E_s}{4} + (E_t - E_s)(\hat{S}_1 \cdot \hat{S}_2) \quad (19)$$

Because the two representations act identically on a basis of states they must do so on all states i.e. they are equivalent. This formulation of the Hamiltonian shows the proportionality to spin as in the Heisenberg model.

$$\hat{H}_{spin} \propto -J(\hat{S}_1 \cdot \hat{S}_2) \quad (20)$$

Where  $J = (E_s - E_t)$  is the energy splitting introduced in (15), here and after known as the coupling constant.

## 2.5 Heisenberg model

The Heisenberg model describes the energy of a large number of spins placed on a n-dimensional lattice. It does not necessarily describe the behaviour of a tangible system, instead it is a tool to study the fundamental behaviour of such a system at a qualitative level. The model is often used in the field of statistical mechanics to study phase transitions of ordered systems, such as ferromagnets. Without making any assumptions concerning the lattice, the most general form of the Heisenberg model concerning spatial coupling is:

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} (J_{ij}^x \hat{S}_i^x \hat{S}_j^x + J_{ij}^y \hat{S}_i^y \hat{S}_j^y + J_{ij}^z \hat{S}_i^z \hat{S}_j^z) \quad (21)$$

where the sums run over all spins and periodic boundary conditions apply. The factor  $\frac{1}{2}$  is included to compensate for the double counting of pairs. Additionally  $J \sim 10\,000$  K so the system has the right energy scale to describe the Curie temperature. The Heisenberg model is a generalisation of the spin Hamiltonian in (20). Note that the coupling constant may vary from pair to pair, and must satisfy  $J_{ij} = J_{ji}$ . In this thesis pairs of non-neighbouring spins are neglected because, in the treated cases, the coupling decreases exponentially with distance similar to the hydrogen case (see figure 1). In the event that coupling between non-neighbouring spins does become important the system becomes more complicated as do all the consequent calculations.

The Heisenberg model in (21) is not the most general formulation of the Heisenberg model concerning spin symmetry. For instance the following one-dimensional model allows for direction-dependent coupling and is referred to as the XYZ-model.

$$\mathcal{H} = \sum_i (J_x \hat{S}_i^x \hat{S}_{i+1}^x + J_y \hat{S}_i^y \hat{S}_{i+1}^y + J_z \hat{S}_i^z \hat{S}_{i+1}^z) \quad (22)$$

where  $J_x, J_y, J_z$  are coupling constants in the different directions. Two types of systems which are often studied are the cases where either  $J_x, J_y, J_z > 0$  or  $J_x, J_y, J_z < 0$ . In the latter case one deals with a ferromagnet where, in the ground state, all spins are orientated in the same direction. Whereas in the antiferromagnetic case,

$J_x, J_y, J_z > 0$ , the ground state is a singlet of total spin  $\vec{S} = \sum_i \vec{S}_i$ . Finally there are the XXZ-model ( $J_x = J_y$ ) and the fully isotropic XXX-model ( $J_x = J_y = J_z$ ). These models will be used later to study spin waves in one dimension. Each of the models have there analogies in higher dimensions.

### 3 Ising model

The Ising model is another special version of the Heisenberg model. The model describes a system of spins that can solely point along one direction. By convention the fixed direction is chosen to be along the z-axis. Every spin in the system must point along this direction, so either up or down. In essence the Ising model is the extreme case of the XYZ-model where  $J_x, J_y \ll J_z \equiv J$ , so putting  $J_x, J_y = 0$  in (22) gives:

$$\mathcal{H} = -J \sum_{\langle i, j \rangle} \hat{S}_i^z \hat{S}_j^z \quad (23)$$

where the sum runs only over nearest neighbour pairs (notation:  $\langle i, j \rangle$ ). The model is used to study a variety of systems such as biological membranes, protein folding and social systems [6, 7, 8]. In this section it will be used to study phase transitions in ferromagnets.

A ferromagnet exhibits a phase transition if at some finite temperature  $T_c$  it goes from an ordered state to a disordered state in a non-smooth fashion. What exactly this means will be discussed throughout this chapter. Intuitively the system is in a disordered state if all spins are orientated randomly and in an ordered state if this is not the case. To make this more precise consider the average magnetisation of the system defined as follows:

$$m = \frac{1}{N} \sum_{i=1}^N \hat{S}_i^z \quad (24)$$

where  $N$  is the total number of spins. The average magnetisation is used to parameterise the phase transition. Plotting the average magnetisation as a function of the temperature will show how the system behaves and whether or not a phase transition occurs. The ground state of the ferromagnetic system described by (23) is the state in which all spins are aligned and the average magnetisation is  $m = \pm 1 \neq 0$ . At high temperatures the system is in a disordered state because of thermal fluctuations so the average magnetisation is  $m = 0$ . This means that the ferromagnetic system is in two different states at either end of the temperature spectrum. However this does not necessarily mean that there is a phase transition as will be illustrated by the next example.

#### 3.1 One-dimensional ferromagnet

Consider a one-dimensional ferromagnet i.e.  $N$  particles on a one-dimensional lattice described by the Ising model. At first assume no periodic boundary conditions. The

Hamiltonian for this system is:

$$\mathcal{H} = -J \sum_{i=1}^{N-1} \hat{S}_i^z \hat{S}_{i+1}^z \quad (25)$$

where, because this is a ferromagnet,  $J > 0$ . Hence the system is in the ground state when all spins are aligned (see figure 2a). Now introduce a single defect then, to minimise the energy, a whole row of spins will change direction (see figure 2b). Since at finite temperature some spins will be flipped the system will be divided into clusters of aligned spins. For a specifically long chain the average magnetisation is expected to be zero, so the system is always in a disordered state ( $m = 0$ ) at finite temperature. Although not hard proof this strongly indicates that there is no phase transition as a function of temperature because a phase transition must always occur at some finite temperature  $T_c$ .



(a) One of the two ground states of the one-dimensional ferromagnetic Ising model



(b) An excited state with the lowest energy above the ground state energy. Because there are no periodic boundary conditions a whole column of spins flip to minimise the energy of the system.

Figure 2: The ground state and an excited state of the one-dimensional ferromagnet without periodic boundary conditions.



(a) An excited state with the lowest energy above the ground state energy. Only one spin is flipped.



(b) Another excited state of with the lowest energy above the ground state energy. An arbitrary number of spins is flipped.

Figure 3: Two excited states of the one-dimensional ferromagnet with periodic boundary conditions that have the same energy.

