Spin waves in frustrated Heisenberg models

Bachelor Project in Physics

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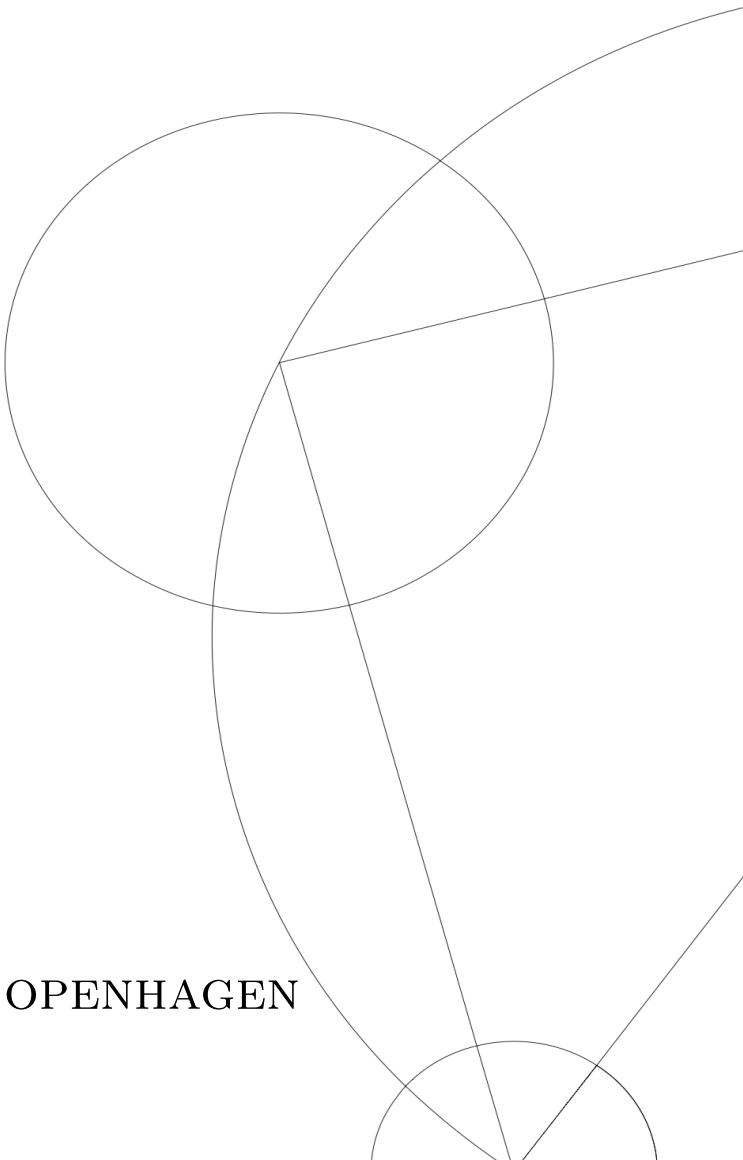

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Abstract

The Heisenberg model is studied with the goal of finding the spin wave dispersion relation. The classical ground state of the Heisenberg model with a Zeeman term is found, and its equation of motion is found and linearized by considering the spin to have small deviations from the ground state. A solution method for the linearized equation of motion is presented in the case where the Zeeman term has no time dependency. The 1-dimensional spiral chain and the antiferromagnetic triangular lattice are solved and their dispersion relations are shown. Finally, solution methods for a time dependent Zeeman term are discussed.

Contents

1 Introduction

The Heisenberg model is a vector model used to describe a lattice of spins on individual sites. An example of such a system is the triangular lattice (displayed on figure 1). The Hamiltonian of the Heisenberg model is on the form:

$$\mathcal{H} = \sum_{ij} J_{ij} \mathbf{s_i} \cdot \mathbf{s_j} \tag{1.1}$$

Where J_{ij} describes the coupling strength between the spin on the i'th and j'th site. For the purpose of this thesis this interaction will be a function of the distance between the sites. Because of this it is useful to think of a site as having nearest neighbours (NN) with the same coupling strength (J_1), next nearest neighbours (NNN) with a different coupling strength (J_2) and so on. This thesis aims to present a classical method of finding spin waves in the Heisenberg model, in particular for frustrated materials.

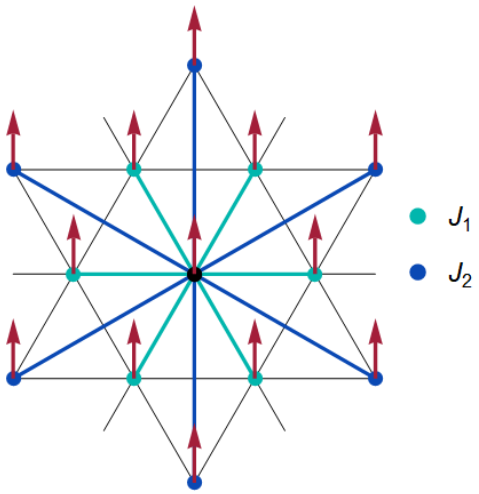


Figure 1: Example of a system where the Heisenberg model can be applied, This is a triangular lattice which has ferromagnetically ordered spins. The nearest neighbour (J_1) and next nearest neighbour (J_2) interactions of the middle site are shown.

A system is said to be frustrated if not all terms in its Hamiltonian can be minimized simultaneously. Frustration can be introduced in a system with antiferromagnetic (AFM) coupling through, for example, the geometry of the material or through the system having both ferromagnetic (FM) and antiferromagnetic couplings. Examples of both of these types of materials are treated in this thesis, in the form of a one dimensional chain with both an FM and AFM coupling, and the AFM triangular lattice.
Frustration can also be introduced into a system through applying a magnetic field, which gives the Hamiltonian a Zeeman term. In a non-ferromagnetically ordered system the magnetic field will not only introduce frustration into the system, but also

break the rotational symmetry of the entire system, as the Hamiltonian will not only depends on the angle differences of the spins, but also their angle to the magnetic field. Frustrations in the Heisenberg model often give rise to interesting properties of the system, including nontrivial magnetic ordering of the ground state[1] and order-by-disorder phenomena[2]. The spin wave dispersion can be measured through neutron scattering[3] and can be used to predict order-by-disorder[2], among other things.
If the magnetic field is oscillating in time, it can drive the spin waves giving rise to a variety of new properties[4]. The driven Heisenberg model is treated with an approach for finding the spin waves in the limit, where the Zeeman Hamiltonian is small compared to the Heisenberg Hamiltonian. A more general approach is also discussed, but it wasn't finished due to the time constraint of this project.

2 Ground States of the Heisenberg Model

In the Heisenberg Model with an external magnetic field $\mathbf{B(t)}$, the Hamiltonian is given by:

$$\mathcal{H} = \sum_{i,j} J_{i,j} \mathbf{s_i} \cdot \mathbf{s_j} - \sum_i g_i \mu_B \mathbf{s_i} \cdot \mathbf{B_i(t)} \tag{2.1}$$

To find the ground state of this Hamiltonian, it is convenient to use the Fourier transform of both the spin and the external magnetic field:

$$\mathbf{s_i} = \sum_{\mathbf{q}} \mathbf{s_q} e^{i\mathbf{R_i}\cdot\mathbf{q}} \qquad \mathbf{B_i} = \sum_{\mathbf{q_B}} \mathbf{B_{q_B}} e^{i\mathbf{R_i}\cdot\mathbf{q_B}} \tag{2.2}$$

For the sake of ease of reading I will split (2.1) into the Heisenberg part ($\mathcal{H}_J$) and the Zeeman part ($\mathcal{H}_B$). Inserting (2.2) into each Hamiltonian:

$$\begin{aligned}
\mathcal{H}_J &= \sum_{\mathbf{q},\mathbf{q'}} \mathbf{s_q} \cdot \mathbf{s_{q'}} \sum_{i,j} J_{i,j} e^{i(\mathbf{q}\cdot\mathbf{R_i}+\mathbf{q'}\cdot\mathbf{R_j})} \\
&= \sum_{\mathbf{q},\mathbf{q'}} \mathbf{s_q} \cdot \mathbf{s_{q'}} \sum_{i,j} J_{i,j} e^{-i\mathbf{q'}\cdot(\mathbf{R_i}-\mathbf{R_j})} \sum_i e^{i\mathbf{R_i}\cdot(\mathbf{q}+\mathbf{q'})} \\
&= \sum_{\mathbf{q}} J(\mathbf{q}) \mathbf{s_q} \cdot \mathbf{s_{-q}}
\end{aligned} \tag{2.3}$$

Where $J(\mathbf{q})$ is given by[5]:

$$J(\mathbf{q}) = \sum_{i,j} J_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R_i}-\mathbf{R_j})} \tag{2.4}$$

As for the Zeeman part of the Hamiltonian:

$$\mathcal{H}_B = -\mu_B \sum_{\mathbf{q},\mathbf{q_B}} \mathbf{s_q} \cdot \mathbf{B_{q_B}} \sum_i g_i e^{i\mathbf{R_i}\cdot(\mathbf{q}+\mathbf{q_B})} \tag{2.5}$$

In the case where g_i is uniform (as is the case in monoatomic materials), the last sum is simply a delta function and (2.5) reduces to:

$$\mathcal{H}_B = \sum_{\mathbf{q}} -g\mu_B \mathbf{s_q} \cdot \mathbf{B_{-q}} \tag{2.6}$$

And the total Hamiltonian becomes:

$$\mathcal{H} = \sum_{\mathbf{q}} \mathbf{s_q} \cdot (J(\mathbf{q})\mathbf{s_{-q}} - g\mu_B \mathbf{B_{-q}}) \tag{2.7}$$

With no magnetic field the way to find the ground state is to minimize $J(\mathbf{q})$ with respect to $\mathbf{q}$[5, 6]. The ground state then becomes:

$$\mathbf{s_{i,0}} = \mathbf{s_Q} e^{i\mathbf{Q}\cdot\mathbf{R_i}} + \mathbf{s_{-Q}} e^{-i\mathbf{Q}\cdot\mathbf{R_i}} \qquad \left.\frac{\partial J(\mathbf{q})}{\partial \mathbf{q}}\right|_{\mathbf{Q}} = 0 \tag{2.8}$$

As it is clear from (2.4) that if $\mathbf{Q}$ is a solution to (2.8) then so is $-\mathbf{Q}$. Note that because $\mathbf{s_{i,0}}$ must be real and have norm $|\mathbf{s_{i,0}}| = 1$ at $\mathbf{B} = \mathbf{0}$, $\mathbf{s_{\pm Q}}$ must be on the form:

$$\mathbf{s_{\pm Q}} = \frac{\hat{\mathbf{u}} \pm i\hat{\mathbf{v}}}{2} \tag{2.9}$$

Where $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ are any orthonormal unit vectors. There are exceptions to the rule that the ground state corresponds to the minimum of $J(\mathbf{q})$[5], but those won't be treated in this thesis.
However when there is a magnetic field the ground state becomes a linear combination of (2.8) and the $\mathbf{s_q}$('s) which couple to the magnetic field. In other words:

$$\mathbf{s_{i,0}} = \alpha\left(\mathbf{s_Q} e^{i\mathbf{Q}\cdot\mathbf{R_i}} + \mathbf{s_{-Q}} e^{-i\mathbf{Q}\cdot\mathbf{R_i}}\right) + \sum_{\mathbf{q_B}} \beta_{\mathbf{q_b}} \mathbf{s_{q_B}} e^{i\mathbf{q_b}\cdot\mathbf{R_i}} \qquad |\mathbf{s_{i,0}}|^2 = 1 \tag{2.10}$$

