Spin Waves on a Honeycomb Lattice: Derivation of the Dispersion Relation

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1 Introduction

In this document we derive the dispersion relation for spin-waves on a Honeycomb lattice. This is worked out following the procedure outlined in Chapters 4, 5.4 of [1].

The basic problem under consideration is the diagonalisation of the Hamiltonian (1) for a ferromagnetic honeycomb lattice with edges of length a. This Hamiltonian has three terms describing distinct effects. The first term with $J > 0$ represents a nearest-neighbour ferromagnetic exchange interaction, which 'encourages' neighbouring spins to align. The second term, proportional to K, is the 'easy-plane' anisotropy term, which forces the spin interaction to be anisotropic. The last term describes the interaction of spin magnetic moment with an external magnetic field.

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \underline{\mathrm{S}}_i \cdot \underline{\mathrm{S}}_j - K \sum_i {S_{iz}}^2 - 2\mu_B B \sum_i S_{iz}. \tag{1}$$

As is visible in Figure 1, the lattice has two separate sublattices: 1 and 2. These are distinct as lattice 1 has a top neighbour in lattice 2, but lattice 2 does not have a top neighbour. A single primitive unit cell has been drawn. As can be seen there are two magnetic sites per unit cell, respectively in lattices 1 and 2.

The subscript $\langle i, j \rangle$ indicates that the first sum should be done over all neighbouring magnetic sites i and j. As lattice 1 is only neighboured by lattice 2 and vice-versa, this sum may be considered to be done over lattice 1, and then repeated for each of the three neighbours of a magnetic site in lattice 1.

Each magnetic site has associated the typical spin operators: $\underline{\mathrm{S}}, S_{x/y/z}, S_{+/-}$. To distinguish sites i, operators are labelled as follows: $S_{i+}^{(1/2)}$, where 1 and 2 are used to label the appropriate lattice for an operator acting on site i.

2 Holstein-Primakoff Transformation

Using the Holstein-Primakoff transformation, which associates a spin state $|m_J\rangle$ with a harmonic oscillator $|S - m\rangle$ state in an infinite dimensional Fock space with corresponding ladder operators $a, a^\dagger, [a, a^\dagger] = 1$, the spin operators $S_{+/-}$ become:

$$S_{i+}^{(1/2)} = \sqrt{2S}\sqrt{1 - \frac{a_i^{\dagger(1/2)} a_i^{(1/2)}}{2S}}\, a_i^{(1/2)}, \qquad S_{i-}^{(1/2)} = \sqrt{2S}\, a_i^{\dagger(1/2)}\sqrt{1 - \frac{a_i^{\dagger(1/2)} a_i^{(1/2)}}{2S}}. \tag{2}$$

Note that $S_{iz}^{(1/2)} = S - a_i^{(1/2)\dagger} a_i^{(1/2)}$.

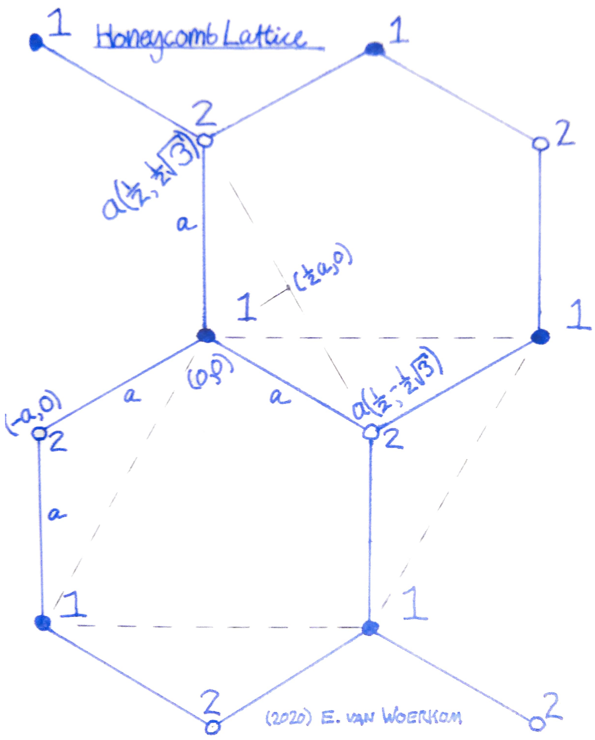

Figure 1: Schematic drawing of two honeycomb lattice hexagons.