The question remains however: what happens when one does assume periodic boundary conditions? The ground state will remain identical, however when one spin flips around there is no longer the guarantee that a whole column will flip as this does not lower the energy any more. Does this mean that only one spin flips at a time? Not necessarily, the length of the column that flips with the spin is arbitrary. This follows from the fundamental assumption of statistical mechanics which says that when a closed system is in equilibrium all microstates are equally likely. The microstates the axiom speaks of are the configurations of the system. Consequently, at a fixed energy, any possible configuration of the system is equally likely. For example the energies of figure 3a and 3b are the same, thus both states are equally likely. Not only these two

examples, but any state that has exactly two antiparallel pairs. Since all these states are equally probable the expected average magnetisation is again zero at finite temperature. Drawing the same conclusions as before this suggests no phase transition as a function of temperature in the one-dimensional case [4]. A mathematical proof for this result can be derived by calculating the free energy of the one-dimensional Ising model exactly using the transfer matrix method. Doing this will result in a smooth expression for the free energy as a function of temperature. However phase transitions must occur in a non-smooth fashion, hence there is no phase transition as a function of temperature.

## 4 Mean field theory

The Ising model has not been solved analytically for more than two dimensions. As ever the goal is to describe real materials so it would be nice to solve the three-dimensional case and compare theory to experiment. Another way to describe a ferromagnetic system is mean field theory. It studies the system by considering a single isolated spin in a mean magnetic field generated by the rest of the spins, hence the name. To make the idea of mean field theory more discrete consider a n-dimensional ferromagnet with periodic boundary conditions. By the philosophy of mean field theory the Hamiltonian for this system can be written as:

$$\mathcal{H} = - \sum_i \vec{H}_{eff} \hat{S}_i \quad (26)$$

where the sum is over all spins each in a field  $\vec{H}_{eff}$  generated by all other spins. When the system is in an ordered state the field  $\vec{H}_{eff}$  for each spin is strong and points along the same direction as each spin hence the energy is low as, expected from the ground state. When the system is in a disordered state the average magnetisation is zero. The field  $\vec{H}_{eff}$  generated by all other spins is weak but is antiparallel to the spin that is being isolated. As a result the energy will be high. This brings to light one of the limitations of mean field theory; it does not accommodate well for local interactions. Mean field theory does not weigh the contribution of individual spins to the effective field  $H_{eff}$ . Even in the disordered state the system is often divided in clusters of aligned spins. When considering a spin in such a cluster mean field theory does not distinguish between a neighbouring spin or a spin far away. This in contrast to the models treated so far which only took into account neighbouring spins. Consequently, in a system where the mean field is zero, mean field theory predicts no correlation between individual spins. Unfortunately the aggregation of spins pointing in the same direction primarily happens near phase transitions, where the system is most interesting.

## 4.1 Mean field theory of the Ising model

Consider a  $n$ -dimensional ferromagnet described by the Ising model<sup>1</sup>:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \hat{S}_i^z \hat{S}_j^z = -J \sum_{\langle i,j \rangle} \hat{S}_i \hat{S}_j \quad (27)$$

where  $J > 0$ . The goal is to rewrite the Hamiltonian in (27) to one as in equation (26). For large  $N$  the effective fields are practically the same for each spin. Using this approximation only one expression for the effective field is required. Also we can rewrite:

$$\hat{S}_i = \langle \hat{S} \rangle + (\hat{S}_i - \langle \hat{S} \rangle) = \langle \hat{S} \rangle + \delta \hat{S}_i \quad (28)$$

where  $m \equiv \langle \hat{S} \rangle$  is the average magnetisation of the system and  $\delta \hat{S}_i = (\hat{S}_i - \langle \hat{S} \rangle)$  is the (small) difference between the spin  $S_i$  and the mean. Then, keeping things up to first order, one obtains:

$$\begin{aligned} \hat{S}_i \hat{S}_j &= (\langle \hat{S} \rangle + \delta \hat{S}_i)(\langle \hat{S} \rangle + \delta \hat{S}_j) \approx \langle \hat{S} \rangle^2 + \langle \hat{S} \rangle(\delta \hat{S}_i + \delta \hat{S}_j) \\ &= -\langle \hat{S} \rangle^2 + \langle \hat{S} \rangle(\hat{S}_i + \hat{S}_j) \end{aligned} \quad (29)$$

This provides a way to rewrite equation (27). Let  $z$  be the number of nearest neighbours and  $N$  the total number of particles then, taking care not to double count pairs, one obtains:

$$\begin{aligned} \mathcal{H} &= -J \sum_{\langle i,j \rangle} \hat{S}_i \hat{S}_j \\ &= -J \sum_{\langle i,j \rangle} \left( -\langle \hat{S} \rangle^2 + \langle \hat{S} \rangle(\hat{S}_i + \hat{S}_j) \right) \\ &= \frac{JNz}{2} \langle \hat{S} \rangle^2 - \frac{Jz}{2} \langle \hat{S} \rangle \sum_i 2\hat{S}_i \\ &= \frac{\tilde{H}Nm}{2} - \tilde{H} \sum_i \hat{S}_i \end{aligned} \quad (30)$$

where  $\tilde{H} = Jz\langle \hat{S} \rangle = Jzm$  is the effective field as in (26). Due to the restriction of the Ising model to nearest neighbour interactions the effective field is only created by the nearest neighbours of each spin instead of all other spins in the system. The constant term can be ignored for now because it will not be important in deriving the qualitative results for this system. The relevant progress resulting from this mean

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<sup>1</sup>I will omit the superscripts to ease the notation

field approach appears when calculating the mean magnetisation:

$$\begin{aligned}
m \equiv \langle \hat{S}_i \rangle &= \frac{\sum_{S_1} \sum_{S_2} \cdots \sum_{S_N} \hat{S}_i e^{-\beta \mathcal{H}}}{\sum_{S_1} \sum_{S_2} \cdots \sum_{S_N} e^{-\beta \mathcal{H}}} \\
&= \frac{e^{-\beta \tilde{H} N m / 2} \prod_{j=1}^N \left( \sum_{S_j} \hat{S}_j e^{\beta \tilde{H} \hat{S}_j} \right)}{e^{-\beta \tilde{H} N m / 2} \prod_{i=1}^N \left( \sum_{S_j} e^{\beta \tilde{H} \hat{S}_j} \right)} \\
&= \frac{2^N \cosh(\beta \tilde{H})^{N-1} \sinh(\beta \tilde{H})}{2^N \cosh(\beta \tilde{H})^N} \\
&= \frac{\sinh(\beta \tilde{H})}{\cosh(\beta \tilde{H})} = \tanh(\beta J z m)
\end{aligned} \tag{31}$$

where  $\beta = 1/(k_B T)$ . This self-consistent expression has either one or three solutions depending on the value of  $\beta J z$ . In the high temperature limit  $\beta J z \leq 1$  there is only one solution:  $m = 0$ , the disordered state. At lower temperatures,  $\beta J z > 1$ , there are three solutions:  $m = 0$  and  $m = \pm \tilde{m}$ . The additional solutions  $m = \pm \tilde{m}$  are a result of the up/down symmetry of the system and correspond to ordered states (see figure 4). It turns out that these ordered states are actually ground states of the system at low