2.1 Uniform magnetic field

In the case of a uniform magnetic field the coupling happens between the minima of (2.3) and $\mathbf{s_0}$. The spin vector $\mathbf{s_{i,0}}$ is then:

$$\mathbf{s_i} = \alpha_i \mathbf{s_{i,B=0}} + \beta_i \hat{\mathbf{B}} \tag{2.11}$$

$$\mathbf{s_{i,B=0}} = \mathbf{s_Q} e^{i\mathbf{Q}\cdot\mathbf{R_i}} + \mathbf{s_{-Q}} e^{-i\mathbf{Q}\cdot\mathbf{R_i}} = \cos(\mathbf{Q}\cdot\mathbf{R_i})\hat{\mathbf{u}} + \sin(\mathbf{Q}\cdot\mathbf{R_i})\hat{\mathbf{v}} \tag{2.12}$$

$\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ are defined in (2.9), and $\hat{\mathbf{B}}$ is the unit vector of the $\mathbf{B}$-field. In general the Hamiltonian (2.7) should be minimized under the normalization constraint:

$$\mathbf{s_{i,0}}^2 = \alpha_i^2 + \beta_i^2 + 2\alpha_i\beta_i \mathbf{s_{i,B=0}} \cdot \hat{\mathbf{B}} = 1 \tag{2.13}$$

Since $\mathbf{s_Q}$ doesn't couple to the magnetic field, you are free to choose $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ independently. While the choice of $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ impacts the spin configuration of the ground state, they are all degenerate. The simplest choice is then $\hat{\mathbf{u}} \cdot \hat{\mathbf{B}} = \hat{\mathbf{v}} \cdot \hat{\mathbf{B}} = 0$, in which case (2.7) should be minimized under the constraint:

$$\mathbf{s_{i,0}}^2 = \alpha^2 + \beta^2 = 1 \tag{2.14}$$

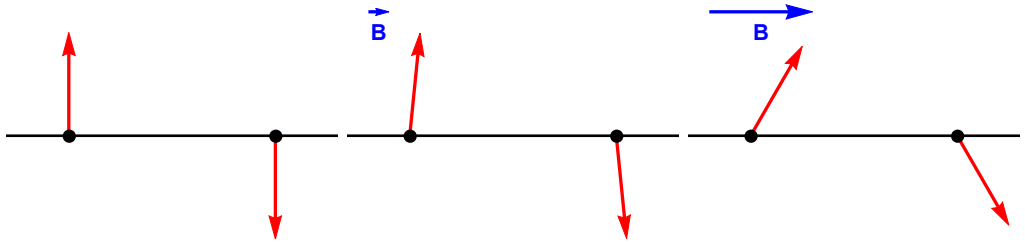
This solution assumes that $\mathbf{Q} \neq \mathbf{0}$. If $\mathbf{Q} = \mathbf{0}$ the ground state is trivial, since there is no longer a difference in the minimum energy state for the Heisenberg term and the Zeeman term in the Hamiltonian. In this case, the spins will be aligned with the $\mathbf{B}$-field. It is convenient to rewrite (2.7) on the form

$$\mathcal{H} = \alpha^2(J(\mathbf{Q}) + J(-\mathbf{Q}))\mathbf{s_Q} \cdot \mathbf{s_{-Q}} + \beta^2 J(\mathbf{0})|\mathbf{s_0}|^2 - \beta g \mu_B |\mathbf{B}| \tag{2.15}$$

$\mathbf{s_0}$ is the Fourier transform with $\mathbf{q} = \mathbf{0}$, and shouldn't be confused with the ground state. Finding the minimum can be done through Lagrange multipliers, and the solution will be:

$$\beta = \frac{g\mu_B|\mathbf{B}|}{2(J(\mathbf{0})|\mathbf{s_0}|^2 - (J(\mathbf{Q}) + J(-\mathbf{Q}))\mathbf{s_Q} \cdot \mathbf{s_{-Q}})} \tag{2.16}$$

And α chosen such that (2.14) holds. A more detailed derivation of this result is shown in appendix A.



(a) $\beta = 0$ *(b)* $\beta = 0.1$ *(c)* $\beta = 0.5$

Figure 2: Ground state of the 1D AFM chain, plotted for different values of β.

Figure 2 shows how the ground state of the 1D AFM chain becomes a linear combination of $\mathbf{s_Q}$ and $\mathbf{s_0}$. The AFM chain has $\mathbf{Q} = \frac{\pi}{a}\hat{\mathbf{x}}$, but as a magnetic field is applied the $\mathbf{Q}$ configuration starts to mix with the $\mathbf{q} = \mathbf{0}$ configuration from the magnetic field. Note that because the magnetic field is orthogonal to $\mathbf{s_Q}$, it is sufficient to use (2.14) as normalization constraint.

3 Equation of Motion

Consider the Hamiltonian (2.1) again:

$$\mathcal{H} = \sum_{i,j} J_{i,j}\mathbf{s_i} \cdot \mathbf{s_j} - \sum_i g_i \mu_B \mathbf{s_i} \cdot \mathbf{B_i(t)} \tag{3.1}$$

The equation of motion for the spins $\mathbf{s_i}$ can be found using Heisenberg equation of motion:

$$\frac{d\mathbf{s_i}}{dt} = -\frac{i}{\hbar}[\mathbf{s_i}, \mathcal{H}] + \frac{\partial \mathbf{s_i}}{\partial t} \tag{3.2}$$

The partial derivative of $\mathbf{s_i}$ is 0, so all that's left is to evaluate the commutator. I will show the calculation for a single component, which should make it clear how this generalizes. First it is convenient to define the local field $\mathbf{H}$ and rewrite the Hamiltonian:

$$\mathcal{H} = \sum_i \mathbf{H_i} \cdot \mathbf{s_i} \qquad \mathbf{H_i} = -g_i \mu_B \mathbf{B_i(t)} + \sum_j J_{i,j} \mathbf{s_j} \tag{3.3}$$

Here $\mathbf{H_i}$ is the local field on site i. To solve this you also need the commutator relations for spin:

$$[s_i^x, s_i^y] = i\hbar s_i^z \qquad [s_i^y, s_i^z] = i\hbar s_i^x \qquad [s_i^z, s_i^x] = i\hbar s_i^y \tag{3.4}$$

Taking the commutator for the x component:

$$-\frac{i}{\hbar}[s_i^x, \mathcal{H}] = -\frac{i}{\hbar}[s_i^x, H_i^x s_i^x + H_i^y s_i^y + H_i^z s_i^z] = H_i^y s_i^z - H_i^z s_i^y \tag{3.5}$$

Which is recognized as the x-component of a cross product. Generalizing this to all three components:

$$\frac{d\mathbf{s_i}}{dt} = \mathbf{H_i} \times \mathbf{s_i} \tag{3.6}$$

This result can also be found through Hamiltons equations, and it is shown how in appendix B. Since $\mathbf{H_i}$ includes a sum over $\mathbf{s_j}$, (3.6) is a nonlinear differential equation. I'm not interested in solving this equation in general, as I'm only interested in the spin waves. Let $\boldsymbol{\sigma_i}$ be a small deviation from the ground state configuration, in which case the spin vector can be written as:

$$\mathbf{s_i} = \mathbf{s_{i,0}} + \boldsymbol{\sigma_i} \qquad\qquad |\mathbf{s_{i,0}}| \gg |\boldsymbol{\sigma_i}| \tag{3.7}$$

Letting $\mathbf{H_{i,0}}$ be the local field from the ground state and any external magnetic field and $\mathbf{H_{i,\sigma}}$ be the local field generated by the spin waves the equation of motion for the spin waves is found to be:

$$\frac{d\boldsymbol{\sigma_i}}{dt} = \mathbf{H_{i,\sigma}} \times \mathbf{s_{i,0}} + \mathbf{H_{i,0}} \times \boldsymbol{\sigma_i} \tag{3.8}$$

Note that there technically is a term with $\mathbf{H_i^\sigma}$ and $\boldsymbol{\sigma_i}$, but it is negligible since it is of order $|\boldsymbol{\sigma_i}|^2$. So (3.8) is the equation of motion of the spin waves. The normalization requirement for $\mathbf{s_i}$ is:

$$1 = |\mathbf{s_i}|^2 \simeq |\mathbf{s_{i,0}}|^2 + 2\mathbf{s_{i,0}} \cdot \boldsymbol{\sigma_i} \qquad \Rightarrow \qquad \mathbf{s_{i,0}} \cdot \boldsymbol{\sigma_i} = 0 \tag{3.9}$$

The solution from (3.8) must fulfill (3.9). Boundary conditions can be chosen to fulfill the requirement at $t = 0$, in which case it is sufficient to show that:

$$\frac{d\boldsymbol{\sigma}_\mathbf{i} \cdot \mathbf{s}_{\mathbf{i},\mathbf{0}}}{dt} = \frac{d\boldsymbol{\sigma}_\mathbf{i}}{dt} \cdot \mathbf{s}_{\mathbf{i},\mathbf{0}} + \boldsymbol{\sigma}_\mathbf{i} \cdot \frac{d\mathbf{s}_{\mathbf{i},\mathbf{0}}}{dt} = \frac{d\boldsymbol{\sigma}_\mathbf{i}}{dt} \cdot \mathbf{s}_{\mathbf{i},\mathbf{0}} = 0 \tag{3.10}$$

The second term is 0 because the magnetic field is assumed to be constant in time, and thus the ground state is as well. Using (3.8), (3.10) becomes:

$$\frac{d\boldsymbol{\sigma}_\mathbf{i}}{dt} \cdot \mathbf{s}_{\mathbf{i},\mathbf{0}} = (\mathbf{H}_{\mathbf{i},\boldsymbol{\sigma}} \times \mathbf{s}_{\mathbf{i},\mathbf{0}} + \mathbf{H}_{\mathbf{i},\mathbf{0}} \times \boldsymbol{\sigma}_\mathbf{i}) \cdot \mathbf{s}_{\mathbf{i},\mathbf{0}} = (\mathbf{s}_{\mathbf{i},\mathbf{0}} \times \mathbf{H}_{\mathbf{i},\mathbf{0}}) \cdot \boldsymbol{\sigma}_\mathbf{i} = 0 \tag{3.11}$$

The spiral order of the ground state makes $\mathbf{H}_{\mathbf{i},\mathbf{0}}$ parallel to $\mathbf{s}_{\mathbf{i},\mathbf{0}}$, assuming the magnetic field is periodic in space. To prove this, consider first the spin part of $\mathbf{H}_{\mathbf{i},\mathbf{0}}$. The sum can be split into sums over the sites at $\mathbf{R}_\mathbf{i} \pm \mathbf{a}$, where $\mathbf{a}$ is any vector between two lattice sites. If I choose my coordinate system such that $\mathbf{s}_{\mathbf{i},\mathbf{0}} = \hat{\mathbf{u}}$ then the sum over these two elements can be written as:

$$(\cos(\mathbf{Q} \cdot \mathbf{a}) + \cos(-\mathbf{Q} \cdot \mathbf{a}))\,\hat{\mathbf{u}} + (\sin(\mathbf{Q} \cdot \mathbf{a}) + \sin(-\mathbf{Q} \cdot \mathbf{a}))\,\hat{\mathbf{v}} = 2\cos(\mathbf{Q} \cdot \mathbf{a})\hat{\mathbf{u}} \tag{3.12}$$

Which is parallel to $\mathbf{s}_{\mathbf{i},\mathbf{0}}$. The same argument holds in the case where the ground state is a superposition of $\mathbf{q}$'s and the argument also holds for the $\mathbf{B}$-field part of $\mathbf{H}$. So normalization holds under the assumption that the $\mathbf{B}$-field is constant in time, periodic in space, and that $\boldsymbol{\sigma}_\mathbf{i}$ is small as compared to $\mathbf{s}_{\mathbf{i},\mathbf{0}}$.

