Spin wave excitations in the 1/2 plateau of the J_1-J_2 model on the square lattice

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Abstract

We investigate the frustrated ground state of the J_1-J_2 model on the square lattice near the Ising limit in the one-half magnetisation plateau, both for spin 1/2 and for general spin S. By calculating the perturbative ground-state energy correction at second order, we demonstrate an order-by-disorder mechanism that selects a periodic state depending on the coupling and Ising parameters. We then map out the full phase diagram as a function of all parameters. Next, we use perturbation theory to compute the single magnon excitations and derive their dispersion relations. In the second part, we perform a leading-order spin-wave expansion around the same one-half plateau state, obtaining an independent set of magnon spectra. It remains to compare the perturbative dispersion relation with the one gathered by the spin wave expansion.

Contents

I. Introduction

In this work, we consider a square lattice with the Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j\rangle_1} \left(J_{1zz} S_i^z S_j^z + J_{1xy} \left(S_i^x S_j^x + S_i^y S_j^y \right) \right. \\ \left. + \sum_{\langle i,j\rangle_2} \left(J_{2zz} S_i^z S_j^z + J_{2xy} \left(S_i^x S_j^x + S_i^y S_j^y \right) \right) - h \sum_i S_i^z . \right.$$

The corresponding lattice can be seen in Fig. 1. Using only the black colored terms, one would get the Ising model. Including the red term introduces a homogeneous magnetic field inside the solid. The blue terms introduce the quantum character of the system.

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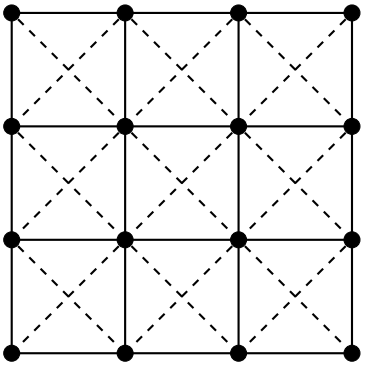


Figure 1: $J_1 - J_2$ square lattice. Solid lines correspond to coupling J_1 and dashed lines to coupling J_2.

Notice that the Hamiltonian preserves the scalar product structure of the Spin, so that we have:

$$[\mathcal{H}, S^z_{tot}] = 0 \quad \text{with} \quad S^z_{tot} = \sum_i S^z_i$$

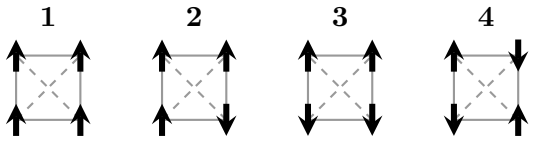
Therefore, the magnetic field couples to a conserved quantity. Our first goal is to identify the parameter regime in which the system is frustrated and to describe the ground-state manifold in the Ising limit. Next, we compute ground-state energy corrections via standard perturbation theory in J_{1xy} and J_{2xy} to see whether the degeneracy is lifted. We then use perturbation theory again to obtain the 1-magnon excitations above the plateau. The result will be valid for any spin S. In the second part of the analysis, we perform a spin-wave calculation (assuming $S \gg 1$) to derive the magnon dispersion relation exactly in J_{1xy} and J_{2xy}. Finally, we compare the two sets of results. A similar analysis was already done in [1] for a triangular lattice and we will take this paper as a guide to analyze this system.

I.1 Ground State in Ising Limit

Let's search for possible ground states in this system. We start by analyzing a single plaquette. If we find a configuration that can be globally expanded, e.g. there emerges a rule which can be satisfied on each plaquette at the same time, then we have found a ground state of the system because

$$\min\{E_G\} = \min\{\sum_{i\in\square} E_i\} \geq \sum_{i\in\square} \min\{E_i\},$$

the sum goes over each square, and E_i is the energy each square contributes. Notice that the energy of a square has to be calculated with care, since we want to avoid double-counting. The edges of the squares are shared so that new coupling constants $\tilde{J}_{1zz} = J_{1zz}/2$, $\tilde{J}_{2zz} = J_{2zz}$ and $\tilde{h} = h/4$ are used. For simplicity, let's start with the spin 1/2 case. How many states are on one square? We have four sites with each site having two different spins and four mirroring axes, so that $Z = 2^4/4 = 4$ per plaquette.



1:

$$E(++++) = \widetilde{J}_1 \; + \; \frac{\widetilde{J}_2}{2} \; - \; 2\,\widetilde{h}$$

2:

$$E(+++-) = -\widetilde{h}$$

3:

$$E(++--) = -\frac{\widetilde{J}_2}{2}$$

4:

$$E(+-+-) = -\widetilde{J}_1 \; + \; \frac{\widetilde{J}_2}{2}$$

Figure 2: Four possible plaquette configurations (top row) and their energies (bottom list).

The different configurations are shown in Fig. 2. The first configuration is a purely ferromagnetic state with no frustration. The fourth configuration is a Néel state. The third configuration forms stripe lines and therefore also has no frustration. The second configuration, however, is interesting in terms of frustration: it can be extended globally, but its extension is not unique. Hence, there is frustration in the 1/2 magnetisation plateau. The parameter range for which this is the ground state is:

$$\left.\begin{aligned} -\tilde{h} &< \tilde{J}_1 + \frac{\tilde{J}_2}{2} - 2\tilde{h} \\ -\tilde{h} &< -\tilde{J}_1 + \frac{\tilde{J}_2}{2} \\ -\tilde{h} &< -\frac{\tilde{J}_2}{2} \end{aligned}\right\} \implies \frac{\tilde{J}_1}{2} - \frac{\tilde{J}_2}{4} < \tilde{h} < \frac{\tilde{J}_1}{2} + \frac{\tilde{J}_2}{4} \ \wedge \ \ \tilde{J}_1 > \tilde{J}_2 > 0$$

From now on, we will work in the parameter range where this configuration is the ground state. For a single plaquette, the ground state is denoted as a $(+++-)$-state, where $+$ stands for spin up and $-$ for spin down. The simplest realization of this pattern is on a 2×2 grid, which admits four ground states:

$$\begin{matrix} -+ & +- \\ ++ & ++ \end{matrix} \qquad \begin{matrix} ++ & ++ \\ -+ & +- \end{matrix}$$

Figure 3: $\frac{1}{2}$-magnetization ground states on a 2x2 grid.

For the 3x3 case, there are significantly more states. To keep track of them, we introduce a notion of symmetry via the translation operator $\mathcal{T}_i^{\mathrm{R/C}}$, which essentially exchanges the spins on a row or a column. We call it the translation operator since it also looks like shifting the antiferromagnetic line up one spot. In Figure 4, this concept is shown on a 3x3 lattice. Since we are working with the ground state manifold, we denote a ground state with $|i\rangle_g$.

$$\begin{matrix} +++ \\ +-+ \\ +++ \end{matrix} = |1\rangle_g\,; \quad \mathcal{T}_2^{\mathrm{R}}\left(|1\rangle_g\right) = \begin{matrix} +++ \\ -+- \\ +++ \end{matrix}$$

$$\begin{matrix} -+- \\ +++ \\ -+- \end{matrix} = |2\rangle_g\,; \quad \mathcal{T}_1^{\mathrm{R}}\mathcal{T}_3^{\mathrm{R}}\left(|2\rangle_g\right) = \begin{matrix} +-+ \\ +++ \\ +-+ \end{matrix}; \mathcal{T}_3^{\mathrm{R}}\left(|2\rangle_g\right) = \begin{matrix} -+- \\ +++ \\ +-+ \end{matrix}; \quad \mathcal{T}_1^{\mathrm{R}}\left(|2\rangle_g\right) = \begin{matrix} +-+ \\ +++ \\ -+- \end{matrix}$$

$$\begin{matrix} +++ \\ +-+ \\ +++ \end{matrix} = |1\rangle_g\,; \quad \mathcal{T}_2^{\mathrm{C}}\left(|1\rangle_g\right) = \begin{matrix} +-+ \\ +++ \\ +-+ \end{matrix}$$

$$\begin{matrix} -+- \\ +++ \\ -+- \end{matrix} = |2\rangle_g\,; \quad \mathcal{T}_1^{\mathrm{C}}\left(|2\rangle_g\right) = \begin{matrix} ++- \\ -++ \\ ++- \end{matrix}; \quad \mathcal{T}_3^{\mathrm{C}}\left(|2\rangle_g\right) = \begin{matrix} -++ \\ ++- \\ -++ \end{matrix}; \quad \mathcal{T}_1^{\mathrm{C}}\mathcal{T}_3^{\mathrm{C}}\left(|2\rangle_g\right) = \begin{matrix} +++ \\ -+- \\ +++ \end{matrix}$$

Figure 4: $\frac{1}{2}$-magnetization ground states on a 3x3 grid.