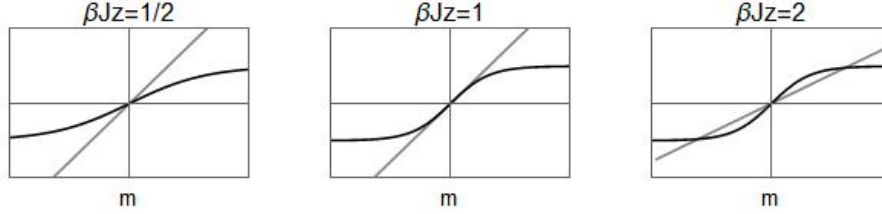


Figure 4: The graphs of  $m$  (gray line) and  $\tanh(\beta J z m)$  (black line) as a function of  $m$  for different values of  $\beta J z$  (temperatures). When  $\beta J z \leq 1$  there is one intersection at  $m = 0$ . When  $\beta J z > 1$  there are two additional intersections at  $m = \pm \tilde{m}$ .

temperatures<sup>2</sup>. Figure 5 shows the average magnetisation as a function of temperature in the case of iron. The average magnetisation decreases continuously from  $m = 1$  at low temperatures until it reaches zero at the Curie temperature (1042 K) and remains zero thereafter. At the Curie temperature the system transitions from an ordered state ( $m \neq 0$ ) to a disordered state ( $m = 0$ ) in a non-smooth way, hence a phase transition occurs. Such a phase transition as in iron is categorised as a continuous phase transition. The temperature at which this transition occurs is given by  $T_c = J z$ , such that  $\beta_c J z = 1$ . This expression allows for the calculation of the coupling constant for iron on a three-dimensional cubic lattice ( $z = 6$ ) from the experimental value for the Curie temperature ( $T_c \sim 1000$  K):  $J \sim 175$  K. This is the value that was used in section 2.3 to compare to the coupling constant for hydrogen.

<sup>2</sup>A derivation of this result can be found in appendix A

Interestingly this result is acquired without assumptions concerning the dimension of the system. The dimension of the system enters the problem through the variable  $z$  (the number of nearest-neighbours). However as was discussed in section 3.1 there is no phase transition in the one-dimensional case, but mean field theory says otherwise. Hence mean field theory fails in one dimension.

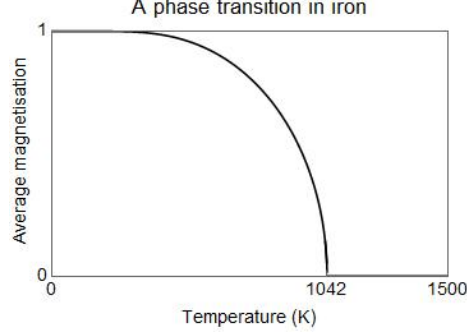


Figure 5: The continuous phase transition in iron. At low temperatures the system is in an ordered state, at high temperatures it is in a disordered state. The phase transition occurs at  $T_c = 1042$  K.

## 5 Ground states of general systems

Up until now the Heisenberg model has only been treated in the extreme case; the Ising model. Although the Ising model has been useful in introducing new concepts such as mean magnetisation, phase transitions and mean field theory it will now make way for more general systems. The Ising model is cast aside because it does not allow for the existence of spin waves. Spin waves are low energy perturbations from the ground state so it is beneficial to find the ground states of the general systems so that we may use these ground states to study spin waves in the next section.

### 5.1 Ferromagnetic Heisenberg model

First of all consider the Heisenberg model on a lattice:

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} (J_{ij}^x \hat{S}_i^x \hat{S}_j^x + J_{ij}^y \hat{S}_i^y \hat{S}_j^y + J_{ij}^z \hat{S}_i^z \hat{S}_j^z) \quad (32)$$

where the sum runs over all sites, not just nearest-neighbour pairs and periodic boundary conditions apply. Later it will be assumed that  $J_{ij}^k > 0$ . Notice that no restriction are made to the dimension of the system. Introduce the raising and lowering operator  $\hat{S}_i^+ = \hat{S}_i^x + i\hat{S}_i^y$  and  $\hat{S}_i^- = \hat{S}_i^x - i\hat{S}_i^y$ , hence  $\hat{S}_i^x = (\hat{S}_i^+ + \hat{S}_i^-)/2$  and



$\hat{S}_i^y = -i(\hat{S}_i^+ - \hat{S}_i^-)/2$ . Equation (32) reduces to:

$$\begin{aligned}\mathcal{H} &= -\frac{1}{2} \sum_{i,j} \left( J_{ij}^x \frac{\hat{S}_i^+ + \hat{S}_i^-}{2} \frac{\hat{S}_j^+ + \hat{S}_j^-}{2} - J_{ij}^y \frac{\hat{S}_i^+ - \hat{S}_i^-}{2} \frac{\hat{S}_j^+ - \hat{S}_j^-}{2} + J_{ij}^z \hat{S}_i^z \hat{S}_j^z \right) \\ &= -\frac{1}{2} \sum_{i,j} \left( \Delta_{ij}^+ \frac{\hat{S}_i^- \hat{S}_j^+ + \hat{S}_i^+ \hat{S}_j^-}{2} + \Delta_{ij}^- \frac{\hat{S}_i^+ \hat{S}_j^+ + \hat{S}_i^- \hat{S}_j^-}{2} + J_{ij}^z \hat{S}_i^z \hat{S}_j^z \right)\end{aligned}\quad (33)$$

where  $\Delta_{ij}^\pm = (J_{ij}^x \pm J_{ij}^y)/2$ . The ground states of the ferromagnetic Ising model are the fully polarised states i.e. the total spin is maximal and all spins are aligned along the z-direction. For example<sup>3</sup>:

$$|\psi\rangle = |S, S\rangle_1 |S, S\rangle_2 \dots |S, S\rangle_N \quad (34)$$

This leads to:

$$\begin{aligned}\mathcal{H}|\psi\rangle &= -\frac{1}{2} \sum_{i,j} \left( 0 + 0 + 0 + \Delta_{ij}^- \frac{\hat{S}_i^- \hat{S}_j^-}{2} |\psi\rangle + J_{ij}^z \hat{S}_i^z \hat{S}_j^z |\psi\rangle \right) \\ &= -\frac{1}{2} \sum_{i,j} \left( S \Delta_{ij}^- [\dots |S, S-1\rangle_i \dots |S, S-1\rangle_j + \dots] + S^2 J_{ij}^z |\psi\rangle \right)\end{aligned}\quad (35)$$

