Spin-Wave Theory Using the Holstein–Primakoff Transformation

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Contents

Note: In these notes we are setting $\hbar = 1$, so the quantities $\epsilon_{\mathbf{k}}$ (energy dispersion relation) and $\omega_{\mathbf{k}}$ (dispersion relation), which are related through $\epsilon_{\mathbf{k}} \equiv \hbar\omega_{\mathbf{k}}$, are equivalent.

1 Introduction

Spin-wave theory refers to any theory in which we find the magnon dispersion of a ferromagnet or antiferromagnet by looking at the fluctuations about its classical ground state. In these notes we look at spin-wave theory using the Holstein–Primakoff transformation, which maps[1] spin operators for a system of spin-S moments on a lattice to bosonic creation and annihilation operators as

$$\begin{aligned} \hat{S}_j^z &= S - \hat{n}_j \,, \\ \hat{S}_j^+ &= \sqrt{2S - \hat{n}_j}\,\hat{b}_j \,, \\ \hat{S}_j^- &= \hat{b}_j^\dagger \sqrt{2S - \hat{n}_j} \,, \end{aligned} \tag{1}$$

where $\hat{b}_j^\dagger$ ($\hat{b}_j$) is a bosonic creation (annihilation) operator at site j that satisfies the bosonic commutation relations

$$[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij} \,, \tag{2}$$

$$[\hat{b}_i, \hat{b}_j] = [\hat{b}_i^\dagger, \hat{b}_j^\dagger] = 0 \,, \tag{3}$$

and $\hat{n}_j = \hat{b}_j^\dagger \hat{b}_j$ is the number operator. In this mapping, the vacuum state has a spin of $+S$ in the z direction and each Holstein–Primakoff boson represents a spin-1 moment in the $-z$ direction, thereby representing a perturbation from the classical ferromagnetic ground state (for antiferromagnets it is slightly more complicated, as discussed in Section 3). With this physical picture in mind, we can see that the factor of $\sqrt{2S - \hat{n}_j}$ in the raising and lowering spin operators are there to limit the number of bosons we can have on a given site to $2S$, since the z-projection of the spin moment at a given site must be between $-S$ and $+S$.

At low temperatures ($k_\mathrm{B}T \ll J$, where J is the exchange energy), the number of perturbations about the classical ground state is very small ($\langle \hat{n}_j \rangle \ll S$), so we can use the linear approximation

$$\begin{aligned} \hat{S}_j^z &= S - \hat{n}_j \,, \\ \hat{S}_j^+ &\approx \hat{b}_j \sqrt{2S} \,, \\ \hat{S}_j^- &\approx \hat{b}_j^\dagger \sqrt{2S} \,. \end{aligned} \tag{4}$$

[1] This mapping preserves the spin commutation relations, as proven in Sections 4.1 and 4.2.

1.1 Useful expressions

1.1.1 Fourier transforms of the bosonic operators

$$
\begin{aligned}
\hat{b}_j^\dagger &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_j} \hat{b}_{\mathbf{k}}^\dagger \,, \\
\hat{b}_j &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} \hat{b}_{\mathbf{k}} \,, \qquad (5) \\
\hat{b}_{\mathbf{k}}^\dagger &= \frac{1}{\sqrt{N}} \sum_{j} e^{i\mathbf{k}\cdot\mathbf{r}_j} \hat{b}_j^\dagger \,, \\
\hat{b}_{\mathbf{k}} &= \frac{1}{\sqrt{N}} \sum_{j} e^{-i\mathbf{k}\cdot\mathbf{r}_j} \hat{b}_j \,, \qquad (6)
\end{aligned}
$$

where N is the number of primitive cells in the lattice.

1.1.2 Orthogonality relations

$$\sum_j e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j} = N\delta_{\mathbf{k}\mathbf{k}'} \,, \tag{7}$$

$$\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} = N\delta_{ij} \,. \tag{8}$$

1.1.3 Binomial approximation

Using the binomial approximation,

$$(1+x)^\alpha \approx 1 + \alpha x \qquad (|x| < 1 \text{ and } |\alpha x| \ll 1) \,, \tag{9}$$

we will approximate $\sqrt{2S - \hat{n}_j}$ as

$$\sqrt{2S - \hat{n}_j} = \sqrt{2S}\sqrt{1 - \frac{\hat{n}_j}{2S}} \approx \sqrt{2S}\left(1 - \frac{\hat{n}_j}{4S}\right) \,. \tag{10}$$