As we can see, by applying the translation operator on two distinct ground states, one can recover the whole ground state manifold. Notice three things:

1. $\left(\mathcal{T}_i^{R/C}\right)^2 = \mathbf{1}$, it is an involution.
2. The ground state manifold is not uniquely defined via these operators, see Fig. 5.
3. Two consecutive shifts of row and column are not allowed, since then the $(+++-)$-state for at least one plaquette is going to be violated.

Even though we have no one-to-one mapping, we can give an upper bound for the number of states Z. Without proof, we assume that in general one needs two reference states from which one can reconstruct all other states. Also, it doesn't matter if we have an even or uneven lattice since we are constructing an upper

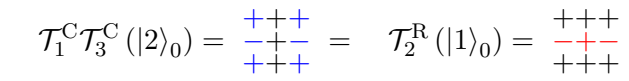


Figure 5: Double counting via the translation operators of the ground-state manifold.

bound. So let's assume it is even. If L is the length of one side of the square, one has $2 \cdot 2^{L/2}$ options for the row shifts and column shifts respectively, so that:

$$\begin{aligned} Z &\leq (2 \cdot 2^{L/2} + 2 \cdot 2^{L/2}) = 4 \cdot 2^{L/2} \\ \Rightarrow S_N &= \frac{1}{N} \ln(Z) \leq \frac{1}{N} \left(\frac{L}{2} \ln(2) + \ln(4) \right) \to 0 \quad \text{for } N \to \infty, N \propto L^2 \end{aligned}$$

Therefore, the system has no residual entropy.

For further analysis, it doesn't matter if we shift the rows or columns since we can shift only one of them and can't mix the two operations. The states are connected via symmetry operations of the Hamiltonian, so if we find a lift in the degeneracy by shifting the rows, for example, we will find the same lift in the states created by shifting the columns. Therefore, for further analysis, we will drop the superscript C/R on the translation operator. This means that for an infinite grid, our ground-state manifold can be parametrized in the fashion shown in Fig. 6.

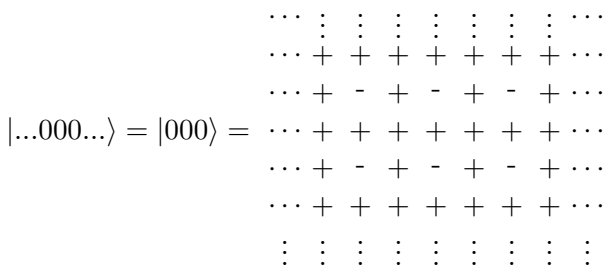
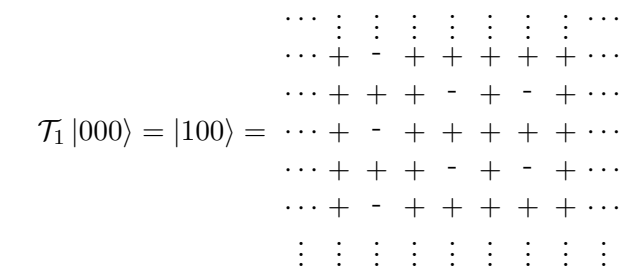


Figure 6: Ground-state with no shifts in the 1/2 magnetization plateau.

The rest of the relevant ground space can be recovered by applying shifts on each second row or not, which can be mapped onto binary numbers:



Let's now determine the energy of the ground state. For that, we wish to make a statement like:

$$E_G = E_{(}++++-) \cdot \#squares$$

The difficulty here is to count the squares. My proposition for this would be

$$E_G = E_{(}++++-) \cdot \#squares = -\tilde{h}(\sqrt{N} - 1)^2 \approx -\tilde{h} \cdot N$$

where we perform a rather naive counting of the possible plaquettes on a finite grid. One must be careful because the coupling constants have been normalized assuming an infinite grid; here, we neglect edge and corner effects in the hope that any residual terms vanish in the limit $N \to \infty$. This concludes our study of

the Ising ground state. In the next section, we proceed to analyze the order-by-disorder phenomenon via perturbation theory.

II. Order by Disorder via Perturbation Theory

We have now established a ground state manifold for our square lattice in the Ising limit. But we want to study the full quantum model. Therefore, we will introduce perturbation theory on the ground state manifold to see if the degeneracy is lifted. We start by introducing the J_{1xy} coupling for the nearest neighbours and assume an infinite grid. The perturbation then is:

$$\mathcal{V} = \sum_{\langle i,j\rangle_1} J_{1xy}\left(S_i^x S_j^x + S_i^y S_j^y\right) = \sum_{\langle i,j\rangle_1} \frac{J_{1xy}}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$$

The subscript in $\langle i,j\rangle_1$ denotes nearest neighbour (a subscript 2 would mean next to neighbour). The last expression indicates that the perturbation allows hopping of a down-spin ($-$) to nearest neighbours. Exchanges of two up-spins ($+$) or two down-spins are not allowed since we are working with spin 1/2, and those operators would annihilate the state. Interestingly, one finds:

$$\langle i|_g^{(0)}\ \mathcal{V}\ |j\rangle_g^{(0)} \ = \ 0,$$

since a single hopp takes the system out of the ground-state manifold. The superscript (0) denotes states in the Ising limit. Furthermore,

$$\sum_{m\neq g} \langle i|_g^{(0)}\ \mathcal{V}\ |\Psi_m\rangle^{(0)}\ \langle\Psi_m|^{(0)}\ \mathcal{V}\ |j\rangle_g^{(0)} \ \propto\ \delta_{ij},$$

and all higher-order terms are diagonal, since it would require an infinite number of hops to change from one ground state to another (i.e., to move an entire antiferromagnetic line). The corresponding energy correction then starts at second order and is already diagonal,

$$E_{n,g} = E_g^{(0)} + J_{1xy}^2 \sum_{m\neq g} \frac{|\,\langle\Psi|_m^{(0)}\,\mathcal{V}\,|n\rangle_g^{(0)}\,|^2}{(E_m^{(0)} - E_g^{(0)})} + \mathcal{O}(J_{1xy}^4).$$

Since only nearest neighbours (and next-nearest neighbours) are involved, the resulting ground-state restriction is 2-periodic, meaning that either $|01010\ldots\rangle$ or $|00000\ldots\rangle$ will be the ground state. Starting from $|00000\ldots\rangle$ and switching on the perturbations □–coupling (J_{1xy}) and ×–coupling (J_{2xy}), which hoppings are now allowed? We can hopp back and forth, so a few intermediate states are illustrated in Fig. 7; the others can be obtained by mirroring around the corresponding symmetry axis, and those symmetry factors have to be included in the calculation.

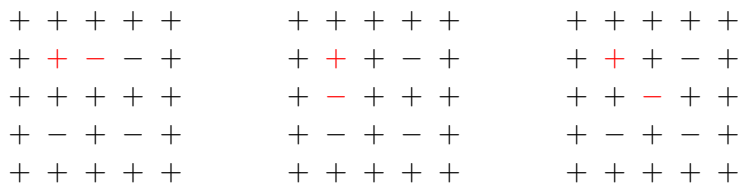


Figure 7: Intermediate states used for second order perturbation theory for the energy correction of the ground-state $|00000...\rangle$(Spin 1/2).