The first three terms vanish because  $\hat{S}_i^+ |S, S\rangle_i = 0$  for all  $i$ . Taking the limiting case  $J_{ij}^x, J_{ij}^y \ll J_{ij}^z$  one finds that  $|\psi\rangle$  is indeed an eigenstate. A second scenario in which  $|\psi\rangle$  is an eigenstate of  $\mathcal{H}$  presents itself when  $\Delta_{ij}^- = 0$  or equivalently  $J_{ij}^x = J_{ij}^y$  for all  $i, j$  turning the model into a XXZ-model. Sticking to the latter scenario for a moment denote by  $\mathcal{H}_0$  the Heisenberg model for which  $J_{ij}^x = J_{ij}^y$  for all  $i, j$ . Define the total spin:  $\hat{S} = \sum_i \hat{S}_i$  then one also finds that:

$$\begin{aligned}[\hat{S}^z, \mathcal{H}] &= -\frac{1}{2} \sum_{i,j} \sum_k \left[ \hat{S}_k^z, J_{ij}^x \hat{S}_i^x \hat{S}_j^x + J_{ij}^y \hat{S}_i^y \hat{S}_j^y + J_{ij}^z \hat{S}_i^z \hat{S}_j^z \right] \\ &= -\frac{1}{2} \sum_{i,j,k} J_{ij}^x (\hat{S}_i^x [\hat{S}_k^z, \hat{S}_j^x] + [\hat{S}_k^z, \hat{S}_i^x] \hat{S}_j^x) + J_{ij}^y (\hat{S}_i^y [\hat{S}_k^z, \hat{S}_j^y] + [\hat{S}_k^z, \hat{S}_i^y] \hat{S}_j^y) \\ &= -\frac{1}{2} \sum_{i,j,k} J_{ij}^x (\hat{S}_i^x \delta_{kj} i \hat{S}_j^y + \delta_{ki} i \hat{S}_i^y \hat{S}_j^x) - J_{ij}^y (i \hat{S}_i^y \delta_{kj} \hat{S}_j^x + i \delta_{ki} \hat{S}_i^x \hat{S}_j^y) \\ &= -\frac{i}{2} \sum_{i,j} J_{ij}^x (\hat{S}_i^x \hat{S}_j^y - \hat{S}_i^y \hat{S}_j^x) - \frac{i}{2} \sum_{i,j} J_{ij}^y (\hat{S}_i^y \hat{S}_j^x - \hat{S}_i^x \hat{S}_j^y) \\ &= -i \sum_{i,j} \Delta_{ij}^- (\hat{S}_i^x \hat{S}_j^y - \hat{S}_i^y \hat{S}_j^x)\end{aligned}\quad (36)$$

<sup>3</sup>The notation that is used is:  $|S_{tot}, m\rangle_i$  where  $S_{tot}$  is the total spin and  $m$  is the spin along the z-direction.

Hence  $[\hat{S}^z, \mathcal{H}_0] = 0$  and analogously  $[\hat{S}^x, \mathcal{H}_0] = 0$ ,  $[\hat{S}^y, \mathcal{H}_0] = 0$ . Therefore  $\mathcal{H}_0$  commutes with  $\hat{S}^2$  and  $\hat{S}^z$ ; thus shares a common basis of eigenstates with  $\hat{S}^2$  and  $\hat{S}^z$ . In addition this means that  $\mathcal{H}_0$  is invariant under rotations in spin space. Consequently every state that is fully polarised is an eigenstate of  $\mathcal{H}_0$ . In a spin-1/2 system there are exactly two fully polarised states: up-and down states. The eigenenergy for any of the polarised states is  $E = -\frac{1}{2}S^2 \sum_{i,j} J_{ij}^z$ . On the other hand the expectation value  $\langle \phi | \mathcal{H}_0 | \phi \rangle$  for an arbitrary product state:  $|\phi\rangle = |S, m_1\rangle_1 \dots |S, m_N\rangle_N$  is:

$$\begin{aligned} \langle \phi | \mathcal{H}_0 | \phi \rangle &= -\frac{1}{2} \sum_{i,j} \left( \Delta_{ij}^+ \frac{\langle \phi | \hat{S}_i^- \hat{S}_j^+ | \phi \rangle}{2} + \Delta_{ij}^- \frac{\langle \phi | \hat{S}_i^+ \hat{S}_j^- | \phi \rangle}{2} + J_{ij}^z \langle \phi | \hat{S}_i^z \hat{S}_j^z | \phi \rangle \right) \\ &= -\frac{1}{2} \sum_{i,j} \left( 0 + 0 + J_{ij}^z \langle \phi | \hat{S}_i^z \hat{S}_j^z | \phi \rangle \right) \\ &= -\frac{1}{2} \sum_{i,j} m_i m_j J_{ij}^z \end{aligned} \tag{37}$$

where the first term vanishes because  $|\phi\rangle$  and  $\hat{S}_i^- \hat{S}_j^+ |\phi\rangle$  are orthogonal and in a similar fashion the second term vanishes as well. Up to this point the derivation holds for general  $J_{ij}^z$ . Considering systems with  $J_{ij}^z \geq 0$  for all  $i, j$  one finds that:

$$\langle \phi | \mathcal{H}_0 | \phi \rangle = -\frac{1}{2} \sum_{i,j} m_i m_j J_{ij}^z \geq -\frac{1}{2} S^2 \sum_{i,j} J_{ij}^z = \langle \psi | \mathcal{H}_0 | \psi \rangle \tag{38}$$

The product states  $|\phi\rangle$  form a basis and thus for every state the energy is larger than:  $\langle \psi | \mathcal{H}_0 | \psi \rangle$ ; the energy of the fully polarised states. Therefore the state  $|\psi\rangle$  and all other fully polarised states are ground states of  $\mathcal{H}_0$  when  $J_{ij}^z > 0$ . Notice that in this derivation no assumptions are made concerning the dimension of the system. However one can show that exclusively in the one-dimensional case there is no ordered state [5]. In section 6.1 the goal is to apply spin wave theory to one-dimensional systems to find the low energy excited states. To this end it will be assumed that the ground state is a fully polarised state i.e. an ordered state. Avoiding this assumption would require spin wave analysis of higher dimensional models. While this is possible, it is quite involved and provides no further qualitative insight since the results are qualitatively no different than those that will be derived from the one-dimensional case using this assumption.

Returning to the general case in (32) one finds that the ground states are not so easily discovered when  $\Delta_{ij}^- \neq 0$ .

## 5.2 Antiferromagnetic Heisenberg model on bipartite lattices

The analysis of the previous section holds for general  $J_{ij}$  up to equation (37). When  $J_{ij} > 0$  one finds that the ground states are the fully polarised states. What happens when  $J_{ij} < 0$ ? If  $J_{ij} < 0$  the fully polarised states are still eigenstates of  $\mathcal{H}_0$  but are no longer ground states; in fact they have the highest energy of any of the normalised

states. In order to find the ground state one might consider taking the opposite of the fully polarised states such that all neighbouring spins are oppositely aligned a.k.a. Néel states. Although this works for the Ising model, it does not fit in general. In fact finding the ground state for the general system is really involved. For instance consider an antiferromagnetic system on a bipartite lattices. In this context, a bipartite lattice is one that can be divided into two disjoint sublattices, A & B, in such a way that every lattice site exclusively interacts with sites from the other sublattice as is the case in the one-dimensional lattice in figure 6.

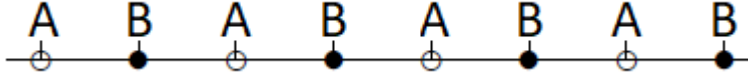


Figure 6: A one-dimensional bipartite lattice divided into two sublattices A & B.