2 Heisenberg ferromagnet

Let's use the Holstein–Primakoff transformation to rewrite the ferromagnetic Heisenberg Hamiltonian,

$$\begin{aligned}\hat{H} &= -J\sum_{\langle ij\rangle}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j && (11)\\ &= -J\sum_{\langle ij\rangle}[\hat{S}_i^z\hat{S}_j^z+\tfrac{1}{2}(\hat{S}_i^+\hat{S}_j^-+\hat{S}_i^-\hat{S}_j^+)]\,, && (12)\end{aligned}$$

where $J>0$, up to order $\mathcal{O}(S^0)$:

$$\begin{aligned}\hat{H} &= -J\sum_{\langle ij\rangle}\left[(S-\hat{n}_i)(S-\hat{n}_j)+\frac{1}{2}\left(\sqrt{2S-\hat{n}_i}\,\hat{b}_i\hat{b}_j^\dagger\sqrt{2S-\hat{n}_j}+\hat{b}_i^\dagger\sqrt{2S-\hat{n}_i}\sqrt{2S-\hat{n}_j}\,\hat{b}_j\right)\right]\\
&\approx -J\sum_{\langle ij\rangle}\left[(S-\hat{n}_i)(S-\hat{n}_j)+S\left[\left(1-\frac{\hat{n}_i}{4S}\right)\hat{b}_i\hat{b}_j^\dagger\left(1-\frac{\hat{n}_j}{4S}\right)+\hat{b}_i^\dagger\left(1-\frac{\hat{n}_i}{4S}\right)\left(1-\frac{\hat{n}_j}{4S}\right)\hat{b}_j\right]\right]\\
&= -J\sum_{\langle ij\rangle}\Bigg[S^2-S\hat{n}_i-S\hat{n}_j+\hat{n}_i\hat{n}_j+S\hat{b}_i\hat{b}_j^\dagger-\frac{1}{4}\hat{b}_i\hat{b}_j^\dagger\hat{n}_j-\frac{1}{4}\hat{n}_i\hat{b}_i\hat{b}_j^\dagger+\frac{1}{16S}\hat{n}_i\hat{b}_i\hat{b}_j^\dagger\hat{n}_j+S\hat{b}_i^\dagger\hat{b}_j\\
&\qquad -\frac{1}{4}\hat{b}_i^\dagger\hat{n}_i\hat{b}_j-\frac{1}{4}\hat{b}_i^\dagger\hat{n}_j\hat{b}_j+\frac{1}{16S}\hat{b}_i^\dagger\hat{n}_i\hat{n}_j\hat{b}_j\Bigg]\\
&\approx -J\sum_{\langle ij\rangle}\left[S^2+S(\hat{b}_i^\dagger\hat{b}_j+\hat{b}_j^\dagger\hat{b}_i-\hat{n}_i-\hat{n}_j)+\frac{1}{4}(4\hat{n}_i\hat{n}_j-\hat{b}_i^\dagger\hat{n}_i\hat{b}_j-\hat{b}_j^\dagger\hat{n}_j\hat{b}_i-\hat{b}_i^\dagger\hat{n}_j\hat{b}_j-\hat{b}_j^\dagger\hat{n}_i\hat{b}_i)\right]\\
&= -\frac{NqJS^2}{2}-J\sum_{\langle ij\rangle}\left[S(\hat{b}_i^\dagger\hat{b}_j+\hat{b}_j^\dagger\hat{b}_i-\hat{n}_i-\hat{n}_j)+\frac{1}{4}[4\hat{n}_i\hat{n}_j-\hat{b}_i^\dagger(\hat{n}_i+\hat{n}_j)\hat{b}_j-\hat{b}_j^\dagger(\hat{n}_i+\hat{n}_j)\hat{b}_i]\right]\\
&= -\frac{NqJS^2}{2}+J\sum_{\langle ij\rangle}\left[S(\hat{b}_i^\dagger-\hat{b}_j^\dagger)(\hat{b}_i-\hat{b}_j)+\frac{1}{4}[\hat{b}_i^\dagger\hat{b}_j^\dagger(\hat{b}_i-\hat{b}_j)^2+(\hat{b}_i^\dagger-\hat{b}_j^\dagger)^2\hat{b}_i\hat{b}_j]\right]\\
&= -\frac{NqJS^2}{2}+JS\sum_{\langle ij\rangle}(\hat{b}_i^\dagger-\hat{b}_j^\dagger)(\hat{b}_i-\hat{b}_j)+\frac{J}{4}\sum_{\langle ij\rangle}[\hat{b}_i^\dagger\hat{b}_j^\dagger(\hat{b}_i-\hat{b}_j)^2+(\hat{b}_i^\dagger-\hat{b}_j^\dagger)^2\hat{b}_i\hat{b}_j]\,,\end{aligned}$$