3 Implementing H-P in the Hamiltonian

To achieve an analytical solution, we make the approximation to first order in $\sqrt{S}$: $S_{i+}^{(1/2)} = \sqrt{2S}a_i^{(1/2)\cdot/\dagger}$. We then proceed to rewrite $\mathcal{H}$ using that $S_{ix}S_{jx} + S_{iy}S_{ix} = (S_{i+}S_{j-} + S_{i-}S_{j+})/2$:

$$
\begin{aligned}
\mathcal{H} =& -J\sum_i^{(1)}\sum_{j=i+\delta}^{(2)}(S_{i+}^{(1)}S_{j-}^{(2)} + S_{i-}^{(1)}S_{j+}^{(2)})/2 + S_{iz}^{(1)}S_{jz}^{(2)} \\
& - K(\sum_i^{(1)} {S_{iz}^{(1)}}^2 + \sum_j^{(2)} {S_{jz}^{(2)}}^2) - 2\mu_B B(\sum_i^{(1)} S_{iz} + \sum_j^{(2)} S_{jz}) \\
\approx & -J\sum_i^{(1)}\sum_{j=i+\delta}^{(2)} 2S(a_i^{(1)}a_j^{(2)\dagger} + a_i^{(1)\dagger}a_j^{(2)})/2 + (S - a_i^{(1)\dagger}a_i^{(1)})(S - a_j^{(2)\dagger}a_j^{(2)}) \\
& - K(\sum_i^{(1)}(S - a_i^{(1)\dagger}a_i^{(1)})^2 + \sum_j^{(2)}(S - a_j^{(2)\dagger}a_j^{(2)})^2) \\
& - 2\mu_B B(\sum_i^{(1)} S - a_i^{(1)\dagger}a_i^{(1)} + \sum_j^{(2)} S - a_j^{(2)\dagger}a_j^{(2)}) \\
=& \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_4.
\end{aligned}
\tag{3}
$$

In doing this approximation, we observe that there is a constant part $\mathcal{H}_0$ proportional to S^2, $\mathcal{H}_2$ which is proportional to S and a 4th order part $\mathcal{H}_4$ which is proportional to S^0:

$$\begin{aligned}
\mathcal{H}_0 =& - NS^2(3J + 2K - 4\mu_B B/S),\\
\mathcal{H}_2 =& - JS \sum_i^{(1)} \sum_{j=i+\delta}^{(2)} a_i^{(1)} a_j^{(2)\dagger} + a_i^{(1)\dagger} a_j^{(2)} - a_i^{(1)\dagger} a_i^{(1)} - a_j^{(2)\dagger} a_j^{(2)}\\
& + K'S(\sum_i^{(1)} a_i^{(1)\dagger} a_i^{(1)} + \sum_j^{(2)} a_j^{(2)\dagger} a_j^{(2)}),\\
\mathcal{H}_4 =& - J \sum_i^{(1)} \sum_{j=i+\delta}^{(2)} a_i^{(1)\dagger} a_i^{(1)} a_j^{(2)\dagger} a_j^{(2)} - K(\sum_i^{(1)} a_i^{(1)\dagger} a_i^{(1)} a_i^{(1)\dagger} a_i^{(1)} + \sum_j^{(2)} a_j^{(2)\dagger} a_j^{(2)} a_j^{(2)\dagger} a_j^{(2)}),\\
K' =& K + 2\mu_B B/S.
\end{aligned} \tag{4}$$

In the equations (4), N stands for the number of unit cells. $\mathcal{H}_0$ represents the classical energy and does not affect spin-wave dynamics because it is constant. $\mathcal{H}_4$ is 4th order and negligible because of two reasons: S is assumed to be large and additionally because the expectation value of $a_i^\dagger a_i$ is already small for a spin-wave (being proportional to $1/N$ as we shall see), and thus $a_i^\dagger a_i a_i^\dagger a_i \sim 1/N^2$, which is vanishingly small. Therefore we need only consider $\mathcal{H}_2$ to analyse spin-wave dynamics.