To show that the Néel states are not the ground states consider the state:

$$|\psi\rangle = \prod_{i \in A} |S, S\rangle_i \prod_{j \in B} |S, -S\rangle_j \quad (39)$$

Then:

$$\begin{aligned} \mathcal{H}|\psi\rangle &= -\frac{1}{2} \sum_{i,j} \left( \Delta_{ij}^+ \frac{S_i^- S_j^+}{2} |\psi\rangle + 0 + 0 + 0 + J_{ij}^z S_i^z S_j^z |\psi\rangle \right) \\ &= -\sum_{i \in A} \sum_{j \in B} \left( \Delta_{ij}^+ \frac{2S}{2} [\dots |S, S-1\rangle_i \dots |S, -S+1\rangle_j \dots] - J_{ij}^z S^2 |\psi\rangle \right) \end{aligned} \quad (40)$$

where the middle three terms vanishes either because  $S_j^- |S, -S\rangle_j = 0$  or  $S_i^+ |S, S\rangle_i = 0$  and  $i \neq j$ . The above equation shows that  $|\psi\rangle$  is generally not an eigenstate of  $\mathcal{H}$ , as promised. The exception is when  $\Delta_{ij}^+ = 0$  or equivalently  $J_{ij}^x = -J_{ij}^y$ . Recall that up to this point no assumptions have been made concerning the signs of  $J_{ij}^k$ . In the event that  $\Delta_{ij}^+ = 0$ ,  $|\psi\rangle$  is again an eigenstate of  $\mathcal{H}$  and one can show, similar to equation (38), that  $|\psi\rangle$  is the ground state for  $J_{ij}^z < 0$ . However since this model represents neither a ferromagnet or antiferromagnet it will not be of interest in the remainder of this thesis.

The search for the exact ground state of the general antiferromagnetic Heisenberg model is very much beyond the scope of this thesis. However there are some nontrivial properties of the ground state which are stated in Marshall's theorem: [9]

*Marshall's theorem (extended by Lieb and Mattis): for the Heisenberg model on a bipartite lattice with sublattices of equal size and  $J_{ij}^k < 0$  for all  $i \in A$  and  $j \in B$  or  $i \in B$  and  $j \in A$ , the ground state  $|\psi_0\rangle$  is non-degenerate and a singlet of total spin i.e.:*

$$\vec{S}|\psi_0\rangle = 0 \quad (41)$$

where  $\vec{S} = \sum_i \vec{S}_i$ . The proof of the theorem is beyond the scope of this thesis, but a universal proof can be found in [11]. Do note that the reverse is not automatically true i.e. a non-degenerate, spin singlet state is not necessarily the ground state as is evident from the example of the Néel state above. The theorem gives at least some idea of the form of the ground state as it must be a spin singlet state. In a spin-1/2 system this is equivalent to having an equal amount of spins up as spins down. The non-degeneracy of the ground state in this type of antiferromagnetic systems also shows another interesting difference from ferromagnetic systems where the ground state is  $(2S + 1)$ - degenerate.

## 6 Spin wave theory

Spin waves are low energy excitations of the ground state and describe the system at low finite temperature where the thermal energy is small. The thermal energy causes fluctuations in the values of individual spins. The Heisenberg model predicts that neighbouring spins will adjust to lower the energy of the system. This behaviour causes a chain reaction that propagates through the system in the shape of a spin wave. The properties of this wave-like behaviour depend on characteristics of the system such as coupling strength, ground states and symmetry. We'll start from the simplest model: the fully isotropic ferromagnetic Heisenberg model and make it more complicated along the way by introducing asymmetry. In every instance the goal is to derive the dispersion relation which will finalise the full description of the motion of the spins and the spin wave.

### 6.1 The isotropic case

Although one can show that in the one-dimensional ferromagnetic Heisenberg model there exists no ordered state [5] it is assumed that such a state does exist. Using this assumption, the results derived from the one-dimensional case are qualitatively no different from those derived from higher-dimensional systems. However the spin wave analysis for higher-dimensional systems is more involved while providing no additional qualitative insight whatsoever.

First consider the isotropic ferromagnetic one-dimensional Heisenberg model:

$$\mathcal{H} = -J \sum_{i=1}^N \hat{S}_i \hat{S}_{i+1} \quad (42)$$

where periodic boundary conditions apply. At absolute zero the system is in the ground state, assume that all spins are aligned i.e. the system is ordered. At finite temperature it happens that a single spin changes due to thermal fluctuations. When this happens the rest of the spins adjust to lower the energy of the system causing the aforementioned wave-like motion. The way to derive the equations of motion for a spin at site  $i$  is a mean field-like approach. Suppose that in the ground state all spins

point in the positive z-direction ( $\vec{S}_i(t) = (0, 0, S)$  for all  $i$ ). The spin at site  $i$  possesses the magnetic moment  $\vec{\mu}_i = \mu_0 \vec{S}_i$  and hence the energy  $-\vec{\mu}_i \vec{B}_i = -J \vec{S}_i (\vec{S}_{i-1} + \vec{S}_{i+1})$  in the magnetic field created by its neighbours  $\vec{B}_i = J(\vec{S}_{i-1} + \vec{S}_{i+1})/\mu_0$ . Introduce a perturbation around the ground state at site  $i$ . Because the magnetic moment and magnetic field at site  $i$  are no longer aligned, a torque  $\vec{\mu}_i \times \vec{B}_i$  is present on the angular momentum  $\vec{S}_i$  resulting in the following equation of motion:

$$\frac{d\vec{S}_i}{dt} = \vec{\mu}_i \times \vec{B}_i = J \vec{S}_i \times (\vec{S}_{i-1} + \vec{S}_{i+1}) \quad (43)$$

These are the so-called Bloch equations. The behaviour of the spins can be seen as a perturbation around the ground state i.e.  $\vec{S}_i(t) = (S_i^x(t), S_i^y(t), S)$  with  $S_i^x(t)$  and  $S_i^y(t)$  small. Using this assumption one can linearise the Bloch-equations:

$$\frac{d\vec{S}_i}{dt} = J \begin{pmatrix} S_i^y(S_{i-1}^z + S_{i+1}^z) - S_i^z(S_{i-1}^y + S_{i+1}^y) \\ S_i^z(S_{i-1}^x + S_{i+1}^x) - S_i^x(S_{i-1}^z + S_{i+1}^z) \\ S_i^x(S_{i-1}^y + S_{i+1}^y) - S_i^y(S_{i-1}^x + S_{i+1}^x) \end{pmatrix} \quad (44)$$

$$\frac{d\vec{S}_i}{dt} = J \begin{pmatrix} S_i^y(2S) - S(S_{i-1}^y + S_{i+1}^y) \\ S(S_{i-1}^x + S_{i+1}^x) - S_i^x(2S) \\ 0 \end{pmatrix} \quad (45)$$