3.1 Solution for a time invariant magnetic field

I want to use the translational symmetry of the ground state to solve equation (3.8), which means using the Fourier transform, because a translationally invariant system conserves $\mathbf{k}$. In order to solve (3.8) I introduce a unit cell (typically the smallest one possible) such that there is translation symmetry between all unit cells. Let $\boldsymbol{\sigma}_\mathbf{i}^n$ be the deviation on the n'th site in the $\mathbf{i}$'th unit cell, $\sigma_\mathbf{i}^{n,m}$ be the m'th component of the same vector, and let $\boldsymbol{\rho}_\mathbf{i}$ be the coordinate of the $\mathbf{i}$'th unit cell. In that case the Fourier transform of $\boldsymbol{\sigma}_\mathbf{i}^n$ is on the form:

$$\boldsymbol{\sigma}_\mathbf{i}^n = \sum_\mathbf{k} \boldsymbol{\sigma}_\mathbf{k}^n e^{i(\mathbf{k} \cdot \boldsymbol{\rho}_\mathbf{i} - \omega t)} \tag{3.13}$$

It is also convenient to introduce $\mathbf{J}_{\mathbf{i},\mathbf{j}}$-matrices, where $J_{\mathbf{i},\mathbf{j}}^{n,m}$ is the J coupling between the n'th atom in the $\mathbf{i}$'th unit cell and the m'th atom in the $\mathbf{j}$'th unit cell. Using this notation and expanding (3.8) you get the equation:

$$\frac{d\boldsymbol{\sigma}_\mathbf{i}^n}{dt} = -g_i \mu_b \mathbf{B}_\mathbf{i}{}^n \times \boldsymbol{\sigma}_\mathbf{i}^n + \sum_\mathbf{j} \sum_m J_{\mathbf{i},\mathbf{j}}^{n,m} (\boldsymbol{\sigma}_\mathbf{j}^m \times \mathbf{s}_{\mathbf{i},\mathbf{0}}{}^n + \mathbf{s}_{\mathbf{j},\mathbf{0}}{}^m \times \boldsymbol{\sigma}_\mathbf{i}^n) \tag{3.14}$$

Where $\mathbf{B_i}^n$ and $\mathbf{s_{i,0}}^n$ is the $\mathbf{B}$-field/spin on the n'th atom in the $\mathbf{i}$'th unit cell (similar to $\boldsymbol{\sigma}_\mathbf{i}^n$). Using (3.13), (3.14) goes on the form:

$$-i\sum_{\mathbf{k}}\omega\boldsymbol{\sigma}_\mathbf{k}^n e^{i(\mathbf{k}\cdot\boldsymbol{\rho}_\mathbf{i}-\omega t)} = \sum_{\mathbf{k}} e^{i(\mathbf{k}\cdot\boldsymbol{\rho}_\mathbf{i}-\omega t)}\left(-g_i\mu_b\mathbf{B_i}^n\times\boldsymbol{\sigma}_\mathbf{k}^n + \sum_{\mathbf{j}}\sum_m J_{\mathbf{i},\mathbf{j}}^{n,m}\left(e^{i\mathbf{k}\cdot(\boldsymbol{\rho}_\mathbf{j}-\boldsymbol{\rho}_\mathbf{i})}\boldsymbol{\sigma}_\mathbf{k}^m\times\mathbf{s_{i,0}}^n + \mathbf{s_{j,0}}^m\times\boldsymbol{\sigma}_\mathbf{k}^n\right)\right) \tag{3.15}$$

Because I have chosen my unit cell such that there is translation symmetry between them, there is no coupling between the different parts of the sum over $\mathbf{k}$. In other words, each part of the sum is equal to the same part on the other side of the equation. So (3.15) simplifies down to:

$$-i\omega\boldsymbol{\sigma}_\mathbf{k}^n = -g\mu_b\mathbf{B_i}^n\times\boldsymbol{\sigma}_\mathbf{k}^n + \sum_{\mathbf{j}}\sum_m J_{\mathbf{i},\mathbf{j}}^{n,m}\left(e^{i\mathbf{k}\cdot(\boldsymbol{\rho}_\mathbf{j}-\boldsymbol{\rho}_\mathbf{i})}\boldsymbol{\sigma}_\mathbf{k}^m\times\mathbf{s_{i,0}}^n + \mathbf{s_{j,0}}^m\times\boldsymbol{\sigma}_\mathbf{k}^n\right) \tag{3.16}$$

When looking at (3.16) it might seem arbitrary that you have to use the ground state and $\mathbf{B}$-field of the $\mathbf{i}$'th unit cell. But since the unit cell is chosen such that there is translational symmetry in the ground state, it is true in general that $\mathbf{B_i}^n = \mathbf{B_j}^n$ and $\mathbf{s_{i,0}}^n = \mathbf{s_{j,0}}^n$ for all values of $\mathbf{i}$ and $\mathbf{j}$.

It might not be clear yet, but (3.16) is an eigenvalue equation. Consider the vector $\boldsymbol{\zeta}_\mathbf{k}$ which, for a unit cell with N atoms, has $3N$ components, which are equal to the x, y and z components of each individual $\boldsymbol{\sigma}_\mathbf{k}^n$ in the unit cell. (3.16) can then be written on the form:

$$-i\omega\boldsymbol{\zeta}_\mathbf{k} = \mathbf{W}(\mathbf{k})\boldsymbol{\zeta}_\mathbf{k} \tag{3.17}$$

Where the matrix $\mathbf{W}(\mathbf{k})$ can be found from (3.16). The eigenvalues of $\mathbf{W}(\mathbf{k})$ are the dispersion relations for the spin waves. This approach for finding the dispersion relation of the spin wave is particularly efficient when the ground state has translational symmetry within a very small number of atoms. If you require a unit cell with more than 2 or 3 atoms, you might have to find the eigenvalues numerically, as opposed to finding them analytically.

Since $\mathbf{W}(\mathbf{k})$ is a $3N\times3N$ matrix it will have $3N$ eigenvalues. With no magnetic field, the spins in the system can all be turned by an arbitrary angle ϕ, since the Hamiltonian only depends on the difference of their angles, but the magnetic field breaks this symmetry, as the Hamiltonian now also depends on the angle the spins have with respect to $\mathbf{B}$. The symmetry in the case with no Zeeman term means you can introduce spin waves with no energy, corresponding to N eigenvalues of $\mathbf{W}$ equal to 0. But when a Zeeman term is introduced, this is no longer possible.

4 One Dimensional Spiral Chain

The setup for this particular problem is a 1D chain with a FM coupling to its nearest neighbor ($J_1 < 0$), and an AFM coupling to its next nearest neighbor ($J_2 > 0$). $J(\mathbf{q})$ is then:

$$J(\mathbf{q}) = 2(J_1 \cos(\mathbf{q}\cdot\mathbf{a}) + J_2 \cos(2\mathbf{q}\cdot\mathbf{a})) \tag{4.1}$$

Where $\mathbf{a}$ is the lattice vector. I choose my coordinate system such that $\mathbf{a} = a\hat{\mathbf{x}}$. If the AFM coupling is stronger than a fourth of the FM coupling the ground state of this system will be a spiral. In this case, $\mathbf{Q}$ can be found to be:

$$\cos(\mathbf{Q}\cdot\mathbf{a}) = -\frac{J_1}{4J_2} \tag{4.2}$$

4.1 Spin waves with no magnetic field

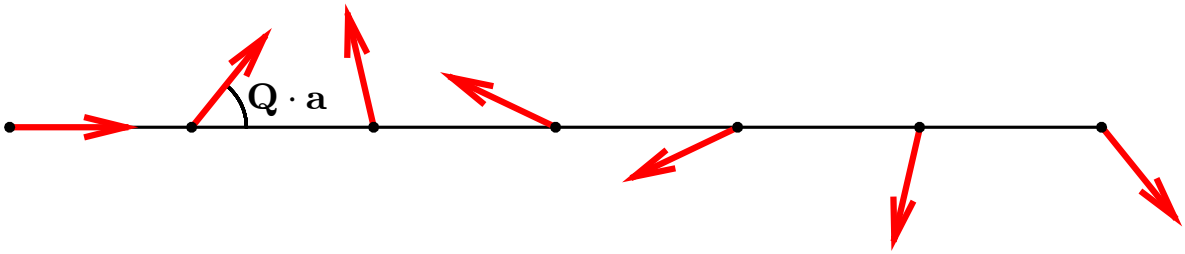


Figure 3: Ground state of the 1D spiral chain with no magnetic field. This particular example is for $\mathbf{Q}\cdot\mathbf{a} = \frac{2\pi}{7}$

A crucial part of the solution method outlined in section 3 is that the ground state has translational symmetry. At arbitrary values of J_1 and J_2, $\mathbf{Q}\cdot\mathbf{a}$ could be an irrational fraction of 2π. So for this particular method to work on this system, it is required that:

$$\mathbf{Q}\cdot\mathbf{a} = \frac{2m\pi}{N} \leq \frac{\pi}{2} \qquad m, N \in \mathbb{Z} \tag{4.3}$$

When this requirement is fulfilled a unit cell consisting of N atoms can be chosen, and there will be translational symmetry. When actually solving this problem it is also much preferred that the value of N is as low as possible since the $\mathbf{W}(\mathbf{k})$ matrix from equation (3.17) is $3N\times 3N$.

Just as in figure 3, the spin wave dispersion relation I will show is for $\mathbf{Q}\cdot\mathbf{a} = \frac{2\pi}{7}$. The dispersion relation can be seen in figure 4. Despite the fact that the $\mathbf{W}(\mathbf{k})$ matrix from equation (3.17) has 21 eigenvalues, there are only 7 non-zero bands. In general it is the case that, when no magnetic field is applied, the $3N\times 3N$ matrix will have N eigenvalues equal to 0 and the other $2N$ will be degenerate in pairs of 2.