4 Converting to Reciprocal Space

To analyse the Hamiltonian appropriately we need to Fourier Transform the operators $a, a^\dagger$. To this end, we define the following transformed operators:

$$\begin{aligned}
a_{\underline{\mathrm{q}}}^{(r)} &= \frac{1}{\sqrt{N}} \sum_i^{(r)} e^{-i\underline{\mathrm{q}}\cdot\underline{\mathrm{R}}_i} a_i^{(r)},\\
a_{\underline{\mathrm{q}}}^{(r)\dagger} &= \frac{1}{\sqrt{N}} \sum_i^{(r)} e^{-i\underline{\mathrm{q}}\cdot\underline{\mathrm{R}}_i} a_i^{(r)\dagger}.
\end{aligned} \tag{5}$$

These operators can be inverted and thus:

$$\begin{aligned}
a_i^{(r)} &= \frac{1}{\sqrt{N}} \sum_{\underline{\mathrm{q}}}^{(r)} e^{i\underline{\mathrm{q}}\cdot\underline{\mathrm{R}}_i} a_{\underline{\mathrm{q}}}^{(r)},\\
a_i^{(r)\dagger} &= \frac{1}{\sqrt{N}} \sum_{\underline{\mathrm{q}}}^{(r)} e^{i\underline{\mathrm{q}}\cdot\underline{\mathrm{R}}_i} a_{\underline{\mathrm{q}}}^{(r)\dagger}.
\end{aligned} \tag{6}$$

It is extremely important to note that the Hermitian conjugate of $a_{\underline{\mathrm{q}}}^{(r)}$ is not $a_{\underline{\mathrm{q}}}^{(r)\dagger}$! This is a weakness of the used FT-notation. Carefully working out the Hermitian conjugate gives (note the minus sign):

$$
\begin{aligned}
(a_{\underline{q}}^{(r)})^\dagger &= a_{-\underline{q}}^{(r)\dagger}, \\
(a_{\underline{q}}^{(r)\dagger})^\dagger &= a_{-\underline{q}}^{(r)}, \\
[a_{\underline{q}}^{(r)}, a_{-\underline{q}'}^{(s)\dagger}] &= \delta_{r,s}\delta_{\underline{q},\underline{q}'}, \\
[a_{\underline{q}}^{(r)}, a_{\underline{q}'}^{(s)}] &= [a_{\underline{q}}^{(r)\dagger}, a_{\underline{q}'}^{(s)\dagger}] = 0.
\end{aligned} \tag{7}
$$

Proceeding to transform each part of $\mathcal{H}_2$:

$$
\begin{aligned}
\sum_i^{(1)} a_i^{(1)\dagger} a_i^{(1)} &= \frac{1}{N} \sum_i^{(1)} \sum_{\underline{q}}^{(1)} e^{i\underline{q}\cdot\underline{R}_i} a_{\underline{q}}^{(1)\dagger} \sum_{\underline{q}'}^{(1)} e^{i\underline{q}'\cdot\underline{R}_i} a_{\underline{q}'}^{(1)} = \frac{1}{N} \sum_i^{(1)} \sum_{\underline{q}}^{(1)} e^{i\underline{q}\cdot\underline{R}_i} a_{\underline{q}}^{(1)\dagger} \sum_{\underline{q}'}^{(1)} e^{-i\underline{q}'\cdot\underline{R}_i} a_{-\underline{q}'}^{(1)} \\
&= \frac{1}{N} \sum_i^{(1)} \sum_{\underline{q}}^{(1)} \sum_{\underline{q}'}^{(1)} e^{i(\underline{q}-\underline{q}')\cdot\underline{R}_i} a_{\underline{q}}^{(1)\dagger} a_{-\underline{q}'}^{(1)} = \frac{1}{N} \sum_{\underline{q}}^{(1)} \sum_{\underline{q}'}^{(1)} N\delta(\underline{q}-\underline{q}') a_{\underline{q}}^{(1)\dagger} a_{-\underline{q}'}^{(1)} \\
&= \sum_{\underline{q}}^{(1)} a_{\underline{q}}^{(1)\dagger} a_{-\underline{q}}^{(1)}
\end{aligned} \tag{8}
$$

Therefore as each point in lattice 1 has three neighbours in lattice 2:

$$
\sum_i^{(1)} \sum_{j=i+\delta}^{(2)} a_j^{(1)\dagger} a_j^{(1)} = 3 \sum_{\underline{q}}^{(1)} a_{\underline{q}}^{(1)\dagger} a_{-\underline{q}}^{(1)} \tag{9}
$$

Similarly:

$$
\begin{aligned}
\sum_j^{(2)} a_j^{(2)\dagger} a_j^{(2)} &= \sum_{\underline{q}}^{(2)} a_{\underline{q}}^{(2)\dagger} a_{-\underline{q}}^{(2)}, \\
\sum_i^{(1)} \sum_{j=i+\delta}^{(2)} a_j^{(2)\dagger} a_j^{(2)} &= 3 \sum_{\underline{q}}^{(2)} a_{\underline{q}}^{(2)\dagger} a_{-\underline{q}}^{(2)}.
\end{aligned} \tag{10}
$$