The right hand side of the last equation had only non-linear terms and thus becomes zero when linearised. The linearised Bloch-equations can be solved using the following ansatz:

$$\begin{aligned} S_n^x(t) &= u e^{i(nka - \omega t)} \\ S_n^y(t) &= v e^{i(nka - \omega t)} \\ S_n^z(t) &= S \end{aligned} \quad (46)$$

where  $u$  and  $v$  are (small) constants,  $k$  is the wave vector and  $a$  is the lattice constant. Filling this ansatz into equation (44) one finds the following eigenvalue equation:

$$-i\omega \begin{pmatrix} u \\ v \end{pmatrix} = JS \begin{pmatrix} 0 & 2 - e^{-ika} - e^{ika} \\ -2 + e^{-ika} + e^{ika} & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} \quad (47)$$

Solving this equation and taking only the positive root one finds the following dispersion relation<sup>4</sup>:

$$\begin{aligned} -\omega^2 + J^2 S^2 (2 - e^{-ika} - e^{ika})^2 &= 0 \\ \omega^2 &= 4J^2 S^2 (1 - \cos ka)^2 \\ \omega(k) &= 2JS(1 - \cos ka) \end{aligned} \quad (48)$$

The corresponding eigenvector is  $u = A, v = -iA$  with  $A$  the (real) amplitude of the initial perturbation. This dispersion relation relates the wave number  $k$  to the frequency of the motion  $\omega$ . A plot of the dispersion relation is shown in figure 7. The

<sup>4</sup>The negative root describes the motion in opposite direction

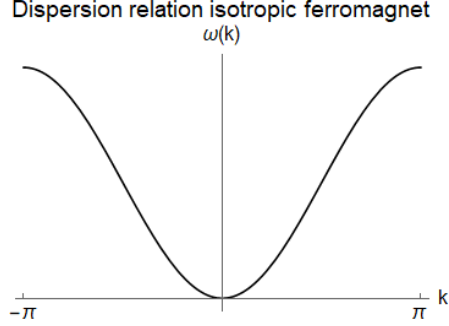


Figure 7: The dispersion relation in natural units ( $a = 1$ ) for the spin wave in an isotropic one-dimensional ferromagnet.

physical motion of a spin at site  $i$  is a counter-clockwise precession around the  $z$ -axis with amplitude  $A$  and frequency  $\omega(k)$  i.e.

$$\begin{aligned}
 S_n^x(t) &= \text{Re}(Ae^{i(nka - \omega(k)t)}) = A \cos(kna - \omega(k)t) \\
 S_n^y(t) &= \text{Re}(iAe^{i(nka - \omega(k)t)}) = -A \sin(kna - \omega(k)t) \\
 S_n^z(t) &= S
 \end{aligned} \tag{49}$$

The spins at neighbouring sites are out of phase by  $ka$ . The motion of the chain of spins can be identified with the motion of a row of identical spinning tops precessing around their  $z$ -axes with a constant phase difference between neighbours. Please do keep in mind that this result is derived from the linearised Bloch equations and thus requires  $A$  to be small.

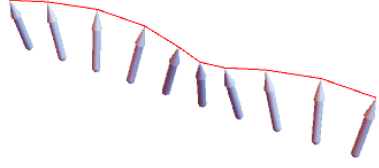
The actual waveform can be found by connecting the spins at neighbouring lattice sites as in figure 8a where the spins are represented by arrows. For the purpose of a clear demonstration the amplitude does not satisfy the requirement  $A \ll a$  (instead  $A \sim 0.4a$ ) used in the linearisation of the Bloch equations. Therefore the wave is not perfectly sinusoidal but is more reminiscent of a cycloid curve. Figure 8b shows a spin wave when  $A \ll a$  which is a sinusoidal wave. The wave will travel in the positive  $x$ -direction with frequency  $f = \omega(k)/(2\pi)$  where  $k$  is determined by the direction of the initial perturbation.

## 6.2 The anisotropic case

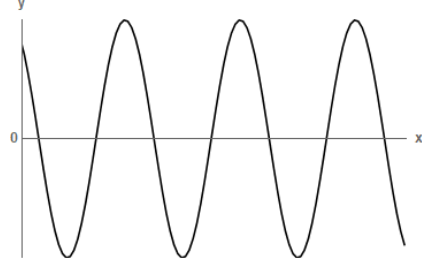
The spin wave analysis from the previous section can be generalised to the anisotropic case. As a stepping stone first consider the case with a single direction being distinct:

$$\hat{\mathcal{H}} = -J \sum_{i=1}^N (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z) \tag{50}$$

where  $\Delta \geq 1$ , because if  $\Delta < 1$  the coupling in the  $z$ -direction would no longer be the strongest and hence the ground state would be different i.e. all spins would



(a) A spin wave (red line) with amplitude  $A \sim 0.4a$  in an array of 10 spins where the spins are represented by arrows.



(b) A spin wave when  $A \ll a = 1$  and  $k = \pi/3$

point along the x- or y-direction. In the event that  $\Delta = 1$  the model reduces to the isotropic model discussed in the previous section. If  $\Delta \rightarrow \infty$  the model becomes a one-dimensional Ising model where a perturbation like the one described in the previous section is not even possible since all spins are parallel to the z-axis at all time. Because  $\Delta \geq 1$  the ground state is identical that of the isotropic case; the fully polarised state  $\vec{S}_i(t) = (0, 0, S)$  for all  $i$ . This time, the spin at site  $i$  has to have the energy:

$$-\vec{\mu}_i \vec{B}_i = -J(S_i^x(S_{i-1}^x + S_{i+1}^x) + S_i^y(S_{i-1}^y + S_{i+1}^y) + \Delta S_i^z(S_{i-1}^z + S_{i+1}^z)) \quad (51)$$

where  $\mu_i = \mu_0 \vec{S}_i$ . Hence the magnetic field produced by the neighbours should be:

$$\vec{B}_i = \frac{J}{\mu_0} \begin{pmatrix} S_{i-1}^x + S_{i+1}^x \\ S_{i-1}^y + S_{i+1}^y \\ \Delta(S_{i-1}^z + S_{i+1}^z) \end{pmatrix} \quad (52)$$

From equation (43) one can now determine the Bloch equations of motion for the anisotropic case:

$$\frac{d\vec{S}_i}{dt} = J \begin{pmatrix} S_i^y(\Delta(S_{i-1}^z + S_{i+1}^z)) - S_i^z(S_{i-1}^y + S_{i+1}^y) \\ S_i^z(S_{i-1}^x + S_{i+1}^x) - S_i^x(\Delta(S_{i-1}^z + S_{i+1}^z)) \\ S_i^x(S_{i-1}^y + S_{i+1}^y) - S_i^y(S_{i-1}^x + S_{i+1}^x) \end{pmatrix} \quad (53)$$

These Bloch equations can be linearised by using the same ansatz as in the isotropic model i.e.  $\vec{S}_i(t) = (S_i^x(t), S_i^y(t), S)$  with  $S_i^x(t)$  and  $S_i^y(t)$  small.