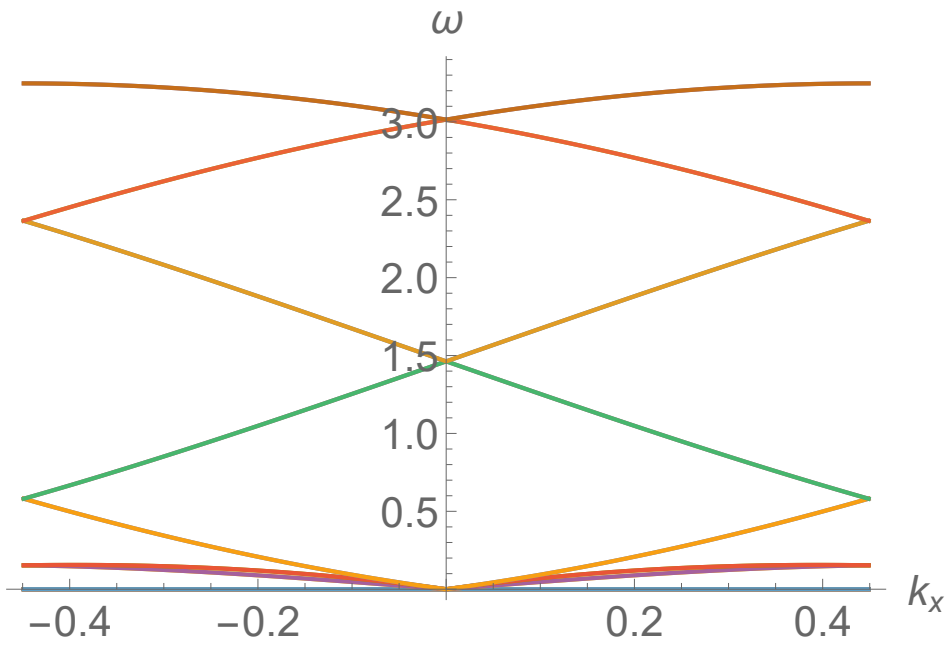


Figure 4: Spin wave dispersion relation for the 1D spiral chain with no magnetic field. This example is for $\mathbf{Q} \cdot \mathbf{a} = \frac{2\pi}{7}$*, meaning a unit cell of 7 atoms, and 7 bands in the dispersion relation.*

4.2 Applying a magnetic field

In the case where a magnetic field is applied to the chain, the ground state from (4.2) needs to be slightly modified. Following the method laid out in section 2.1, the Hamiltonian (2.7) can be written as:

$$\begin{aligned}\mathcal{H} &= 2\alpha^2 J(\mathbf{Q})\mathbf{s}_{\mathbf{Q}} \cdot \mathbf{s}_{-\mathbf{Q}} + \beta^2 J(\mathbf{0}) - \beta g\mu_B|\mathbf{B}| \\ &= 2\alpha^2(J_1\cos(\mathbf{Q}\cdot\mathbf{a}) + J_2\cos(2\mathbf{Q}\cdot\mathbf{a})) + 2\beta^2(J_1+J_2) - \beta g\mu_B|\mathbf{B}| \\ &= \alpha^2\left(-2J_2 - \frac{J_1^2}{4J_2}\right) + 2\beta^2(J_1+J_2) - \beta g\mu_B|\mathbf{B}| \end{aligned} \tag{4.4}$$

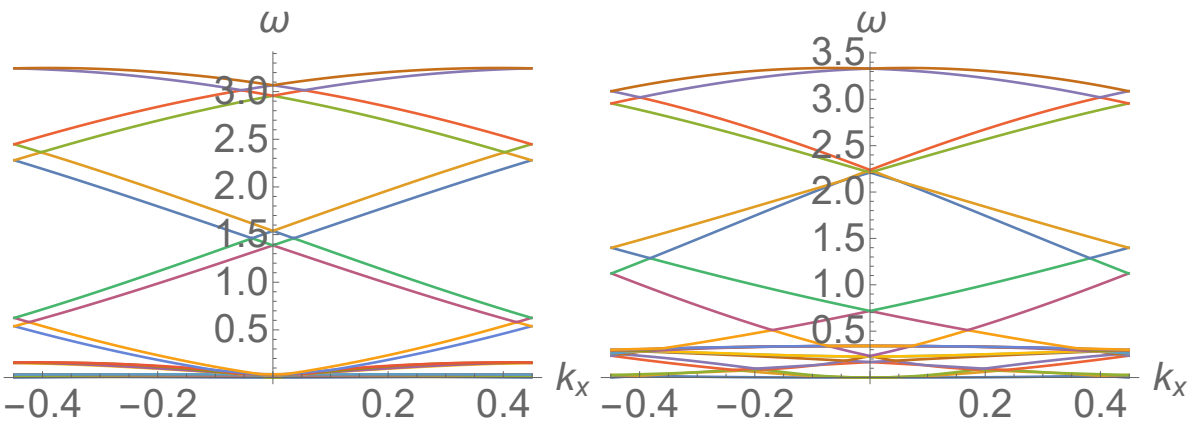
For convenience I define:

$$E_{\mathbf{Q}} = -2J_2 - \frac{J_1^2}{4J_2} \qquad E_{\mathbf{0}} = 2(J_1+J_2) \qquad E_{\mathbf{B}} = -g\mu_B|\mathbf{B}| \tag{4.5}$$

And I choose $\mathbf{s}_{\mathbf{Q}}$'s plane to be perpendicular to the magnetic field, so I have to minimize (4.4) under the constraint (2.14). This gives two different solutions depending on the values of (4.5):

$$\beta = \frac{-E_{\mathbf{B}}}{2(E_{\mathbf{0}} - E_{\mathbf{Q}})} \qquad \alpha^2 = 1 - \frac{E_{\mathbf{B}}^2}{4(E_{\mathbf{0}} - E_{\mathbf{Q}})^2} \tag{4.6}$$

$$\beta = 1 \qquad \alpha = 0 \tag{4.7}$$



(a) Dispersion relation for $\beta = 0.05$ *(b) Dispersion relation for $\beta = 0.5$*

Figure 5: Spin wave dispersion relations for the 1D spiral chain in an external magnetic field. This figure shows the dispersion relation for both a small magnetic field and a large one.

(4.6) breaks down when $|E_{\mathbf{B}}| > 2|E_{\mathbf{0}} - E_{\mathbf{Q}}|$ (since α must be real), and so (4.7) becomes the solution for big **B**-fields, whereas (4.6) is the solution for smaller fields. Figure 5 shows the dispersion relation of the spin waves with two different values of β. For the small β (figure 5a) you can see how the degeneracy of the dispersion relation (figure 4) is lifted, but it still looks very similar to figure 4. Whereas when you apply a large field (figure 5b), so the ground state is significantly different, the original shape of the dispersion relation is lost.

5 Triangular Lattice

The triangular lattice is a 2D lattice arranged in equilateral triangles. I will consider a model with an antiferromagnetic coupling to the nearest neighbor (J_1) and the next nearest neighbor (J_2). In other words, $J_1 > 0$ and $J_2 > 0$. The Fourier transform of J, as defined in equation (2.4), can be found to be:

$$\begin{aligned} J(\mathbf{q}) =& J_1 \left(2\cos(q^x a) + 4\cos\left(\frac{q^x a}{2}\right)\cos\left(\frac{\sqrt{3}q^y a}{2}\right)\right) \\ &+ J_2 \left(2\cos\left(\sqrt{3}q^y a\right) + 4\cos\left(\frac{3q^x a}{2}\right)\cos\left(\frac{\sqrt{3}q^y a}{2}\right)\right) \end{aligned} \tag{5.1}$$

Q will depend on the ratio $\alpha = \frac{J_2}{J_1}$. The ground state of the triangular lattice will have two different forms, depending on α. I will treat the solutions for $\alpha < \frac{1}{8}$ (low NNN coupling) and for $\frac{1}{8} < \alpha < 1$ (high NNN coupling)[1].

5.1 Low NNN coupling

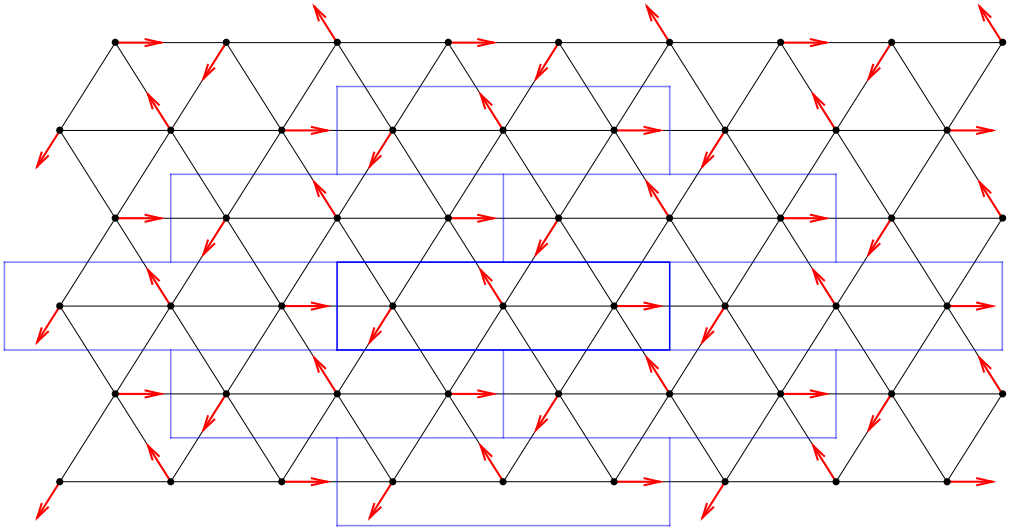


Figure 6: The ground state of the triangle lattice for $\alpha < \frac{1}{8}$. The rectangles are unit cells, all of which have couplings to the middle cell.

For low NNN coupling the ground state can be chosen to be on the form $\mathbf{Q} = \frac{4\pi}{3a}\hat{\mathbf{x}}$. This corresponds to a 120° magnetic order. The ground state is plotted on figure 6. As shown in the figure, I choose a unit cell with 3 atoms, since that's the smallest unit cell possible. With the selection of the unit cell shown in figure 6, the lattice vectors are $\mathbf{a_1} = \sqrt{3}a\hat{\mathbf{y}}$ and $\mathbf{a_2} = \frac{3}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}}$. This selection makes the Brillouin zone a regular hexagon with sides of length $|\mathbf{K}| = \frac{4\pi}{3\sqrt{3}a}$. The dispersion relations are plotted in figure 7 and 8.

Previous studies of the triangular lattice have found the Brillouin zone to contain three Goldstone nodes[7, 8]. In those studies the unit cell is taken to only include 1 atom, in which case they have one band with two of the Goldstone nodes are found on the K points in the Brillouin zone and one in Γ. Because I choose a larger unit cell, I find all three Goldstone nodes in Γ, one for each of the bands I find. This is because their K points have the same coordinates as my reciprocal lattice vectors. So when their Brillouin zone is translated into mine, all their K points are translated to Γ. This is described in greater detail in appendix C.