Note how the interaction term transforms with an extra factor $\Gamma_{\underline{q}} = \frac{1}{3}\sum_{\delta}^{(2)} e^{-i\underline{q}\cdot\underline{\delta}}$:

$$\begin{aligned}
\sum_{i}^{(1)}\sum_{j=i+\delta}^{(2)} a_i^{(1)\dagger}a_j^{(2)} &= \frac{1}{N}\sum_{i}^{(1)}\sum_{j=i+\delta}^{(2)}\sum_{\underline{q}}^{(1)} e^{i\underline{q}\cdot\underline{R}_i}a_{\underline{q}}^{(1)\dagger}\sum_{\underline{q}'}^{(2)} e^{i\underline{q}'\cdot\underline{R}_j}a_{\underline{q}'}^{(2)} \\
&= \frac{1}{N}\sum_{i}^{(1)}\sum_{j=i+\delta}^{(2)}\sum_{\underline{q}}^{(1)}\sum_{\underline{q}'}^{(2)} e^{i(\underline{q}\cdot\underline{R}_i-\underline{q}'\cdot\underline{R}_j)}a_{\underline{q}}^{(1)\dagger}a_{-\underline{q}'}^{(2)} \\
&= \frac{1}{N}\sum_{i}^{(1)}\sum_{\underline{q}}^{(1)}\sum_{\underline{q}'}^{(2)} e^{i(\underline{q}\cdot\underline{R}_i-\underline{q}'\cdot\underline{R}_i)}a_{\underline{q}}^{(1)\dagger}a_{-\underline{q}'}^{(2)}\sum_{\delta}^{(2)} e^{-i\underline{q}'\cdot\underline{\delta}} \\
&= \sum_{\underline{q}}^{(1)}\sum_{\underline{q}'}^{(2)} \delta(\underline{q}-\underline{q}')a_{\underline{q}}^{(1)\dagger}a_{-\underline{q}'}^{(2)}\sum_{\delta}^{(2)} e^{-i\underline{q}'\cdot\underline{\delta}} \\
&= \sum_{\underline{q}}^{(1)} a_{\underline{q}}^{(1)\dagger}a_{-\underline{q}}^{(2)}\sum_{\delta}^{(2)} e^{-i\underline{q}\cdot\underline{\delta}} = 3\sum_{\underline{q}}^{(1)} a_{\underline{q}}^{(1)\dagger}a_{-\underline{q}}^{(2)}\Gamma_{\underline{q}}.
\end{aligned} \tag{11}$$

Similarly:

$$\sum_{i}^{(1)}\sum_{j=i+\delta}^{(2)} a_i^{(1)}a_j^{(2)\dagger} = 3\sum_{\underline{q}}^{(1)} a_{\underline{q}}^{(1)}a_{-\underline{q}}^{(2)\dagger}\Gamma_{\underline{q}}. \tag{12}$$

Applying these transforms we get:

$$\mathcal{H}_2 = S\sum_{\underline{q}}(3J+K')(a_{\underline{q}}^{(1)\dagger}a_{-\underline{q}}^{(1)} + a_{\underline{q}}^{(2)\dagger}a_{-\underline{q}}^{(2)}) - 3J\Gamma_{\underline{q}}(a_{\underline{q}}^{(1)\dagger}a_{-\underline{q}}^{(2)} + a_{\underline{q}}^{(1)}a_{-\underline{q}}^{(2)\dagger}). \tag{13}$$

Which can be rewritten into equation (14) using some inversions of $\underline{q}$ and finally into the form of equation (15), which can be used to find an analytical solution.

$$\mathcal{H}_2 = S\sum_{\underline{q}}(3J+K')(a_{-\underline{q}}^{(1)\dagger}a_{\underline{q}}^{(1)} + a_{-\underline{q}}^{(2)\dagger}a_{\underline{q}}^{(2)}) - 3J(\Gamma_{\underline{q}}^{*}a_{-\underline{q}}^{(1)\dagger}a_{\underline{q}}^{(2)} + \Gamma_{\underline{q}}a_{\underline{q}}^{(1)}a_{-\underline{q}}^{(2)\dagger}). \tag{14}$$