$$\frac{d\vec{S}_i}{dt} = J \begin{pmatrix} S_i^y(2\Delta S) - S(S_{i-1}^y + S_{i+1}^y) \\ S(S_{i-1}^x + S_{i+1}^x) - S_i^x(2\Delta S) \\ 0 \end{pmatrix} \quad (54)$$

Using the ansatz as in (46) one finds the following dispersion relation:

$$\omega(k) = 2JS(\Delta - \cos ka) \quad (55)$$

The dispersion relation in the above equation is plotted in figure 9 for different values of  $\Delta$ . The overall motion of the spins will remain the same i.e. precession around the

z-axis like spinning tops as in (49). The only difference is the angular frequency with which the motion takes place. The parameter  $\Delta$  can be seen as the tuning peg on a guitar; the higher  $\Delta$ , the higher the tension in the guitar string, the higher the frequency when the string gets plucked. As expected setting  $\Delta$  to 1 returns the isotropic dispersion relation. At the beginning of this section it was suggested that the described perturbations could not take place in the limit  $\Delta \rightarrow \infty$ . This is clear from the dispersion relation as well; the frequency diverges for  $\Delta \rightarrow \infty$  meaning that the energy needed to excite a spin wave would be infinite. Alternatively, using the guitar string analogy, one can not pluck an infinitely tight guitar string<sup>5</sup>.

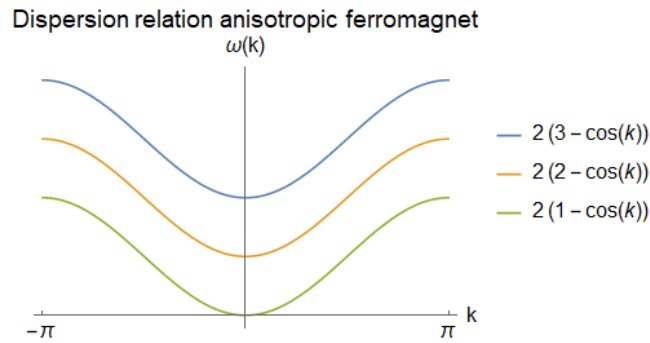


Figure 9: The dispersion relation for the spin wave in an anisotropic one-dimensional ferromagnet.

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<sup>5</sup>I realise the metaphor does not hold in practice as the guitar string would break long before reaching infinite tension.



### 6.3 The antiferromagnetic case

So far all systems discussed in this section have been ferromagnetic. Now it is time to take a step back and look at the antiferromagnetic system described by:

$$\hat{\mathcal{H}} = -J \sum_{i=1}^N \hat{\vec{S}}_i \hat{\vec{S}}_{i+1} \quad (56)$$

where  $J < 0$ . The exact ground state of such a general antiferromagnetic system is more complex than one might expect at first glance. However there is a more straightforward alternative: the Néel state i.e. the ground state of the antiferromagnetic Ising model from section 3. It was shown in the section 5.2 that the Néel state is actually not the ground state of the system, it is not even an eigenstate. Nevertheless it is a good enough approximation to the ground state to apply perturbation theory and retrieve the spin waves. The neighbouring spins in the Néel state are oppositely aligned and by convention point along the z-axis. A perturbation from the Néel state causes, as in the ferromagnet, a spin wave. The derivation of the Bloch equations is completely identical to that of the isotropic ferromagnetic case:

$$\frac{d\vec{S}_i}{dt} = J \begin{pmatrix} S_i^y (S_{i-1}^z + S_{i+1}^z) - S_i^z (S_{i-1}^y + S_{i+1}^y) \\ S_i^z (S_{i-1}^x + S_{i+1}^x) - S_i^x (S_{i-1}^z + S_{i+1}^z) \\ S_i^x (S_{i-1}^y + S_{i+1}^y) - S_i^y (S_{i-1}^x + S_{i+1}^x) \end{pmatrix} \quad (57)$$

where  $J < 0$ . Since, in the Néel state, the system is an alternating array of "up"- and "down" spins the perturbation from the ground state of each spin is described by:  $\vec{S}_i(t) = (S_i^x(t), S_i^y(t), (-1)^i S)$  with  $S_i^x(t)$  and  $S_i^y(t)$  small. This ansatz can be used to linearise the Bloch-equations:

$$\frac{d\vec{S}_i}{dt} = (-1)^{i-1} J \begin{pmatrix} S_i^y (2S) + S (S_{i-1}^y + S_{i+1}^y) \\ -S (S_{i-1}^x + S_{i+1}^x) - S_i^x (2S) \\ 0 \end{pmatrix} \quad (58)$$

Make the following ansatz for the case that  $n$  is even:

$$\begin{aligned} S_n^x(t) &= A e^{i(kna - \omega t)} \\ S_n^y(t) &= -i A e^{i(kna - \omega t)} \\ S_{n+1}^x(t) &= B e^{i(kna - \omega t)} \\ S_{n+1}^y(t) &= -i B e^{i(kna - \omega t)} \end{aligned} \quad (59)$$

Filling this ansatz into the equations of motion for even and odd  $i$  one finds two equations:

$$i\omega A = JS(-2iA - 2iB \cos(ka)) \quad (60a)$$

$$i\omega B = -JS(-2iB - 2iA \cos(ka)) \quad (60b)$$

Combining these two equations into one eigenvalue equation gives:

$$\omega \begin{pmatrix} A \\ B \end{pmatrix} = 2JS \begin{pmatrix} -1 & -\cos(ka) \\ \cos(ka) & 1 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \quad (61)$$

The characteristic equation now results in the positive dispersion relation as plotted in figure 10.

$$\begin{aligned}\omega^2 - (2JS)^2 + (2JS)^2 \cos(ka)^2 &= 0 \\ \omega^2 &= (2JS)^2(1 - \cos(ka)^2) \\ \omega &= 2JS|\sin(ka)|\end{aligned}\tag{62}$$

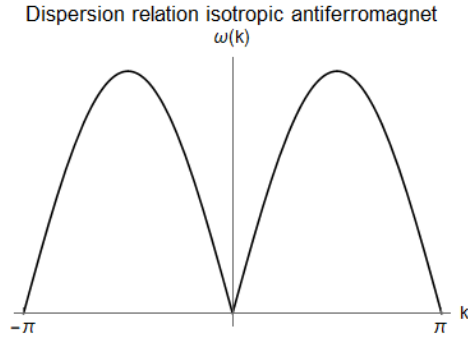
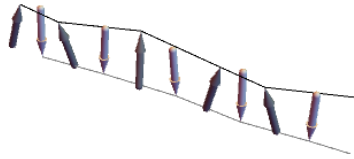
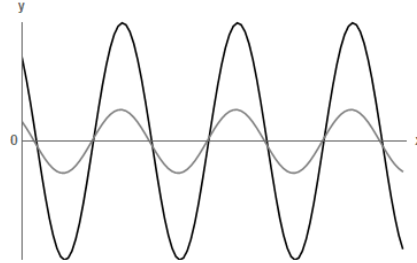


Figure 10: The positive dispersion relation of the one-dimensional isotropic antiferromagnet.