5.2 High NNN coupling

In the case where $\frac{1}{8} < \alpha < 1$ the ground state can be chosen to be $\mathbf{Q} = \frac{2\pi}{\sqrt{3}a}\hat{\mathbf{y}}$[1] and the resulting ground state is plotted in figure 9. As with every other Heisenberg model the ground state is degenerate when you rotate all spins by the same angle. This particular ground state has a further degeneracy (also plotted in figure 9), which can

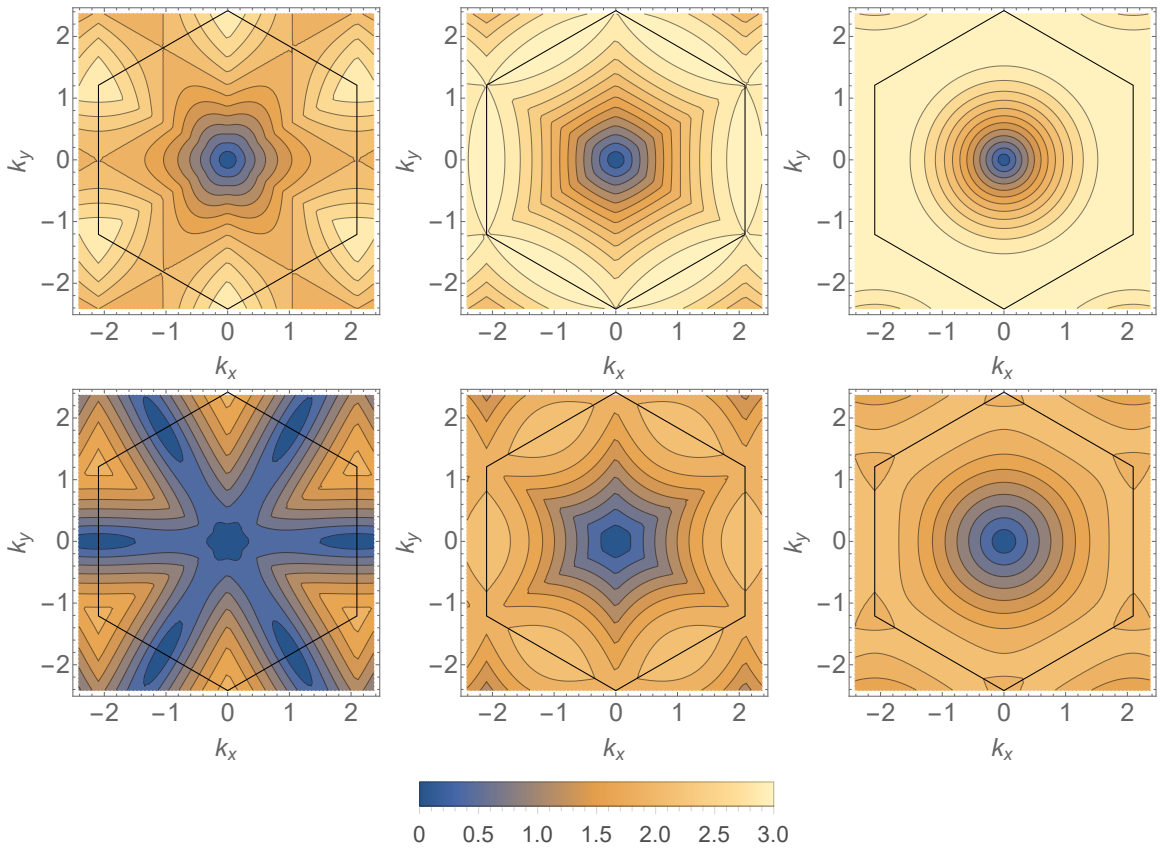


Figure 7: Contour plots of the Spin wave dispersion relations in the triangular lattice with no magnetic field. The edge of the Brillouin Zone is marked with a black line. First row: Dispersion relations for the three bands with $\alpha = 0$. Second row: Dispersion relations for $\alpha = \frac{1}{8}$.

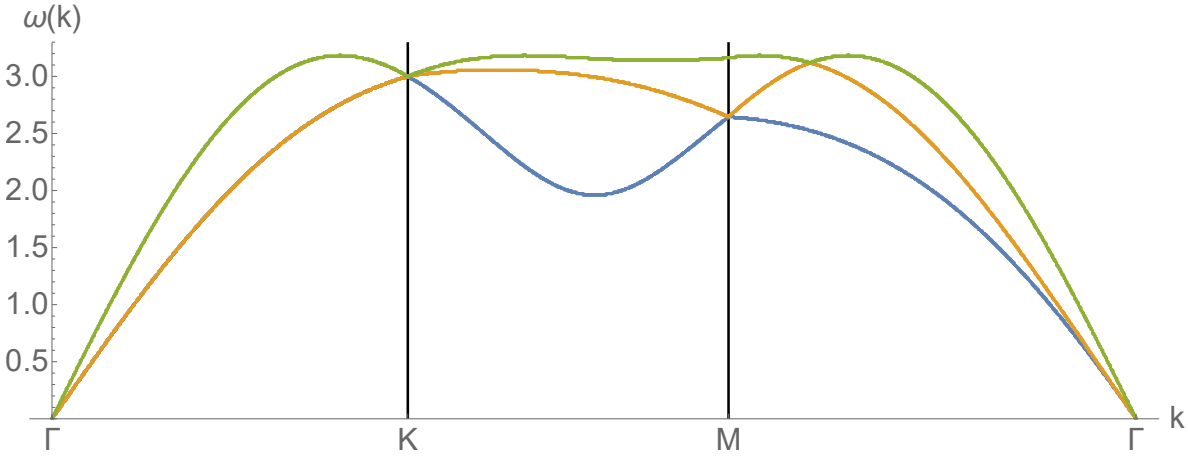


Figure 8: Cut through the Brillouin zone of the triangular lattice for $\alpha = 0$

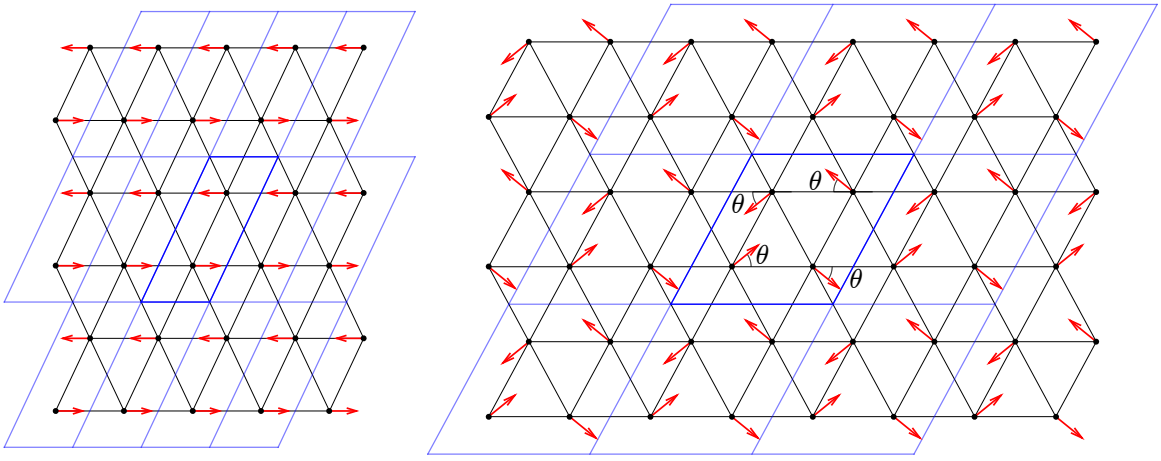


Figure 9: The ground state of the triangular lattice for $\frac{1}{8} < \alpha < 1$ (High NNN coupling). The chosen unit cell is plotted with the ground state. Left: Unit cell choice at $\theta = 0$. Right: Unit cell choice at arbitrary θ

be parameterized by an angle θ[1]. This symmetry leads to there being only 2 bands, instead of the expected 4.

In the case where $\theta = 0$ the Brillouin zone is a rectangle with sides $|\mathbf{K_1}| = \frac{2\pi}{a}\hat{\mathbf{x}}$ and $|\mathbf{K_2}| = \frac{2\pi}{\sqrt{3}a}\hat{\mathbf{y}}$. The dispersion relations for this choice of unit cell is plotted in figure 11. The θ degeneracy comes from the fact that the sum of the cosines of all the angle differences is θ independent. However if $\theta = \frac{n\pi}{2}$ ($n \in \mathbb{Z}$), then it is again possible to choose a unit cell with only 2 atoms and still have translation symmetry. Due to this degeneracy in the ground state, it is a candidate for looking for order-by-disorder, and to do so I need to find the entropy of the ground state as a function of θ[2]. The part of the entropy of the ground state which is related to the spin waves is given by:

$$S(\theta) = \text{const} - \frac{2\pi^2}{\sqrt{3}a^2}\int d\mathbf{k}^2 \log(\omega(\mathbf{k}, \theta)) \tag{5.2}$$

Which is the integral over the Brillouin zone[2]. Since the ground state is identical for θ and $\theta + \frac{\pi}{2}$, it is sufficient to only consider θ to be in the interval of $[0, \frac{\pi}{2}]$. The results of this integral (for $\alpha = \frac{1}{8}$) is plotted on figure 10, and it is clear that the states which maximize entropy are those at $\theta = \frac{n\pi}{2}$. The ground state will be the state which minimizes the free energy $F = E - TS$, which for $T > 0$ are the states with maximum entropy. These are exactly the states at $\theta = \frac{n\pi}{2}$ as is consistent with previous studies results[1].

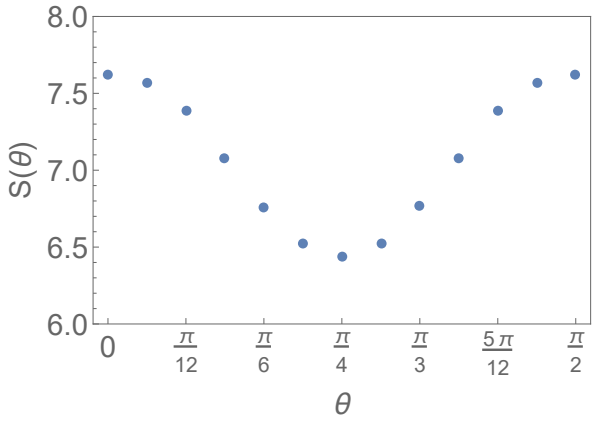


Figure 10: Entropy of the ground state plotted for select values of the parameter θ. The entropy was found through numerical integration over the Brillouin zone.