The corresponding matrix element for such an excited state looks like

$$\langle\Psi|_m^{(0)}\,\mathcal{V}\,|n\rangle_g^{(0)} = \sum_{\langle i,j\rangle_1}\frac{J_{1xy}}{2}\,\langle\Psi|_m^{(0)}\left(S_i^+S_j^- + S_i^-S_j^+\right)|n\rangle_g^{(0)} = \frac{J_{1xy}}{2}$$

$$\text{since}\quad S^+|\downarrow\rangle = |\uparrow\rangle \quad \text{no other factors occur.}$$
$$S^-|\uparrow\rangle = |\downarrow\rangle$$

Nicely, we don't have to calculate overlap integrals since the excited Ising states after the action of the potential are either orthogonal or coincide. For the spin 1/2 case, we also don't get Spin-factors. The only careful thing one has to pay attention to is the counting of how many such states exist. Let's look at a single $-$, there are $N/4$ of those so that we define:

$$\frac{N}{4}E_i = E$$

There are four hopping terms regarding the $\square$-coupling, 2 (=symmetry factor) going to exchange up and down, and two sidewards; therefor,e the energy change per site is:

$$\begin{aligned}\gamma(E) :&= \frac{1}{(E-E_g)} \quad E_g = -\tilde{h}N\\ E_{\square,i}(|00\rangle) &= 2\frac{J_{1xy}^2}{4}\gamma\left(-\tilde{h}(N-4)+2E(++++)+2E(++--)\right)\\ &\quad + 2\frac{J_{1xy}^2}{4}\gamma\left(-\tilde{h}(N-4)+2E(++++)+2E(++--)\right)\\ &= \frac{J_{1xy}^2}{2\tilde{J}_1}\end{aligned}$$

Where the argument of γ is the energy of the intermediate state, for which one has to check the plaquettes violating the $(+++-)$-rule. An important fact regarding the result is that it is independent of h. A dependence for example $\propto 1/h$, would be strange, since this parameter is coupled to a conserved quantity and therefore the energy shouldn't vary if the perturbation is turned on. A similar thing holds for the $\times$-coupling (J_{2xy}). Four terms are contributing and all are the same due to symmetry:

$$\begin{aligned}E_{\times,i}(|00\rangle) &= 4\frac{J_{2xy}^2}{4}\gamma\left(-2\tilde{h}(N-6)+3E(++++)+3E(+-+-)\right)\\ &= \frac{J_{2xy}^2}{3\tilde{J}_2}\end{aligned}$$

Therefore:

$$E_i(|00\rangle) = E_{g,i}^{(0)} + \frac{J_{1xy}^2}{2\tilde{J}_1} + \frac{J_{2xy}^2}{3\tilde{J}_2} \quad \text{with} \quad E_{g,i}^{(0)} = \frac{4}{N}E_g^{(0)}$$

Let's look at the alternating $|01\rangle$ state. The intermediate excited states are shown in Fig. 8

$$\begin{array}{ccccc}+&+&+&-&+\\+&+&-&+&+\\+&+&+&-&+\\+&-&+&+&+\\+&+&+&-&+\end{array}\qquad\begin{array}{ccccc}+&+&+&-&+\\+&+&+&+&+\\+&-&+&-&+\\+&-&+&+&+\\+&+&+&-&+\end{array}\qquad\begin{array}{ccccc}+&+&+&-&+\\+&+&+&+&+\\+&+&-&-&+\\+&-&+&+&+\\+&+&+&-&+\end{array}$$

Figure 8: Intermediate states used for second order perturbation theory for the energy correction of the ground-state $|01010...\rangle$ (Spin 1/2).

The exact same steps as for the $|00000...\rangle$-state are done resulting in:

$$E_{\square,i}(|01\rangle) = \frac{J_{1xy}^2}{4\tilde{J}_2} + \frac{J_{1xy}^2}{4\tilde{J}_1}$$
$$E_{\times,i}(|01\rangle) = \frac{J_{2xy}^2}{2\tilde{J}_1 + \tilde{J}_2}$$

So that

$$E_i(|01\rangle) = E_{g,i}^{(0)} + \frac{J_{1xy}^2}{4\tilde{J}_2} + \frac{J_{1xy}^2}{4\tilde{J}_1} + \frac{J_{2xy}^2}{2\tilde{J}_1 + \tilde{J}_2}$$

We have found the energy corrections up to the first non-vanishing order in perturbation theory. By inspecting the sign of ΔE, one determines which state is the ground state:

$$E_i(|00\rangle) - E_i(|01\rangle) = J_{1xy}^2 \left(\frac{1}{4}\Big(\frac{1}{\tilde{J}_1} - \frac{1}{\tilde{J}_2}\Big) + R^2 \Big(\frac{1}{3\,\tilde{J}_2} - \frac{1}{2\,\tilde{J}_1 + \tilde{J}_2}\Big)\right) \quad \text{with} \quad R = \frac{J_{2xy}}{J_{1xy}}.$$

As a matter of fact, the phase transition at $\Delta E = 0$ defines a line in the phase diagram:

$$0 = \Delta E \implies \tilde{J}_2 = \tilde{J}_1\Big(\tfrac{8}{3}\,R^2 - 2\Big).$$

Keeping the constraints for a possible transition due to the change of the Ising parameters restricts R to:

$$R_{\min} = \sqrt{\frac{6}{8}}, \quad R_{\max} = \sqrt{\frac{9}{8}}.$$

The corresponding phase diagram as a function of the parameters is given in Fig. 9.

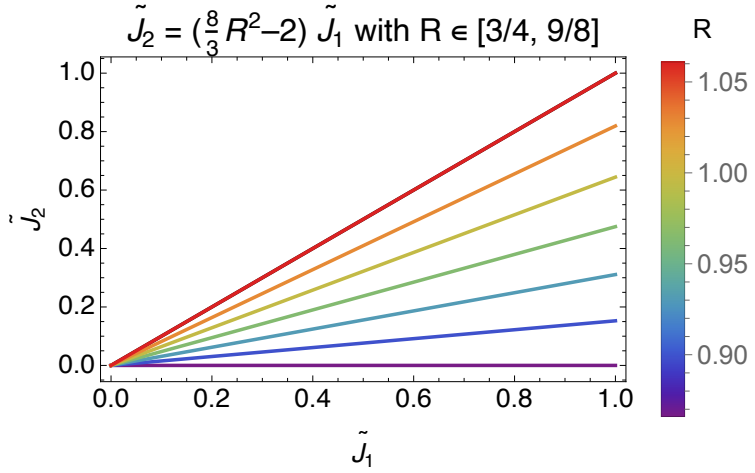


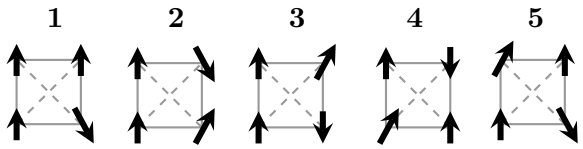
Figure 9: Phasediagramm of groundstatemanifold. The colorful lines indicate a phase transition between the $|00000...\rangle$ and the $|01010...\rangle$-state. The upper triangle is a forbidden parameter region.

II.1 General Spin Perturbation Theory

We are now going to redo the calculation, but for a general spin. I believe that the ground state has a similar pattern ($\uparrow\uparrow\uparrow\downarrow$) with energy:

$$E_g = -\tilde{h}SN$$

A formal proof still needs to be created. We again start with degenerate perturbation theory. For that, we first need a few new Ising energies from our new states that can arise seen in Fig. 11:



1:

$$E(\uparrow\uparrow\uparrow\searrow) = 2\,\widetilde{J}_1 S + \widetilde{J}_2 S - \widetilde{h}\,(2S+1)$$

2:

$$E(\uparrow\uparrow\searrow\nearrow) = \widetilde{J}_1(2S-1) - \widetilde{h}\,(2S)$$

3:

$$E(\uparrow\uparrow\nearrow\downarrow) = -\widetilde{J}_2 S - \widetilde{h}\,(2S-1)$$

4:

$$E(\uparrow\downarrow\uparrow\nearrow) = -2\,\widetilde{J}_1 S + \widetilde{J}_2 S - \widetilde{h}\,(2S-1)$$

5:

$$E(\uparrow\searrow\uparrow\nearrow) = \widetilde{J}_2(2S-1) - 2S\,\widetilde{h}$$

Figure 10: Possible configurations with different energies for general spin in the Ising limit.