$$\begin{bmatrix} a_{\underline{q}}^{(1)} \\ a_{\underline{q}}^{(2)} \\ a_{-\underline{q}}^{(1)\dagger} \\ a_{-\underline{q}}^{(2)\dagger} \end{bmatrix}^{\dagger} \frac{S}{2} \begin{bmatrix} (3J+K') & -3J\Gamma_{\underline{q}}^{*} & 0 & 0 \\ -3J\Gamma_{\underline{q}} & (3J+K') & 0 & 0 \\ 0 & 0 & (3J+K') & -3J\Gamma_{\underline{q}} \\ 0 & 0 & -3J\Gamma_{\underline{q}}^{*} & (3J+K') \end{bmatrix} \begin{bmatrix} a_{\underline{q}}^{(1)} \\ a_{\underline{q}}^{(2)} \\ a_{-\underline{q}}^{(1)\dagger} \\ a_{-\underline{q}}^{(2)\dagger} \end{bmatrix} \tag{15}$$

Note: the matrix in equation (15) differs markedly from that given in 5.37 in Section 5.4 of [1] on three points:

1. K' is absent from the bottom-left and top-right submatrices, which are empty, in contrast with 5.37.

2. K' has a positive instead of negative sign as in 5.37.

3. $\Gamma_{\underline{q}}$ and $\Gamma_{\underline{q}}^{*}$ should be interchanged in the bottom-right submatrix of 5.37.

5 Retrieving the Dispersion Relation

The matrix in (15) is called $\underline{\text{L}}$. To retrieve the dispersion relation, the eigenvalues of $\underline{\mathcal{L}} = \underline{\text{N}} \cdot \underline{\text{L}}$ as a function of $\underline{\text{q}}$ should be calculated, where $\underline{\text{N}} = \left[\begin{smallmatrix} I & 0 \\ 0 & -I \end{smallmatrix}\right]$:

$$\underline{\mathcal{L}} = \frac{3JS}{2}\begin{bmatrix} (1+K'/3J) & -\Gamma^*_{\underline{\text{q}}} & 0 & 0 \\ -\Gamma_{\underline{\text{q}}} & (1+K'/3J) & 0 & 0 \\ 0 & 0 & -(1+K'/3J) & \Gamma_{\underline{\text{q}}} \\ 0 & 0 & \Gamma^*_{\underline{\text{q}}} & -(1+K'/3J) \end{bmatrix} \tag{16}$$

Equation (16) differs on two points from 5.39 in [1]:

1. K' is absent in 5.39 as it has been set to zero.
2. The $\Gamma_{\underline{\text{q}}}$ symbols in the bottom-right submatrix of 5.37 should have a negative sign.
3. Once again, $\Gamma_{\underline{\text{q}}}$ and $\Gamma^*_{\underline{\text{q}}}$ should be interchanged in the bottom-right submatrix of 5.37.

Equation (16) has the characteristic equation:

$$\left[\left(1 + K'/3J - \frac{\varepsilon}{3JS/2}\right)^2 - |\Gamma_{\underline{\text{q}}}|^2\right] \cdot \left[\left(-1 - K'/3J - \frac{\varepsilon}{3JS/2}\right)^2 - |\Gamma_{\underline{\text{q}}}|^2\right] = 0 \tag{17}$$

Finally, this gives the following eigenvalue solutions for the dispersion relation:

$$\begin{aligned} \varepsilon_{1/2} &= \frac{3JS}{2}\left(1 + K'/3J \pm |\Gamma_{\underline{\text{q}}}|\right), \\ \varepsilon_{3/4} &= \frac{-3JS}{2}\left(1 + K'/3J \pm |\Gamma_{\underline{\text{q}}}|\right). \end{aligned} \tag{18}$$

Furthermore $|\Gamma_q|^2$ has a range between 0 and 1:

$$\begin{aligned} |\Gamma_q|^2 &= \frac{1}{9}|e^{q_x a} + e^{-i\frac{a}{2}(q_x + q_y\sqrt{3})} + e^{-i\frac{a}{2}(q_x - q_y\sqrt{3})}|^2 \\ &= \frac{1}{9}\left(1 + 4\cos^2\left(\frac{aq_y\sqrt{3}}{2}\right) + 4\cos\left(\frac{aq_y\sqrt{3}}{2}\right)\cos\left(\frac{aq_x 3}{2}\right)\right) \end{aligned} \tag{19}$$

References

[1] *"Spin-Wave Theory and its Applications to Neutron Scattering and THz Spectroscopy"*, Fishman R, Fernandez-Baca F., Room, T., Morgan & Claypool Publishers (2018).