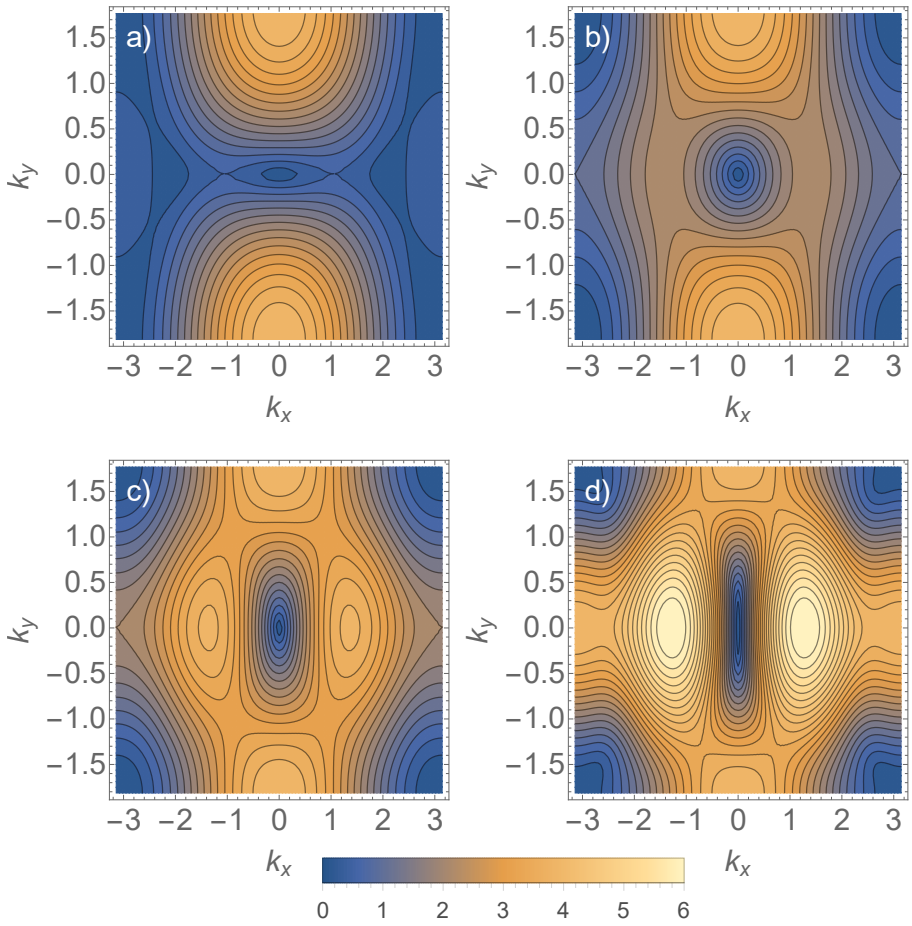


Figure 11: Contour plots of the spin wave dispersion relations in the triangular lattice with no magnetic field. The four different plots have α values of: a) $\alpha = \frac{1}{8}$, b) $\alpha = \frac{1}{4}$, c) $\alpha = \frac{1}{2}$, d) $\alpha = 1$ and all have $\theta = 0$, as is clear from the shape of the Brillouin zone.

6 Solution for time dependent magnetic field

To find the ground state, the time dependency of α and β in equation (2.10) must be found for the case where the magnetic field is time dependent. For the sake om simplicity, I will consider the case where the magnetic field is uniform in space, and I will also assume it is periodic in time. In that case the magnetic field can be written on the form:

$$\mathbf{B}(t) = \mathbf{B_0}\tau(t) \tag{6.1}$$

Where $\tau(t)$ is a periodic function of t. Minimizing (2.15) under the constraint (2.14), α and β are on the form:

$$\beta = \frac{-E_{\mathbf{B}}}{2(E_{\mathbf{0}} - E_{\mathbf{Q}})} \qquad \alpha^2 = 1 - \frac{E_{\mathbf{B}}^2}{4(E_{\mathbf{0}} - E_{\mathbf{Q}})^2} \tag{6.2}$$

Where I have defined

$$E_{\mathbf{Q}} = (J(\mathbf{Q}) + J(-\mathbf{Q}))\mathbf{s}_{\mathbf{Q}} \cdot \mathbf{s}_{-\mathbf{Q}} \qquad E_{\mathbf{0}} = J(\mathbf{0})|\mathbf{s}_{\mathbf{0}}|^2 \qquad E_{\mathbf{B}} = -g\mu_B|\mathbf{B}| \tag{6.3}$$

It is now clear that β is proportional to $\mathbf{B}$, meaning it is also proportional to $\tau(t)$. In this case α and β can be written on the form:

$$\beta = \beta_0\tau(t) \qquad \alpha = \sqrt{1-\beta^2} = \sqrt{1-\beta_0^2\tau(t)^2} \simeq 1 - \frac{\beta_0^2\tau(t)^2}{2} \tag{6.4}$$

The Taylor expansion is only true under the assumption that $\beta \ll 1$. The equation of motion from section 3.1 is:

$$\frac{d\boldsymbol{\zeta}_{\mathbf{k}}}{dt} = \mathbf{W}'(\mathbf{k}, t)\boldsymbol{\zeta}_{\mathbf{k}} \tag{6.5}$$

Where $\mathbf{W}'(\mathbf{k}, t)$ is defined as in (3.17). Since $\mathbf{W}'$ is assumed to be periodic Floquet theory[9] says that the solution must be on the form:

$$\boldsymbol{\zeta}_{\mathbf{k}} = e^{(\chi + i\omega)t}\mathbf{P}(t) \tag{6.6}$$

Where $\mathbf{P}(t)$ is periodic in t with the same period as τ(t). For normalization to hold I have to ensure that $\chi \leq 0$, since if not my assumption that $|\mathbf{s_{i,0}}| \gg |\boldsymbol{\sigma}_{\mathbf{i}}|$ no longer holds for all values of t. If $\mathbf{W}$ is an $3N \times 3N$ matrix, then there are $3N$ solutions all with different values of χ and ω. Floquet theory also states that:

$$T\sum_{n=1}^{N}\mu_n = \int_0^T dt' \,\mathrm{Tr}(\mathbf{W}'(\mathbf{k}, t')) \tag{6.7}$$

Where T is the period of $\mathbf{W}'$, and $\mu_n = \chi_n + i\omega_n$. Since $\mathbf{W}'$ is traceless (because all terms in (3.16) are cross products), the set of μ_n must sum to 0, meaning that if there are any solutions with $\chi > 0$ there must also be solutions which are dampened by the

oscillating field. Since the solutions can be driven by the magnetic field, it is necessary to introduce a damping term into the equation of motion (3.6). (6.5) is rewritten to include said term:

$$\frac{d\boldsymbol{\zeta}_{\mathbf{k}}}{dt} = \mathbf{W}'(\mathbf{k},t)\boldsymbol{\zeta}_{\mathbf{k}} - \gamma\boldsymbol{\zeta}_{\mathbf{k}} \tag{6.8}$$

Then $e^{-\gamma t}\boldsymbol{\zeta}_{\mathbf{k}}$ is a solution (as can be seen from inserting it into (6.8)), and the γ can be manually fitted to stop any of the solutions from having an exponentially scaling amplitude. Furthermore since $\mathbf{P}(t)$ (as defined in (6.6)) is periodic, it can be expanded in the basis of $e^{in\omega_{\mathbf{B}}t}$ where $\omega_{\mathbf{B}} = \frac{2\pi}{T}$ and n is some integer. The general solution will then have ω's which couple to the $\omega_{\mathbf{B}}$ of the $\mathbf{B}$-field.

As in Section 3, to ensure the normalization holds, it is necessary to require $\mathbf{s_{i,0}} \cdot \boldsymbol{\sigma}_{\mathbf{i}} = 0$. In the time independent case this was done by choosing $\boldsymbol{\sigma}_{\mathbf{i}}$ to be orthogonal to the ground state at some point t_0, and then showing that $\frac{d\mathbf{s_{i,0}}\cdot\boldsymbol{\sigma}_{\mathbf{i}}}{dt} = 0$. All the arguments made in that case still hold in the time dependent case with the exception that $\frac{d\mathbf{s_{i,0}}}{dt} = 0$, which is no longer true.

This means $\frac{d\mathbf{s_{i,0}}\cdot\boldsymbol{\sigma}_{\mathbf{i}}}{dt} = \frac{d\mathbf{s_{i,0}}}{dt} \cdot \boldsymbol{\sigma}_{\mathbf{i}}$, which means that for this derivative to be 0, $\boldsymbol{\sigma}_{\mathbf{i}}$ must be simultaneously orthogonal to $\mathbf{s_{i,0}}$ and $\dot{\mathbf{s}}_{\mathbf{i,0}}$. One can deduce that this requirement can only hold if:

$$\dot{\boldsymbol{\sigma}}_{\mathbf{i}} \times (\mathbf{s_{i,0}} \times \ddot{\mathbf{s}}_{\mathbf{i,0}}) = 0 \qquad \Rightarrow \qquad \dot{\boldsymbol{\sigma}}_{\mathbf{i}} \cdot \ddot{\mathbf{s}}_{\mathbf{i,0}} = 0 \tag{6.9}$$

Since $\dot{\boldsymbol{\sigma}}_{\mathbf{i}}$ is known from (3.14), this dot product can be evaluated and it is in general not equal to 0. However, because $\mathbf{s_{i,0}}$ and $\boldsymbol{\sigma}_{\mathbf{i}}$ have the same period (with the exception of the exponential function in equation (6.6)), you can choose them to be orthogonal at some time t_0 and then they will also be orthogonal at all times $t = t_0 + nT$. Furthermore, if $\chi - \gamma \leq 0$ the amplitude of $\boldsymbol{\sigma}_{\mathbf{i}}$ will either remain constant or fall exponentially.

6.1 Perturbation approach

To solve (6.5), rewrite (3.8) on the form:

$$\frac{d\boldsymbol{\zeta}_{\mathbf{k}}}{dt} = \left(\mathbf{W}(\mathbf{k}) + \eta\boldsymbol{\Gamma}(\mathbf{k},t)\right)\boldsymbol{\zeta}_{\mathbf{k}} \tag{6.10}$$

Where all time dependent elements of $\mathbf{W}(\mathbf{k})$ (as defined in equation (3.17)) have been pulled out, and will be treated as a perturbation. η is then some (small) dimensionless quantity used to track the order of the perturbation. In other words, the solution $\boldsymbol{\zeta}_{\mathbf{k}}$ should be on the form:

$$\boldsymbol{\zeta}_{\mathbf{k}} = \sum_m \eta^m \boldsymbol{\zeta}_{\mathbf{k},m} \tag{6.11}$$

The 0'th order solution is the same solution as that in (3.17). Collecting first order terms you get the equation:

$$\frac{d\boldsymbol{\zeta}_{\mathbf{k},1}}{dt} = \mathbf{W}(\mathbf{k})\boldsymbol{\zeta}_{\mathbf{k},1} + \boldsymbol{\Gamma}(\mathbf{k},t)\boldsymbol{\zeta}_{\mathbf{k},0} \tag{6.12}$$

Since $\boldsymbol{\zeta}_{\mathbf{k},0}$ is already known from the 0'th order equation, the last term is completely independent of $\boldsymbol{\zeta}_{\mathbf{k},1}$. This is, in other words, a inhomogeneous linear differential equation. The homogeneous solution is identical to that from equation (3.17), so it doesn't add anything to the overall solution (6.11). The inhomogeneous solution can be found using the method of varying constants (this method is described in appendix D). Let the matrix $\boldsymbol{\Phi}(\mathbf{k},t)$ have the solutions to the homogeneous problem (the eigenvectors of $\mathbf{W}(\mathbf{k})$ multiplied by $e^{\lambda t}$ where λ is an eigenvalue of $\mathbf{W}$) as columns. In that case the inhomogeneous solution will be on the form:

$$\boldsymbol{\zeta}_{\mathbf{k},1} = \boldsymbol{\Phi}(\mathbf{k},t)\int^t dt' \boldsymbol{\Phi}^{-1}(\mathbf{k},t')\boldsymbol{\Gamma}(\mathbf{k},t')\boldsymbol{\zeta}_{\mathbf{k},0} \tag{6.13}$$