We recover the old results if $S = \frac{1}{2}$ is inserted. Let's calculate the new matrix elements since now we get factors due to the larger spin. The general formula is:

$$S^+ |m\rangle = \sqrt{S(S+1) - m(m+1)}\,|m+1\rangle$$
$$S^- |m\rangle = \sqrt{S(S+1) - m(m-1)}\,|m-1\rangle$$

In our case S^- will always act on $|S\rangle$ and S^+ will always act on $|-S\rangle$ so that:

$$S^+ |-S\rangle = \sqrt{2S}\,|-S+1\rangle$$
$$S^- |S\rangle = \sqrt{2S}\,|S-1\rangle$$

So that any matrix element in the perturbation theory becomes:

$$\langle\Psi|_m^{(0)}\,\mathcal{V}\,|n\rangle_g^{(0)} = 2S\frac{J_{xy}}{2} \quad \Rightarrow \quad |\,\langle\Psi|_m^{(0)}\,\mathcal{V}\,|n\rangle_g^{(0)}\,|^2 = S^2 J_{xy}$$

We again start with the $|00\rangle$ state and repeat the calculation done in the previous section. The intermediate states can be seen in Fig. 11. This results in

$$E_{\square,i}(|00\rangle) = \frac{4J_{1xy}^2 S^2}{\widetilde{J}_1(8S-2)}$$
$$E_{\times,i}(|00\rangle) = \frac{4J_{2xy}^2 S^2}{\widetilde{J}_2(8S-1)}$$

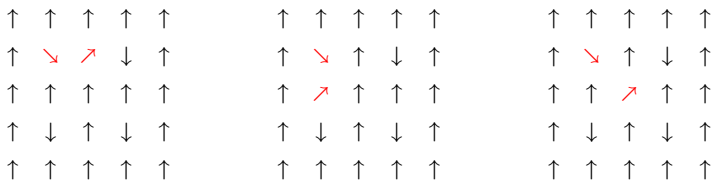


Figure 11: Intermediate states used for second order perturbation theory for the energy correction of the ground-state $|00000...\rangle$(general Spin).

So that we get the energy correction:

$$E_i(|00\rangle) = E^{(0)}_{g,i} + \frac{J^2_{1xy}S}{\tilde{J}_1(2-\frac{1}{2S})} + \frac{2J^2_{2xy}S}{3\tilde{J}_2}$$

Now we do the same thing for the $|01\rangle$ ground-state. The intermediate states can be seen in Fig. 12.

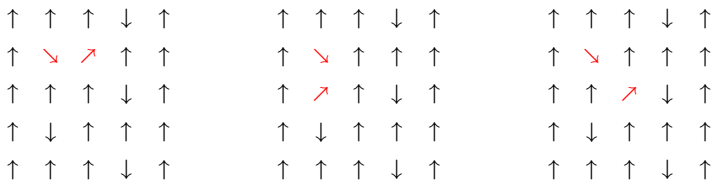


Figure 12: Intermediate states used for second order perturbation theory for the energy correction of the ground-state $|01010...\rangle$(general Spin).

This results in:

$$E_{\square,i}(|01\rangle) = \frac{2J^2_{1xy}S^2}{\tilde{J}_1(4S-2)+4\tilde{J}_2S} + \frac{2J^2_{1xy}S^2}{\tilde{J}_1(8S-2)}$$
$$E_{\times,i}(|01\rangle) = \frac{4J^2_{2xy}S^2}{\tilde{J}_1 4S + \tilde{J}_2(4S-1)}$$

So that we get the energy correction:

$$E_i(|01\rangle) = E^{(0)}_{g,i} + \frac{J^2_{1xy}S}{\tilde{J}_1(2-\frac{1}{S})+2\tilde{J}_2} + \frac{J^2_{1xy}S}{\tilde{J}_1(4-\frac{1}{S})} + \frac{J^2_{2xy}S}{\tilde{J}_1+\tilde{J}_2(1-\frac{1}{4S})}$$

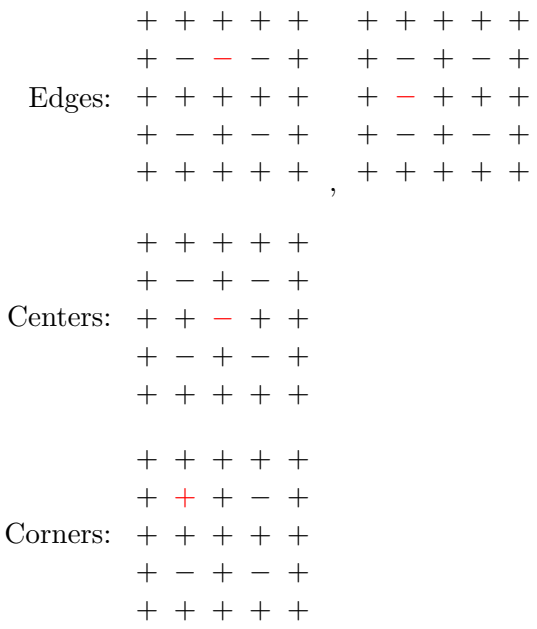
The difference is then:

$$E_i(|00\rangle) - E_i(|01\rangle) = J^2_{1xy}S\left(\frac{1}{\tilde{J}_1(2-\frac{1}{2S})} - \frac{1}{\tilde{J}_1(2-\frac{1}{S})+2\tilde{J}_2} - \frac{1}{\tilde{J}_1(4-\frac{1}{S})}\right)$$
$$+ J^2_{2xy}S\left(\frac{1}{\tilde{J}_2(2-\frac{1}{4S})} - \frac{1}{\tilde{J}_1+\tilde{J}_2(1-\frac{1}{4S})}\right)$$

If one inserts $S=\frac{1}{2}$, one gets the same result as in the previous chapter!

III. 1-Magnons via Perturbation Theory

We expect that the lowest excitations that can occur in our system are flips of single spins, 1-magnon states. A proof still needs to be done. Let's stick to the $|00\rangle$-ground-state in spin 1/2 first. In our Ising Model, we can have three different kinds of 1 Magnon excitations, which can be seen in Fig. 13.



with Energy

$$E_{Ed} = 4E(++--) + (N-4)E(+++-)$$
$$= -N\tilde{h} + 2\tilde{h} - 2\tilde{J}_2$$

with Energy

$$E_{Ce} = 4E(+-+-) + (N-4)E(+++-)$$
$$= 2\tilde{J}_2 - 4\tilde{J}_1 + 4\tilde{h} - N\tilde{h}$$

with Energy

$$E_{Co} = 4E(+++\!+) + (N-4)E(+++-)$$
$$= 4\tilde{J}_1 + 2\tilde{J}_2 - 4\tilde{h} - N\tilde{h}$$

Figure 13: 1-Magnon states for spin 1/2 of the $|00\rangle$ ground-state.

III.1 Edge-Magnons:

We now have to do degenerate perturbation theory where the matrix $\langle i|^{(0)}_{Ed}\,\mathcal{V}\,|j\rangle^{(0)}_{Ed}$ is not diagonal, so that we have to diagonalize this matrix to get the energies. We note that the interaction is split into nearest and next to nearest neighbor terms $\mathcal{V} = \mathcal{V}_\square + \mathcal{V}_\times$, and that in first order there is no nearest neighbor coupling, the next magnon is one diagonal distanced. Therefore, we investigate the Matrix:

$$\langle\alpha|^{(0)}_{Ed}\,\mathcal{V}_\times\,|\beta\rangle^{(0)}_{Ed} = \frac{\tilde{J}_{2xy}}{2}\sum_{\langle i,j\rangle_2}\langle\alpha|^{(0)}_{Ed}\,S^+_iS^-_j + S^+_jS^-_i\,|\beta\rangle^{(0)}_{Ed}$$

The situation can be seen in Fig. 14.