First of all an important difference to note between this dispersion relation and the one for a ferromagnetic system is its behaviour for small  $k$ . The dispersion relation in (62) is linear for small  $k$  whereas the dispersion relation in (48) goes like  $k^2$  in this regime.



(a) A small piece of a one-dimensional antiferromagnetic system in which one can distinguish between two sublattices (dark and light) each with their own spin wave.



(b) The two spin waves that present in the sublattices of the one-dimensional antiferromagnetic system.

Figure 11: Spin waves in a one-dimensional antiferromagnetic system with  $k = \pi/3$  and  $B = A(2 - \sqrt{3})$

The eigenvector corresponding to the positive dispersion relation is:

$$(A, B) = C(-1 + \sin(ka), \cos(ka))\tag{63}$$

where  $C$  is a real number. The motion of a spin at site  $i$  is again a circular precessing motion with frequency  $\omega$  for all  $i$ . The main difference with the ferromagnetic case is that the amplitude of the motion is no longer the same for all spins. One can divide the one-dimensional lattice into two sublattices; one containing all the odd numbered lattice sites and the other containing all even numbered lattice sites (see figure 11a). At odd numbered lattice sites the circular motion of a spin has an amplitude  $|B| = |-1 + \sin(ka)|$  and spins point 'downwards' while at even numbered lattice sites the amplitude is equal to  $|A| = |\cos(ka)|$  and spins point 'upwards'. Either sublattice produces a spin-wave with frequency  $f = \omega(k)/(2\pi)$  and the corresponding amplitude (see figure 11b).

## 7 Discussion

What is the origin of coupling between magnetic moments and what role play quantum effects in the interaction? How do magnetic systems with different coupling behave at various temperatures?

Two neutral atoms sufficiently close to each other will interact due to Coulomb interaction. As a result of Pauli's exclusion principle the total wave function needs to be antisymmetric under exchange of electrons. A direct consequence is the splitting of energy levels, which in turn causes the coupling. If the spin singlet has the lowest energy the coupling constant will be negative and one deals with an antiferromagnetic system. Conversely a ferromagnetic system has a positive coupling constant which implies that the spin triplet has the lowest energy. In the case of hydrogen the coupling constant is  $J \approx -6.6 \cdot 10^4 \text{K}$  which is sufficiently strong to describe the experimentally observed properties of a magnetic system.

The Heisenberg model is a formulation of the Hamiltonian of a composite system such that it only acts on the spin degrees of freedom of the system. One of the special cases of the Heisenberg model is the Ising model. One-dimensional systems described by the Ising model have no mean magnetisation at finite temperature and therefore can not undergo a phase transition. Mean field theory shows that the one-dimensional case is the exception rather than the rule as higher dimensional ferromagnetic systems do undergo a phase transition at a finite critical temperature. The critical temperature for ferromagnetic systems is linearly dependent on the coupling constant.

A general one-dimensional ferromagnetic system does not immediately lose its mean magnetisation at finite temperature. Instead when a low energy thermal fluctuation occurs other magnetic moments will adjust producing a wave-like motion through the medium known as a spin wave. Solving the linear Bloch equations results in a dispersion relation that describes the angular motion of the spins and thus the propagation of the spin wave. For ferromagnetic systems the frequency grows quadratically as a function of the wave vector in the regime of small wave vectors. For small perturbations the spin wave is approximately sinusoidal with a frequency  $f = \omega(k)/(2\pi) \sim k^2$ .

The ground state of the homogeneous antiferromagnetic Heisenberg model is not the

Néel state; the ground state of the corresponding Ising model. Marshall's theorem does give a general idea of the form of the ground state; it is non-degenerate and a singlet of total spin. Spin waves in antiferromagnetic systems are produced on both sublattices and propagate with the same frequency but different amplitudes correlated as  $-1 + \sin(ka) : \cos(ka)$ . An important difference with the ferromagnetic systems is that the dispersion relation behaves linearly for small wave vectors instead of quadratically.

## 8 Conclusion

In one-dimensional ferromagnetic- and antiferromagnetic systems a low energy thermal fluctuation manifests itself as a spin wave. Spin waves are perturbations from the ground state and are approximately sinusoidal. The dispersion relation for the motion of the spins and the spin wave is quadratic for ferromagnetic systems while linear for antiferromagnetic systems in the regime of small wave vectors. In antiferromagnetic systems the wave-like motion is different on both sublattices; the frequency is identical, but the amplitude is not.

The spin wave analysis in this thesis has been restricted to small amplitudes and one-dimensional systems. A more complete theory about spin waves would include a more in depth study of the non-linear Bloch equations as to include larger fluctuations. It would also be interesting to know how magnetic systems behave at higher temperatures, for example room temperature. In conclusion more research will be needed to fully understand those whimsical refrigerator magnets.

# Appendices

## A Ground state of the ferromagnetic Ising model

The ground states of the Ising model are the ordered states with mean magnetisation:  $m = \pm \tilde{m}$  because they correspond to a minimum in the free energy. The free energy as a function of the mean magnetisation is:

$$\begin{aligned}
 F &= -\frac{1}{\beta} \log(Z) \\
 &= -\frac{1}{\beta} \log \left( \sum_{S_1} \sum_{S_2} \dots \sum_{S_N} e^{-\beta \mathcal{H}} \right) \\
 &= -\frac{1}{\beta} \log \left( e^{-\beta \tilde{H} N m / 2} (e^{\beta \tilde{H} N} + e^{-\beta \tilde{H} N}) \right) \\
 &= -\frac{N}{\beta} \left( \log(2 \cosh(\beta \tilde{H})) - \frac{1}{2} \beta \tilde{H} m \right)
 \end{aligned} \tag{64}$$

where  $\tilde{H} = Jz m$ . The difference in the free energy between an ordered state ( $m = \tilde{m}$ ) and a disordered state ( $m = 0$ ) is:

$$\begin{aligned}
 \Delta F &= F|_{m=\tilde{m}} - F|_{m=0} = \int_0^{\tilde{m}} \frac{dF}{dm} dm \\
 &= -\frac{N}{\beta} \int_0^{\tilde{m}} \left( \frac{2 \sinh(\beta Jz m)}{2 \cosh(\beta Jz m)} \beta Jz - \beta Jz m \right) dm \\
 &= Jz N \int_0^{\tilde{m}} (m - \tanh(\beta Jz m)) dm
 \end{aligned} \tag{65}$$

Going back to the graphical solution in figure 4 it follows that the integral is negative because the area under the line is smaller than the area under the tanh function between  $m = 0$  and  $m = \tilde{m}$ . Therefore the free energy is smaller when  $m = \tilde{m}$ . Due to symmetry the same is true for  $m = -\tilde{m}$ . Hence at absolute zero the system is in an ordered state.

## **9 Acknowledgement**

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