The process of finding $\boldsymbol{\zeta}_{\mathbf{k},m}$ can be done iteratively since in general:

$$\frac{d\boldsymbol{\zeta}_{\mathbf{k},m}}{dt} = \mathbf{W}(\mathbf{k})\boldsymbol{\zeta}_{\mathbf{k},m} + \boldsymbol{\Gamma}(\mathbf{k},t)\boldsymbol{\zeta}_{\mathbf{k},m-1} \Rightarrow \tag{6.14}$$

$$\boldsymbol{\zeta}_{\mathbf{k},m} = \boldsymbol{\Phi}(\mathbf{k},t)\int^t dt' \boldsymbol{\Phi}^{-1}(\mathbf{k},t')\boldsymbol{\Gamma}(\mathbf{k},t')\boldsymbol{\zeta}_{\mathbf{k},m-1} \tag{6.15}$$

It is worth noting that $\boldsymbol{\Phi}(\mathbf{k},t)$ is always on the same form, since the solution to the homogeneous equation is the same for all m (and its columns are also the general solution for $\boldsymbol{\zeta}_{\mathbf{k},0}$).
This method is most efficient when solving for a time dependent magnetic field which is very weak. But if the magnetic field has a very simple time dependency ($\mathbf{B} \propto \cos(\omega_{\mathbf{B}} t)$ for example) the integral from equation (6.15) will always be on a simple form since all time dependency in $\boldsymbol{\Phi}$ will be on the form $e^{i\omega t}$ (although in general ω will not be the same for all columns). This also means the the rows in $\boldsymbol{\Phi}^{-1}$ will have time dependency on the form $e^{-i\omega t}$, with the ω from the corresponding column in $\boldsymbol{\Phi}$.
An example of a solution is plotted on figure 12. This particular solution is of a 1D AFM chain with a driving frequency $\omega_{\mathbf{B}}$ ten times higher than the ω of the time independent solution. The β_0 (as defined in equation (6.4)) is $\frac{1}{8}$ and the solution is evolved to the third order in η. It is especially evident from the y-coordinates of the spin waves how the time independent frequency combines with the frequency of the magnetic field. The driving of the magnetic field can also be seen in the form of an amplitude increase, again especially evident in the y-coordinates.

6.2 Fourier approach

Similar to the approach in the time independent problem, this approach takes advantage of the Fourier transform to turn (3.14) into an algebraic equation. But because the ground state and the magnetic field are now time dependent it is convenient to Fourier

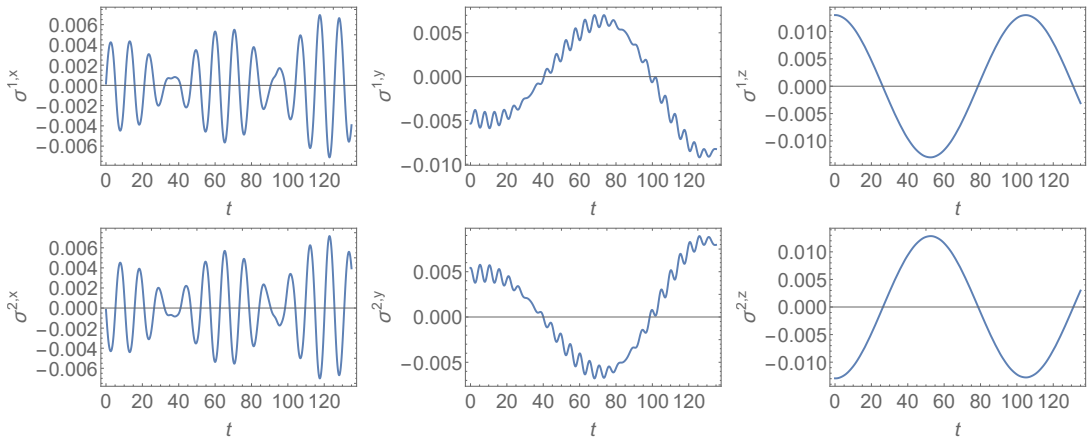


Figure 12: Example solution of the time dependent problem using the perturbation approach. This is a solution of the AFM 1D chain, evolved to the third order in η with no damping term.

transform both the spin wave itself, but also the magnetic field and the ground state:

$$\boldsymbol{\sigma}_{\mathbf{i}}^{n} = \sum_{\mathbf{k}} \int d\omega \boldsymbol{\sigma}_{\mathbf{k}}^{n}(\omega) e^{i(\mathbf{k}\cdot\boldsymbol{\rho}_{\mathbf{i}} - \omega t)} \tag{6.16}$$

$$\mathbf{B}_{\mathbf{i}}{}^{n}(t) = \int d\omega \mathbf{B}_{\mathbf{i}}{}^{n}(\omega) e^{-i\omega t} \tag{6.17}$$

$$\mathbf{s}_{\mathbf{i}}{}^{n}(t) = \int d\omega \mathbf{s}_{\mathbf{i}}{}^{n}(\omega) e^{-i\omega t} \tag{6.18}$$

This way the time dependency of $\boldsymbol{\sigma}_{\mathbf{i}}^{n}$ is trivial. These Fourier transforms can be used in equation (3.14), but in order to do so the cross products need to be evaluated. I will do this on component form, using the antisymmetric symbol, instead of doing it on vector form since it makes the integrals easier to evaluate:

$$\begin{aligned}(\mathbf{B}_{\mathbf{i}}{}^{n} \times \boldsymbol{\sigma}_{\mathbf{i}}^{n})^{u} &= \epsilon_{uvw} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\boldsymbol{\rho}_{\mathbf{i}}} \iint d\omega d\omega' B_{\mathbf{i}}^{n,v}(\omega) \sigma_{\mathbf{k}}^{n,w}(\omega') e^{-i(\omega+\omega')t} \\ &= \epsilon_{uvw} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\boldsymbol{\rho}_{\mathbf{i}}} \int d\Omega e^{-i\Omega t} (B_{\mathbf{i}}^{n,v} * \sigma_{\mathbf{k}}^{n,w})(\Omega)\end{aligned} \tag{6.19}$$

Where $(B_i^{n,v} * \sigma_i^{n,w})$ is the convolution between the v'th coordinate of $\mathbf{B}_{\mathbf{i}}{}^{n}(\omega)$ and the w'th coordinate of $\boldsymbol{\sigma}_{\mathbf{i}}^{n}$. The other cross products from (3.14) can be evaluated in the same way. If the **B**-field is periodic (with period T), the Fourier transform is a sum of Dirac delta functions:

$$\mathbf{B}_{\mathbf{i}}{}^{n}(\omega) = \sum_{\eta} \mathbf{B}_{\mathbf{i},\eta}^{n} \delta(\omega - \frac{2\eta\pi}{T}) \qquad \eta \in \mathbb{Z} \tag{6.20}$$

The same argument applies for the ground state. For shorthand I will introduce $\omega_{\mathbf{B}} = \frac{2\pi}{T}$. The convolutions from the cross products will couple the ω of the spin wave itself to $\omega + \eta\omega_{\mathbf{B}}$ (similar to the result from the perturbation approach). Using these results, (3.14) collapses to:

$$-i\omega\sigma^{n,u}_{\mathbf{k}}(\omega) = \epsilon_{uvw}\sum_{\eta}\left(-g\mu_B B^{n,v}_{\mathbf{i},\eta}\sigma^{n,w}_{\mathbf{k}}(\omega+\eta\omega_{\mathbf{B}}) + \sum_{\mathbf{j}}\sum_{m} J^{n,m}_{\mathbf{i},\mathbf{j}}\left(e^{i\mathbf{k}\cdot(\boldsymbol{\rho}_{\mathbf{j}}-\boldsymbol{\rho}_{\mathbf{i}})}s^{n,w}_{\mathbf{i},0,\eta}\sigma^{m,v}_{\mathbf{k}}(\omega+\eta\omega_{\mathbf{B}}) + s^{m,v}_{\mathbf{j},0,\eta}\sigma^{n,w}_{\mathbf{k}}(\omega+\eta\omega_{\mathbf{B}})\right)\right) \quad (6.21)$$

I have not found a way to solve this equation, but it is likely the best approach for finding an exact solution as opposed to an approximate solution, as is done in the perturbation approach.

7 Conclusion

The Heisenberg model was studied with the goal of finding spin waves in frustrated systems. As the spin waves are small deviations from the ground state, it was necessary to find the ground state of the frustrated system. The ground state was found through a Fourier transform of the Hamiltonian, both with and without a Zeeman term from an external magnetic field.

The equation of motion of the Heisenberg model was derived and linearized through only considering small deviations from the ground state. By assuming no time dependency of the Zeeman term, the differential equation was turned algebraic through a Fourier transform, and the translational symmetry of the ground state was used to diagonalize the spin wave in $\mathbf{k}$-space. The, now linearized and algebraic, equation was shown to be on the form of an eigenvalue equation, with the spin waves given by the eigenvectors and the dispersion relation given by the eigenvalues.

The equation of motion was solved for the 1D spiral chain and the antiferromagnetic triangular lattice. Through the solution of the 1D spiral chain, it was shown how the Zeeman term breaks the rotational symmetry of the Heisenberg Hamiltonian, and gives rise to three times as many bands as the Heisenberg model without a Zeeman term does. The triangular lattice was, through the dispersion of the spin waves, shown to have order-by-disorder when $\frac{1}{8} < \frac{J_2}{J_1} < 1$.

Finally, the case of a time dependent Zeeman term was discussed. Issues with normalization of the spin vectors were shown, and partially solved through the introduction of a damping term in the equation of motion. Two methods of solving the equation of motion were discussed, one based on treating the time dependent Zeeman term as a perturbation and another Fourier transformed the time coordinate in order to turn the

equation of motion into an algebraic equation. However, the solution of the resulting algebraic equation was not found.

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A Finding the Ground State through Lagrange Multipliers

Minimizing (2.15) under (2.14) can be done through the method of Lagrange Multipliers. Consider the function:

$$\mathcal{L}(\alpha,\beta,\lambda) = \alpha^2(J(\mathbf{Q}) + J(-\mathbf{Q}))\mathbf{s_Q}\cdot\mathbf{s_{-Q}} + \beta^2 J(\mathbf{0})|\mathbf{s_0}|^2 - \beta g\mu_B|\mathbf{B}| - \lambda(\alpha^2+\beta^2-1)$$

The α, β and λ which solve the equation $\nabla\mathcal{L} = \mathbf{0}$ is then a local extremum of (2.15) under the constraint of (2.14). Solving this requires solving three equations with three unknowns, namely:

$$2\alpha((J(\mathbf{Q}) + J(-\mathbf{Q}))\mathbf{s_Q}\cdot\mathbf{s_{-Q}} - \lambda) = 0$$
$$2\beta(J(\mathbf{0}|\mathbf{s_0}| - \lambda) - g\mu_B|\mathbf{B}| = 0$$
$$\alpha^2+\beta^2-1=0$$

The first equation has two possible solutions, namely $\lambda = (J(\mathbf{Q})+J(-\mathbf{Q}))\mathbf{s_Q}\cdot\mathbf{s_{-Q}}$ and $\alpha = 0$. Since $\alpha = 0$ is the local maximum (unless the magnetic field is strong enough), let's consider the case where $\alpha \neq 0$. Using the value of λ in the second equation, one can find:

$$\beta = \frac{g\mu_B|\mathbf{B}|}{2(J(\mathbf{0}|\mathbf{s_0}| - (J(\mathbf{Q})+J(-\mathbf{Q}))\mathbf{s_Q}\cdot\mathbf{s_{-Q}})}$$

Once this value of β is found, α can be found through the third equation.