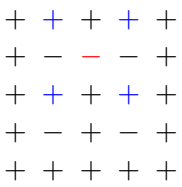


Figure 14: Edge-Magnon for spin 1/2 (flip is denoted red) and potential hopping to neighbouring Edge-Magnons (blue)

so that we get:

$$\langle\alpha|^{(0)}_{Ed}\,\mathcal{V}\,|\beta\rangle^{(0)}_{Ed} = \frac{\tilde{J}_{2xy}}{2}\sum_{\vec{\tau}}\delta\left(\beta - (\alpha + \vec{\tau})\right)$$

With τ being the diagonal vectors to the next-to-nearest neighbour sites. Let's now introduce a change of basis to diagonalise this matrix via the Edge-Magnon states:

$$\left|\vec{k}\right\rangle_{Ed} := \frac{1}{N}\sum_i e^{-i\vec{k}\vec{R}_i}\,|i\rangle_{Ed} \quad ,\vec{k} = \begin{pmatrix}k_x\\k_y\end{pmatrix}$$

So that:

$$\begin{aligned}\left\langle \vec{k}\right|_{Ed}\mathcal{V}\left|\vec{k}'\right\rangle_{Ed} &= \frac{1}{N^2}\sum_i\sum_j e^{-i\vec{k}\vec{R}_i}e^{i\vec{k}'\vec{R}_j}\left\langle i\right|_{Co}\mathcal{V}\left|j\right\rangle_{Ed}\\ &= \frac{\tilde{J}_{2xy}}{2N^2}\sum_{\vec{\tau}}\sum_i\sum_j e^{-i\vec{k}\vec{R}_i}e^{i\vec{k}'\vec{R}_j}\delta\left(j-(i+\vec{\tau})\right)\\ &= \frac{\tilde{J}_{2xy}}{2N^2}\sum_{\vec{\tau}}\sum_i e^{-i\vec{R}_i(\vec{k}-\vec{k}')}e^{i\vec{k}'\vec{\tau}}\\ &= \frac{\tilde{J}_{2xy}}{2}\delta\left(\vec{k}-\vec{k}'\right)\sum_{\vec{\tau}}e^{i\vec{k}\vec{\tau}}\end{aligned}$$

the vectors τ by a given lattice constant a are:

$$a\begin{pmatrix}1\\1\end{pmatrix}, a\begin{pmatrix}1\\-1\end{pmatrix}, a\begin{pmatrix}-1\\1\end{pmatrix}, a\begin{pmatrix}-1\\-1\end{pmatrix}$$

So that

$$E^{(1)}_{Ed}(\vec{k}) = \tilde{J}_{2xy}\left(\cos\left(a(k_x+k_y)\right)+\cos\left(a(k_x-k_y)\right)\right)$$

Changing to general Spin, will just get a Factor $2S$-plopping outside due to the matrix element, so that:

$$E^{(1)}_{Ed}(\vec{k}) = \tilde{J}_{2xy}2S\left(\cos\left(a(k_x+k_y)\right)+\cos\left(a(k_x-k_y)\right)\right)$$

III.2 Center-Magnons

Regarding the Center-Magnons the first order perturbation theory vanishes, since we need two hopps to get to another Center-Magnon:

$$\left\langle\alpha\right|^{(0)}_{Ce}\mathcal{V}\left|\beta\right\rangle^{(0)}_{Ce} = 0$$

and we have to go straight to second order perturbation theory. The matrix we have to diagonalise is of the form:

$$\begin{aligned}M^{\alpha\beta} &= \sum_m \frac{\left\langle\alpha\right|_{Ce}\mathcal{V}\left|\psi\right\rangle_m\left\langle\psi\right|_m\mathcal{V}\left|\beta\right\rangle_{Ce}}{E_{Ce}-E_m}\\ &= \sum_m\Big(\frac{\left\langle\alpha\right|_{Ce}\mathcal{V}_\square\left|\psi\right\rangle_m\left\langle\psi\right|_m\mathcal{V}_\square\left|\beta\right\rangle_{Ce}}{E_{Ce}-E_m}+\frac{\left\langle\alpha\right|_{Ce}\mathcal{V}_\square\left|\psi\right\rangle_m\left\langle\psi\right|_m\mathcal{V}_\times\left|\beta\right\rangle_{Ce}}{E_{Ce}-E_m}\\ &+\frac{\left\langle\alpha\right|_{Ce}\mathcal{V}_\times\left|\psi\right\rangle_m\left\langle\psi\right|_m\mathcal{V}_\square\left|\beta\right\rangle_{Ce}}{E_{Ce}-E_m}+\frac{\left\langle\alpha\right|_{Ce}\mathcal{V}_\times\left|\psi\right\rangle_m\left\langle\psi\right|_m\mathcal{V}_\times\left|\beta\right\rangle_{Ce}}{E_{Ce}-E_m}\Big)\\ &= M_1^{\alpha\beta}+M_2^{\alpha\beta}+M_3^{\alpha\beta}+M_4^{\alpha\beta}\end{aligned}$$

The cross terms $M_2^{\alpha\beta}$, $M_3^{\alpha\beta}$ are zero since there is no possibility to jump to another Center-Magnon. Let's have a look at $M_1^{\alpha\beta}$. We can now jump twice, first to any intermediate state (which is not a Center-Magnon) and then to a Center-Magnon. Since we are now only using nearest neighbours, we have four intermediate states, which all look similar, and are Edge-Magnons:

$$\begin{array}{ccccc}+&+&+&+&+\\+&-&+&-&+\\+&+&+&-&+\\+&-&+&-&+\\+&+&+&+&+\end{array}$$

Therefore, we have:

$$M_1^{\alpha\beta} = \sum_{\vec{\tau}} \frac{\langle\alpha|_{Ce}\,\mathcal{V}_\square\,|\alpha+\vec{\tau}\rangle_{Ed}\,\langle\alpha+\vec{\tau}|_{Ed}\,\mathcal{V}_\square\,|\beta\rangle_{Ce}}{E_{Ce}-E_{Ed}}$$

Where $\vec{\tau}$ are vectors pointing to the nearest neighbours. The final states can be either hopping back to the Center-Magnon α or to the neighbouring Center-Magnon, which is $2\vec{\tau}$ distant. Therefore, we have:

$$M_1^{\alpha\beta} = \frac{1}{E_{Ce}-E_{Ed}}\left[C_{\text{Self}}\,\delta(\beta-\alpha) + \sum_{\vec{\tau}}\delta(\beta-(\alpha+2\vec{\tau}))\right]$$

For the following calculations, we will ignore the self-energy term, as it is cumbersome to compute. Many additional terms contribute to it, such as hopping back and forth elsewhere on the lattice, so we introduce an unknown constant $\mathcal{C}_{\text{self}}$. Since it is a diagonal term, it will just add a constant to the dispersion relation and will not contribute to a $\vec{k}$ dependent factor. Let us now proceed to diagonalise the matrix. Once again, we perform a change of basis to the Center-Magnon states:

$$\left|\vec{k}\right\rangle_{Ce} := \frac{1}{N}\sum_i e^{-i\vec{k}\vec{R}_i}\,|i\rangle_{Ce} \quad ,\vec{k} = \begin{pmatrix}k_x\\k_y\end{pmatrix}$$

So that:

$$\begin{aligned}
M_1^{\alpha\beta} - \delta_{\alpha\beta}\,\tilde{C}_{\text{Self},\square} &= \sum_m \frac{\left\langle\vec{k}\right|_{Ce}\mathcal{V}_\square\,|\psi\rangle_m\,\langle\psi|_m\,\mathcal{V}_\square\left|\vec{k}'\right\rangle_{Ce}}{E_{Ce}-E_m}\\
&= \frac{1}{N^2}\sum_i\sum_j e^{-i\vec{k}\vec{R}_i}e^{i\vec{k}\vec{R}_j}\sum_m\frac{\langle i|_{Ce}\,\mathcal{V}_\square\,|\psi\rangle_m\,\langle\psi|_m\,\mathcal{V}_\square\,|j\rangle_{Ce}}{E_{Ce}-E_m}\\
&= \frac{1}{N^2}\sum_i\sum_j e^{-i\vec{k}\vec{R}_i}e^{i\vec{k}\vec{R}_j}\frac{1}{E_{Ce}-E_{Co}}\left[\sum_{\vec{\tau}}\delta(j-(i+2\vec{\tau}))\right]\\
&= \frac{\delta(\vec{k}-\vec{k}')}{E_{Ce}-E_{Co}}\left(\sum_{\vec{\tau}}e^{i\vec{k}\vec{\tau}}\right)
\end{aligned}$$