B Classical Derivation of the Equation of Motion

In this classical model I will consider the spin to be an angular momentum, which means it must be on the form

$$\mathbf{s_i} = \mathbf{r_i}\times\mathbf{p_i}$$

And so in accordance with Hamilton's equations the time derivative must be:

$$\dot{\mathbf{s_i}} = \dot{\mathbf{r_i}}\times\mathbf{p_i} + \mathbf{r_i}\times\dot{\mathbf{p_i}} = \frac{\partial\mathcal{H}}{\partial\mathbf{p_i}}\times\mathbf{p_i} - \mathbf{r_i}\times\frac{\partial\mathcal{H}}{\partial\mathbf{r_i}}$$

Just as in the quantum mechanical derivation (section 3.1) it is convenient to define the local field (3.3). This section will make use of the antisymmetric symbol (ϵ_{ijk}) and of Einstein notation. The following identity will also come in handy a couple of times:

$$\epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$$

Having defined the local field, the Hamiltonian can be written on the form:

$$\mathcal{H} = \sum_i \epsilon_{uvw}H_i^u r_i^v p_i^w$$

And the l'th component of $\dot{\mathbf{s}}_\mathbf{i}$:

$$\dot{s}_i{}^l = \epsilon_{lmn}\left(\frac{\partial \mathcal{H}}{\partial p_i^m}p_i^n - r_i^m\frac{\partial \mathcal{H}}{\partial r_i^n}\right) = \epsilon_{lmn}\left(p_i^n\epsilon_{uvm}H_i^u r_i^v + r_i^m\epsilon_{uvn}H_i^u p_i^v\right)$$

Using the above identity this expression can be collapsed to the form:

$$\dot{s}_i{}^l = p_i^n\left(H_i^n r_i^l - H_i^l r_i^n\right) + r_i^n\left(p_i^n H_i^l - p_i^l H_i^n\right) = H_i^n\left(r_i^l p_i^n - r_i^n p_i^l\right)$$

It might not be immediately obvious that this is the cross product from (3.6) so in order to explicitly show that lets rewrite (3.6) to the same form:

$$s_i^n = \epsilon_{nuv}r_i^u p_i^v \qquad \Rightarrow \qquad \dot{s}_i{}^l = \epsilon_{lmn}H_i^m s_i^n = \epsilon_{lmn}\epsilon_{nuv}H_i^m r_i^u p_i^v = H_i^n\left(r_i^l p_i^n - r_i^n p_i^l\right)$$

So you can find the equation of motion without having to involve quantum mechanics.

C Translating the Brillouin Zone of the Triangular Lattice

The spin wave dispersion relation that I find for the triangular lattice is compared to previously found dispersion relations in section 5. Because I used a different unit cell from the results I'm comparing to, the Brillouin zone (BZ) from the previous studies has to be translated so it can be compared with mine.

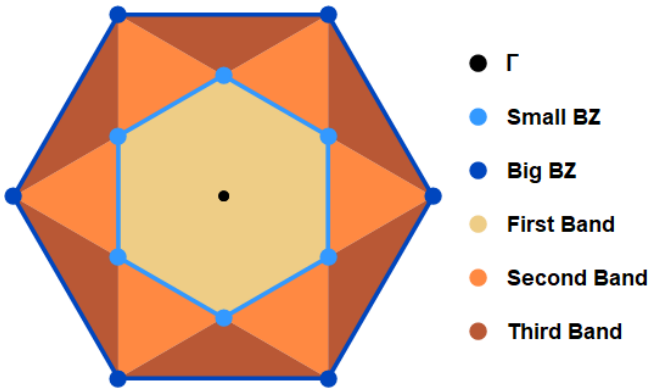

Figure 13: Plot of both the Brillouin zone of the unit cell with 1 atom (Big BZ) and the unit cell with 3 atoms (small BZ). The colored areas on the figure indicate which parts of the big BZ become which bands in the small BZ.

Both of the Brillouin zones are plotted on figure 13. Because the K points of the Big BZ are reciprocal lattice vectors for the small BZ, all the K points from the big BZ will be translated into the center point Γ.
The important thing to keep in mind when comparing the two BZ is that the big BZ

describes the phase change of the spin waves between each site, whereas the small BZ describes the phase change between each unit cell. The K points for the big BZ have $\mathbf{k}$ such that there is translational symmetry every 3 atoms, which is exactly why they correspond to Γ in the small unit cell. The $\mathbf{k}$ vectors in the small BZ describe the phase that the spin waves pick up between unit cells, and so if there is translational symmetry every 3 atoms the spin waves shouldn't pick up a phase between unit cells.
Another way of thinking about this is that in the small BZ, the eigenvectors of $\mathbf{W}$ have the spiral order within the unit cell built into it. Because the eigenvectors have 9 entries corresponding to the x-, y- and z-components of each atom in the unit cell, they can have the spiral order from the K points in the big unit cell built into them, so it is unnecessary to take phase changes that happen within the unit cell into consideration when building the Brillouin zone.

D Short Introduction to Lagrange's Method of Variation of Constants

This method can be used when solving problems on the form:

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{f}(t)$$

Where $\mathbf{A}$ is some constant matrix. The solution to the homogeneous problem will span the solution space, meaning the solution can be written as a linear combination of these solutions:

$$\mathbf{x} = \mathbf{\Phi}\mathbf{c}(t)$$

Where the columns of $\mathbf{\Phi}$ are the solutions to the homogeneous problem and $\mathbf{c}(t)$ is the column vector with the (time dependent) expansion coefficients. Using the solution on this form on the original problem, you find:

$$\dot{\mathbf{\Phi}}\mathbf{c}(t) + \mathbf{\Phi}\dot{\mathbf{c}}(t) = \mathbf{A}\mathbf{\Phi}\mathbf{c}(t) + \mathbf{f}(t)$$

Since $\mathbf{\Phi}$ is the solution for the inhomogeneous problem, this equation simplifies down to:

$$\mathbf{\Phi}\dot{\mathbf{c}}(t) = \mathbf{f}(t) \qquad \Rightarrow \qquad \dot{\mathbf{c}}(t) = \mathbf{\Phi}^{-1}\mathbf{f}(t)$$

The solution to the differential equation can, through integration, be found to be on the form:

$$\mathbf{x} = \mathbf{\Phi}\int^{t} dt' \mathbf{\Phi}^{-1}\mathbf{f}(t')$$

E Mathematica Code for the Triangular Lattice

```
Clear["Global`*"]
(*Define the number of atoms in the unit
 cell and the number of unit cells it couples to*)
nuc := 3;
nmatrix := 9;
(*Write out all the J_ij Matrices as defined in section 3.1 of the thesis*)
Jmat0 := {{0, J1, 0}, {J1, 0, J1}, {0, J1, 0}};
Jmat1 := {{J2, 0, 0}, {J1, J2, 0}, {J1, J1, J2}};
Jmat2 := {{J2, 0, 0}, {0, J2, 0}, {0, 0, J2}};
Jmat3 := {{J2, J1, J1}, {0, J2, J1}, {0, 0, J2}};
Jmat4 := {{0, 0, 0}, {0, 0, 0}, {J1, 0, 0}};
Jmat5 := {{0, 0, J1}, {0, 0, 0}, {0, 0, 0}};
Jmat6 := {{J2, 0, 0}, {J1, J2, 0}, {J1, J1, J2}};
Jmat7 := {{J2, 0, 0}, {0, J2, 0}, {0, 0, J2}};
Jmat8 := {{J2, J1, J1}, {0, J2, J1}, {0, 0, J2}};
JFull = {Jmat0, Jmat1, Jmat2, Jmat3, Jmat4, Jmat5, Jmat6, Jmat7, Jmat8};

(*Define the ground state of each atom in the unit cell with no B field*)
θ[m_] := (4 * π / 3) * (m - 1);
ϕ[m_] = π / 2;
sQ[m_] := {Sin[θ[m]] Cos[ϕ[m]], Sin[θ[m]] Sin[ϕ[m]], Cos[θ[m]]};

(*Define the ρ vectors which are the coordinates of the unit
 cell. These should be in the same "order" as the J_ij matrices*)
a1 := {0, Sqrt[3]};
a2 := (1 / 2) * {3, Sqrt[3]};
avec := {{0, 0}, a1 - a2, a1, a2, a1 - 2 * a2, -a1 + 2 * a2, -a2, -a1, -a1 + a2};

(*Define matricies which correspond to the front factor in H_σ and H_0 respectively*)
Jσmat[kx_, ky_] := Sum[JFull[[k]] * Exp[-I * avec[[k]].{kx, ky}], {k, nmatrix}];
Js0mat := Sum[JFull[[k]], {k, nmatrix}];

(*The σ's here are used to keep track of which coordinates of ς couple to which*)
σ := Table[ds[i, j], {i, nuc}, {j, 3}];

(*Define the strength and direction of the B field*)
B0 := 0;
sB := {0, 0, 1};
B := B0 * sB;
Bmat := {{0., B[[3]], -B[[2]]}, {-B[[3]], 0., B[[1]]}, {B[[2]], -B[[1]], 0.}}
Bfullmat := ArrayFlatten[Table[Bmat * KroneckerDelta[i, j], {i, nuc}, {j, nuc}]];

(*The relevant energies for calculating β and
 α are found from the J(q) for the triangular lattice*)
EQ := -3 * J1 + 6 * J2;
E0 := 6 * (J1 + J2)
EB := -B0;

(*Note that this normalization assumes that sB is orthogonal to sQ*)
β := Min[{-EB / (2 * (E0 - EQ)), 1}];
α := Sqrt[1 - β^2];
```

```
(*The final ground state is found*)
s0[m_] := α * sQ[m] + β * sB;

(*Find the equation of motion for the a'th atom in the unit cell*)
hmat[a_, kx_, ky_] := Sum[Js0mat[[b, a]] * Cross[s0[b], σ[[a]]] +
    Jσmat[kx, ky][[b, a]] * Cross[σ[[b]], s0[a]], {b, nuc}];

(*Gather all these equations of motion up into one big vector*)
hmatbig[kx_, ky_] := Table[hmat[a, kx, ky], {a, nuc}];

(*Pull out the coefficients of the σ matrix to find the W'matrix*)
Wmat[kx_, ky_] = Transpose[Table[Coefficient[Flatten[hmatbig[kx, ky]],
      ds[Floor[(a - 1) / 3] + 1, Mod[a - 1, 3] + 1]], {a, 3 * nuc}]] - Bfullmat;
```