With the same $\vec{\tau}$ being:

$$a\begin{pmatrix}1\\0\end{pmatrix}, a\begin{pmatrix}0\\-1\end{pmatrix}, a\begin{pmatrix}-1\\0\end{pmatrix}, a\begin{pmatrix}0\\1\end{pmatrix}$$

Resulting in:

$$E^{(1)}_{Ce,\square}(\vec{k}) - E^{(1)}_{Ce,self,\square} = \frac{\tilde{J}^2_{1xy}}{E_{Ce}-E_{Ed}}\left(\cos(2ak_x)+\cos(2ak_y)\right)$$

The same procedure must now be applied to the $\times$ interaction. Here, a magnon can hop completely diagonally up along a cross or first up and then down along another cross. In this case, two intermediate states are reached, which are three-magnon states. Their energies are denoted by $E_{3,\diagup}$ and $E_{3,\hat{}}$. The matrix in position space is given by:

$$M_1^{\alpha\beta} - \delta_{\alpha\beta}\,\tilde{C}_{\text{Self},\times} = \frac{1}{E_{Ce}-E_{3,\diagup}}\sum_{\vec{\tau}}\delta(\beta-(\alpha+2\vec{\tau})) + \frac{1}{E_{Ce}-E_{3,\hat{}}}\sum_{\vec{\tau}_{1,2}}\delta(\beta-(\alpha+\tau_1+\tau_2))$$

This results in:

$$\begin{aligned} E^{(2)}_{Ce}(\vec{k}) - E^{(2)}_{Ce,self} &= \frac{\tilde{J}^2_{1xy}}{E_{Ce} - E_{Ed}} \left(\cos\left(2ak_x\right) + \cos\left(2ak_y\right)\right) \\ &+ \frac{\tilde{J}^2_{2xy}}{E_{Ce} - E_{3,\nearrow}} \left(\cos\left(2a(k_x + k_y)\right) + \cos\left(2a(k_x - k_y)\right)\right) \\ &+ \frac{\tilde{J}^2_{2xy}}{E_{Ce} - E_{3,\hat{}}} \left(\cos\left(2ak_x\right) + \cos\left(2ak_y\right)\right) \end{aligned}$$

Let's calculate the energy fractions:

$$\begin{aligned} \frac{1}{E^{(0)}_{Ed} - E^{(0)}_{Ce}} &= \frac{1}{4(\tilde{J}_1 - \tilde{J}_2)} \\ \frac{1}{E_{Ce} - E_{3,\nearrow}} &= \frac{-1}{2\tilde{J}_2} \end{aligned}$$

For the spin 1/2 system we have $E_{3,\hat{}} = E_{3,\nearrow}$ Therefore, the energy corrections read:

$$\begin{aligned} E^{(2)}_{Ce}(\vec{k}) - E^{(2)}_{Ce,self} &= \frac{\tilde{J}^2_{1xy}}{4(\tilde{J}_2 - \tilde{J}_1)} \left(\cos\left(2ak_x\right) + \cos\left(2ak_y\right)\right) \\ &- \frac{\tilde{J}^2_{2xy}}{2\tilde{J}_2} \left(\cos\left(2a(k_x + k_y)\right) + \cos\left(2a(k_x - k_y)\right) + \cos\left(2ak_x\right) + \cos\left(2ak_y\right)\right) \end{aligned}$$

III.2.1 General Spin

For the general spin case, we have to calculate the general spin Energies of Center/Edge-Magnon and the two 3-Magnon intermediate states..

$$\begin{array}{ccccc} \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \uparrow & \nearrow & \uparrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \end{array} \qquad \begin{array}{ccccc} \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \nearrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \end{array}$$

$$\begin{aligned} E^{(0)}_{Ce} &= (N-4)E(\uparrow\uparrow\uparrow\downarrow) + 4E(\uparrow\downarrow\uparrow\nearrow) \\ &= 4\tilde{h} - 2\tilde{h}SN + 4\tilde{J}_2 S - 8\tilde{J}_1 S \end{aligned} \qquad \begin{aligned} E^{(0)}_{Ed} &= (N-4)E(\uparrow\uparrow\uparrow\downarrow) + 4E(\uparrow\uparrow\nearrow\downarrow) \\ &= 4\tilde{h} - 2\tilde{h}SN - 4\tilde{J}_2 S \end{aligned}$$

The energy denominators the evaluated to:

$$\begin{aligned} \frac{1}{E^{(0)}_{Ed} - E^{(0)}_{Ce}} &= \frac{1}{8S(\tilde{J}_1 - \tilde{J}_2)} \\ \frac{1}{E_{Ce} - E_{3,\hat{}}} &= \frac{1}{2\tilde{J}_2(1 - 4S)} \\ \frac{1}{E_{Ce} - E_{3,/}} &= \frac{1}{2\tilde{J}_2(1 - 4S)} \end{aligned}$$

By setting $S = 1/2$ and the rescaling of the coupling constants, it coincides with the non general case!

Inserting those new denominators results in:

$$E^{(1)}_{Ce}(\vec{k}) - E^{(1)}_{Ce,self} = \frac{\tilde{J}^2_{1xy}S}{8(\tilde{J}_2 - \tilde{J}_1)}\left(\cos(2ak_x) + \cos(2ak_y)\right) + \frac{\tilde{J}^2_{2xy}S^2}{2\tilde{J}_2(1-4S)}\left(\cos(2a(k_x+k_y)) + \cos(2a(k_x-k_y)) + \cos(2ak_x) + \cos(2ak_y)\right)$$

IV. Spin-Wave Expansion

We start by defining 4 sublattices A;B;C;D. All are square lattices with twice the lattice constant. The A lattice sits on the Corners of the squares.

$$\begin{array}{ccccccc} & +^D & & +^C & & +^D & \\ +^B & & -^A & & +^B & & -^A \\ & +^D & & +^C & & +^D & \\ +^B & & -^A & & +^B & & -^A \\ & +^D & & +^C & & +^D & \end{array}$$

We apply a rotation to the A lattice, so that we have no bosons in our ground-state by introducing a unitary transformation. Solving the regular Hamiltonian system is equivalent to solving a rotated one:

$$\mathcal{H}|\psi\rangle = E|\psi\rangle \Leftrightarrow \left(U^{-1}\mathcal{H}U\right)U^{-1}|\psi\rangle = EU^{-1}|\psi\rangle \quad \Rightarrow \quad \tilde{\mathcal{H}} = U^{-1}\mathcal{H}U$$

We choose U as follows:

$$U = \bigotimes_{i\in A} U_i \quad \text{with} \quad U_i = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \sigma_x$$

That way we turned S^z around

$$\begin{aligned} U_i^\dagger S_i^z U_i &= -S_i^z \\ U_i^\dagger S_i^y U_i &= -S_i^y \\ U_i^\dagger S_i^x U &= S_i^x \end{aligned}$$

Inserting this and changing notation slightly: Vectors are normal letters, $\tilde{J}_{1zz} = J_1$, $\tilde{J}_{2zz} = J_2$

$$\begin{aligned} \mathcal{H} &= J_1 \sum_{<i,j>_1} S_i^z S_j^z + J_{1xy} \sum_{<i,j>_1} \left(S_i^x S_j^x + S_i^y S_j^y\right) \\ &+ J_2 \sum_{<i,j>_2} S_i^z S_j^z + J_{2xy} \sum_{<i,j>_2} \left(S_i^x S_j^x + S_i^y S_j^y\right) \\ &= J_1 \sum_{<i,j>_1 \in B,C,D} S_i^z S_j^z + \frac{J_{1xy}}{2} \sum_{<i,j>_1 \in B,C,D} \left(S_i^+ S_j^- + S_i^- S_j^+\right) \\ &- J_1 \sum_{i\in A} \sum_{j\in n.n.(i)} S_i^z S_j^z + J_{1xy} \sum_{i\in A} \sum_{j\in n.n.(i)} \left(S_i^x S_j^x - S_i^y S_j^y\right) \\ &+ J_2 \sum_{<i,j>_2 \in B,C,D} S_i^z S_j^z + \frac{J_{2xy}}{2} \sum_{<i,j>_2 \in B,C,D} \left(S_i^+ S_j^- + S_i^- S_j^+\right) \\ &- J_2 \sum_{i\in A} \sum_{j\in n.n.n.(i)} S_i^z S_j^z + J_{2xy} \sum_{i\in A} \sum_{j\in n.n.n.(i)} \left(S_i^x S_j^x - S_i^y S_j^y\right) \end{aligned}$$

With that we introduce a Hohlstein-Primakoff transformation:

$$\begin{aligned}
S_i^+ &= S_i^x + iS_i^y = \sqrt{2S - n_i}a_i \\
S_i^- &= S_i^x - iS_i^y = a_i^\dagger 2S - n_i \\
\Leftrightarrow \quad S_i^x &= \frac{1}{2}\left(\sqrt{2S - n_i}a_i + a_i^\dagger\sqrt{2S - n_i}\right) \\
S_i^y &= \frac{1}{2i}\left(\sqrt{2S - n_i}a_i - a^\dagger\sqrt{2S - n_i}\right) \\
S_i^z &= S - n_i, \quad n_i = a_i^\dagger a_i
\end{aligned}$$

Putting this in the Hamiltonian and neglecting $\mathcal{O}(a^2)$ terms gives:

$$\begin{aligned}
H_{LSWT} = &-\frac{1}{2}NSh - h\sum_{i\in B,C,D} n_i + h\sum_{i\in A} n_i \\
&+ \sum_{<i,j>_1\in B,C,D} (n_i + n_j)(-J_1 S) + J_{1xy}(a_i a_j^\dagger + a_i^\dagger a_j) \\
&+ \sum_{i\in A}\sum_{j\in n.n.(A)} J_1 S(n_i + n_j) + \frac{J_{1xy}}{2}S(a_i a_j + a_i^\dagger a_j^\dagger) \\
&+ \sum_{<i,j>_2\in B,C,D} (n_i + n_j)(-J_2 S) + J_{2xy}(a_i a_j^\dagger + a_i^\dagger a_j) \\
&+ \sum_{i\in A}\sum_{j\in n.n.n.(A)} J_2 S(n_i + n_j) + \frac{J_{2xy}}{2}S(a_i a_j + a_i^\dagger a_j^\dagger)
\end{aligned}$$

Now we are going to transform the sums to be local with the vectors:

$$\tau_1 \in \{\pm a\vec{e}_x, \pm a\vec{e}_y\} \quad \tau_2 \in \{\pm a(\vec{e}_x + \vec{e}_y), \pm a(\vec{e}_x - \vec{e}_y)\}$$

So that we get:

$$\begin{aligned}
&= -\frac{1}{2}NSh - h\sum_{i\in B,C,D} n_i + h\sum_{i\in A} n_i \\
&+ \sum_{i\in D}\sum_{\tau_1}(n_i + n_{i+\tau_1})(-J_1 S) + J_{1xy}(a_i a_{i+\tau_1}^\dagger + a_i^\dagger a_{i+\tau_1}) \\
&+ \sum_{i\in A}\sum_{\tau_1} J_1 S(n_i + n_{i+\tau_1}) + \frac{J_{1xy}}{2}S(a_i a_{i+\tau_1} + a_i^\dagger a_{i+\tau_1}^\dagger) \\
&+ \sum_{i\in D}\sum_{\tau_2}(n_i + n_{i+\tau_2})(-J_2 S) + J_{2xy}(a_i a_{i+\tau_2}^\dagger + a_i^\dagger a_{i+\tau_2}) \\
&+ \sum_{i\in A}\sum_{\tau_2} J_2 S(n_i + n_{i+\tau_2}) + \frac{J_{2xy}}{2}S(a_i a_{i+\tau_2} + a_i^\dagger a_{i+\tau_2}^\dagger) \\
&= -\frac{1}{2}NSh + h\left(\sum_{i\in A} n_i + \sum_{i\in B,C,D} n_i\right) \\
&+ 4S(J_1 + J_2)\left(\sum_{i\in A} n_i - \sum_{i\in D} n_i\right) \\
&+ \sum_{\tau_1}\left(\sum_{i\in A}\frac{J_{1xy}}{2}S(a_i a_{i+\tau_1} + a_i^\dagger a_{i+\tau_1}^\dagger) + \sum_{i\in D} J_{1xy}(a_i a_{i+\tau_1}^\dagger + a_i^\dagger a_{i+\tau_1})\right) \\
&+ \sum_{\tau_2}\left(\sum_{i\in A}\frac{J_{2xy}}{2}S(a_i a_{i+\tau_2} + a_i^\dagger a_{i+\tau_2}^\dagger) + \sum_{i\in D} J_{2xy}(a_i a_{i+\tau_2}^\dagger + a_i^\dagger a_{i+\tau_2})\right)
\end{aligned}$$

We will now go fourierspace and introduce:

$$a_i = \sqrt{\frac{4}{N}} \sum_k e^{ik\cdot r_i} a_{\alpha_i}(k) \quad \text{with} \quad (\alpha_1, \alpha_2, \alpha_3, \alpha_4) = (A, B, C, D)$$

The technical details of the fouriertransformations can be seen in A. The resulting Hamiltonian takes a similar structure to that in [1]:

$$\mathcal{H} = -\frac{1}{2} NSh + \sum_k A^\dagger(k) L_k A(k)$$

with $A(k) = \begin{bmatrix} a_A(k) & a_B(k) & a_C(k) & a_D(k) & a_A^\dagger(-k) & a_B^\dagger(-k) & a_C^\dagger(-k) & a_D^\dagger(-k) \end{bmatrix}^T$

$$L_k = \begin{bmatrix} \tilde{E}(k) & F(k) \\ F(k) & E(k) \end{bmatrix}$$

and the individual matrices being

$$\tilde{E}(k) = \begin{bmatrix} h + 4S(J_1 + J_2) & 0 & 0 & 0 \\ 0 & -h - 4S(J_1 + J_2) & 0 & 0 \\ 0 & 0 & -h - 4S(J_1 + J_2) & 0 \\ J_{2xy}(\sum_{\tau_2} e^{ik\cdot\tau_2}) & J_{1xy}(e^{-ik_y} + e^{ik_y}) & J_{1xy}(e^{-ik_x} + e^{ik_x}) & -h - 4S(J_1 + J_2) \end{bmatrix}$$

$$E(k) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ J_{2xy}(\sum_{\tau_2} e^{ik\cdot\tau_2}) & J_{1xy}(e^{-ik_y} + e^{ik_y}) & J_{1xy}(e^{-ik_x} + e^{ik_x}) & 0 \end{bmatrix}$$

$$F(k) = \begin{bmatrix} 0 & \frac{J_{1xy}S}{2}(e^{-ik_x} + e^{ik_x}) & \frac{J_{1xy}S}{2}(e^{-ik_y} + e^{ik_y}) & \frac{J_{2xy}S}{2}(\sum_{\tau_2} e^{ik\cdot\tau_2}) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Therefore our hamiltonian can be rewritten as four sums like:

$$\mathcal{H} = -\frac{1}{2} NSh + \sum_k \tilde{E}_{\alpha\beta}(k) a_\alpha^\dagger(k) a_\beta(k) + E_{\alpha\beta}(-k) a_\alpha(k) a_\beta^\dagger(k) + F_{\alpha\beta}(k) a_\alpha^\dagger(k) a_\beta^\dagger(-k) + F_{\alpha\beta}(k) a_\alpha(-k) a_\beta(k)$$

where $\alpha, \beta \in \{(1, A), (2, B), (3, C), (4, D)\}$. Now that we have our hamiltonian we are interested in the corresponding energies. For that we will you the Heisenberg equation of motion:

$$\dot{a} = i[\mathcal{H}, a]$$

The only difference is that $a \mapsto A$. The eigenvalues of the matrix then will be our energies. Let's start, we will use following two identities:

$$[BC, A] = [B, A]C + B[C, A] \quad \left[a_\gamma(k), a_\alpha^\dagger(k')\right] = \delta_{\alpha,\gamma}\delta_{k,k'}$$

So that we find:

$$\dot{A} = \begin{bmatrix} -(\tilde{E}(k) + E^T(-k)) & -(F(k) + F^T(-k)) \\ F(k) + F^T(-k) & \tilde{E}^T(-k) + E(k) \end{bmatrix} A$$

This now has to be typed into mathematica, which will then diagonalize the 8 by 8 matrix.

Appendix A: Fouriertransformations

Necessary are 5 Fourier-transformations of terms of the type:

$$\sum_{i\in A} n_i \quad \sum_{i\in A} a_i a_{i+\tau} \quad \sum_{i\in A} a_i^\dagger a_{i+\tau}^\dagger \quad \sum_{i\in A} a_i^\dagger a_{i+\tau} \quad \sum_{i\in A} a_i^\dagger a_{i+\tau}$$

$\sum_{i\in A} n_i$:

$$\begin{aligned}\sum_{i\in A} n_i &= \frac{4}{N}\sum_{i\in A}\sum_k\sum_{k'} e^{-ik\cdot r_i} e^{ik'\cdot r_i} a_A^\dagger(k) a_A(k') = \sum_k a_A^\dagger(k) a_A(k) \\ &= \sum_k \begin{bmatrix} a_A(k)^\dagger \\ a_B(k)^\dagger \\ a_C(k)^\dagger \\ a_D(k)^\dagger \\ a_A(-k) \\ a_B(-k) \\ a_C(-k) \\ a_D(-k) \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a_A(k) \\ a_B(k) \\ a_C(k) \\ a_D(k) \\ a_A^\dagger(-k) \\ a_B^\dagger(-k) \\ a_C^\dagger(-k) \\ a_D^\dagger(-k) \end{bmatrix}\end{aligned}$$

$\sum_{i\in A} a_i a_{i+\tau}$:

$$\begin{aligned}\sum_{i\in A} a_i a_{i+\tau} &= \frac{4}{N}\sum_{i\in A}\sum_k\sum_{k'} e^{ik\cdot r_i} e^{ik'\cdot(r_i+\tau)} a_A(k) a_{\alpha_{i+\tau}}(k') \\ &= \sum_k e^{ik\cdot\tau} a_A(k) a_{\alpha_{i+\tau}}(-k) \\ &\overset{\alpha=B}{=} \sum_k e^{-ik\cdot\tau} a_A(-k) a_B(k) \\ &= \sum_k \begin{bmatrix} a_A(k)^\dagger \\ a_B(k)^\dagger \\ a_C(k)^\dagger \\ a_D(k)^\dagger \\ a_A(-k) \\ a_B(-k) \\ a_C(-k) \\ a_D(-k) \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{-ik\cdot\tau} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a_A(k) \\ a_B(k) \\ a_C(k) \\ a_D(k) \\ a_A^\dagger(-k) \\ a_B^\dagger(-k) \\ a_C^\dagger(-k) \\ a_D^\dagger(-k) \end{bmatrix}\end{aligned}$$

$\sum_{i\in A} a_i^\dagger a_{i+\tau}^\dagger$:

$$\begin{aligned}
\sum_{i\in A} a_i^\dagger a_{i+\tau}^\dagger &= \frac{4}{N}\sum_{i\in A}\sum_k\sum_{k'} e^{-ik\cdot r_i}e^{-ik'\cdot(r_i+\tau)}a_A^\dagger(k)a_{\alpha_{i+\tau}}^\dagger(k') \\
&= \sum_k e^{-ik\cdot\tau}a_A^\dagger(k)a_{\alpha_{i+\tau}}^\dagger(-k) \\
&\overset{\alpha=B}{=} \sum_k e^{-ik\cdot\tau}a_A^\dagger(k)a_B^\dagger(-k) \\
&= \sum_k \begin{bmatrix} a_A(k)^\dagger \\ a_B(k)^\dagger \\ a_C(k)^\dagger \\ a_D(k)^\dagger \\ a_A(-k) \\ a_B(-k) \\ a_C(-k) \\ a_D(-k) \end{bmatrix} \begin{bmatrix} 0&0&0&0&0&e^{-ik\cdot\tau}&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \end{bmatrix} \begin{bmatrix} a_A(k) \\ a_B(k) \\ a_C(k) \\ a_D(k) \\ a_A^\dagger(-k) \\ a_B^\dagger(-k) \\ a_C^\dagger(-k) \\ a_D^\dagger(-k) \end{bmatrix}
\end{aligned}$$

$\sum_{i\in A} a_i^\dagger a_{i+\tau}$:

$$\begin{aligned}
\sum_{i\in A} a_i a_{i+\tau}^\dagger &= \frac{4}{N}\sum_{i\in A}\sum_k\sum_{k'} e^{ik\cdot r_i}e^{-ik'\cdot(r_i+\tau)}a_A(k)a_{\alpha_{i+\tau}}^\dagger(k') \\
&= \sum_k e^{-ik\cdot\tau}a_A(k)a_{\alpha_{i+\tau}}^\dagger(k) \\
&\overset{\alpha=B}{=} \sum_k e^{ik\cdot\tau}a_A(-k)a_B^\dagger(-k) \\
&= \sum_k \begin{bmatrix} a_A(k)^\dagger \\ a_B(k)^\dagger \\ a_C(k)^\dagger \\ a_D(k)^\dagger \\ a_A(-k) \\ a_B(-k) \\ a_C(-k) \\ a_D(-k) \end{bmatrix} \begin{bmatrix} 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&e^{ik\cdot\tau}&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \end{bmatrix} \begin{bmatrix} a_A(k) \\ a_B(k) \\ a_C(k) \\ a_D(k) \\ a_A^\dagger(-k) \\ a_B^\dagger(-k) \\ a_C^\dagger(-k) \\ a_D^\dagger(-k) \end{bmatrix}
\end{aligned}$$

$\sum_{i\in A} a_i^\dagger a_{i+\tau}$:

$$\begin{aligned}
\sum_{i\in A} a_i^\dagger a_{i+\tau} &= \frac{4}{N}\sum_{i\in A}\sum_k\sum_{k'} e^{-ik\cdot r_i}e^{ik'\cdot(r_i+\tau)}a_A^\dagger(k)a_{\alpha_{i+\tau}}(k') \\
&= \sum_k e^{ik\cdot\tau}a_A^\dagger(k)a_{\alpha_{i+\tau}}(k) \\
&\overset{\alpha=B}{=} \sum_k e^{ik\cdot\tau}a_A^\dagger(k)a_B(k) \\
&= \sum_k \begin{bmatrix} a_A(k)^\dagger \\ a_B(k)^\dagger \\ a_C(k)^\dagger \\ a_D(k)^\dagger \\ a_A(-k) \\ a_B(-k) \\ a_C(-k) \\ a_D(-k) \end{bmatrix} \begin{bmatrix} 0&e^{ik\cdot\tau}&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \end{bmatrix} \begin{bmatrix} a_A(k) \\ a_B(k) \\ a_C(k) \\ a_D(k) \\ a_A^\dagger(-k) \\ a_B^\dagger(-k) \\ a_C^\dagger(-k) \\ a_D^\dagger(-k) \end{bmatrix}
\end{aligned}$$

References

[1] Achille Mauri and Frédéric Mila. *Slow convergence of spin-wave expansion and magnon dispersion in the 1/3 plateau of the triangular XXZ antiferromagnet*. Jan. 7, 2025. DOI: 10.48550/arXiv.2501.03887. arXiv: 2501.03887[cond-mat]. URL: http://arxiv.org/abs/2501.03887 (visited on 02/19/2025).

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