where N is the number of sites on the lattice and q is the coordination number of the lattice. The Hamiltonian is therefore of the form

$$\hat{H} = -\frac{NqJS^2}{2}+\hat{H}_1+\hat{H}_2+\mathcal{O}\left(\frac{1}{S}\right)\,, \tag{13}$$

where the first term is the classical ground-state energy of the ferromagnet and

$$\begin{aligned}\hat{H}_1 &= JS\sum_{\langle ij\rangle}(\hat{b}_i^\dagger - \hat{b}_j^\dagger)(\hat{b}_i - \hat{b}_j)\\ &= -JS\sum_{\langle ij\rangle}(\hat{b}_i^\dagger\hat{b}_j + \hat{b}_j^\dagger\hat{b}_i) + qJS\sum_i \hat{n}_i\,, \end{aligned}\tag{14}$$

$$\begin{aligned}\hat{H}_2 &= \frac{J}{4}\sum_{\langle ij\rangle}[\hat{b}_i^\dagger\hat{b}_j^\dagger(\hat{b}_i - \hat{b}_j)^2 + (\hat{b}_i^\dagger - \hat{b}_j^\dagger)^2\hat{b}_i\hat{b}_j]\\ &= -\frac{J}{4}\sum_{\langle ij\rangle}[4\hat{n}_i\hat{n}_j - \hat{b}_i^\dagger(\hat{n}_i + \hat{n}_j)\hat{b}_j - \hat{b}_j^\dagger(\hat{n}_i + \hat{n}_j)\hat{b}_i]\,. \end{aligned}\tag{15}$$

The $\hat{H}_1$ term contains the magnon dispersion relation, and $\hat{H}_2$ and higher-order terms are magnon–magnon interaction terms. At low temperatures, since $\langle\hat{n}_j\rangle \ll S$, we can ignore these higher-order terms and just keep the ground-state energy term and terms quadratic in bosonic operators (i.e., $\hat{H}_1$); this is referred to as *linear spin-wave theory.* Note that we could have more quickly and easily obtained the correct expression for the ground-state energy and $\hat{H}_1$ if we had used the linear approximations in Eqs. 4 to begin with.[2] We can rewrite the sum over nearest neighbors in $\hat{H}_1$ as

$$\sum_{\langle ij\rangle}(\hat{b}_i^\dagger\hat{b}_j + \hat{b}_j^\dagger\hat{b}_i) = \frac{1}{2}\sum_i\sum_{\boldsymbol{\delta}}(\hat{b}_i^\dagger\hat{b}_{i+\boldsymbol{\delta}} + \hat{b}_{i+\boldsymbol{\delta}}^\dagger\hat{b}_i)\,,\tag{16}$$

where the sum over $\boldsymbol{\delta}$ is carried out over the nearest-neighbor vectors $\boldsymbol{\delta}_1$, $\boldsymbol{\delta}_2$, … , $\boldsymbol{\delta}_q$, the operator $\hat{b}_{i+\boldsymbol{\delta}}$ annihilates a boson at the site whose position is $\mathbf{r}_i + \boldsymbol{\delta}$, and the factor of 1/2 is to avoid double counting. Let's now rewrite $\hat{H}_1$ in momentum space:

$$\begin{aligned}\hat{H}_1 &= -\frac{JS}{2N}\sum_i\sum_{\boldsymbol{\delta},\mathbf{k},\mathbf{k}'}(e^{-i\mathbf{k}\cdot\mathbf{r}_i}e^{i\mathbf{k}'\cdot(\mathbf{r}_i+\boldsymbol{\delta})}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}'} + e^{-i\mathbf{k}'\cdot(\mathbf{r}_i+\boldsymbol{\delta})}e^{i\mathbf{k}\cdot\mathbf{r}_i}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}'}) + qJS\sum_{\mathbf{k}}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}}\\ &= -\frac{JS}{2}\sum_{\boldsymbol{\delta},\mathbf{k}}(e^{i\mathbf{k}\cdot\boldsymbol{\delta}} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}})\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}} + qJS\sum_{\mathbf{k}}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}}\\ &= -JS\sum_{\boldsymbol{\delta},\mathbf{k}}\cos(\mathbf{k}\cdot\boldsymbol{\delta})\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}} + qJS\sum_{\mathbf{k}}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}}\\ &= qJS\sum_{\mathbf{k}}\left[1 - \frac{1}{q}\sum_{\boldsymbol{\delta}}\cos(\mathbf{k}\cdot\boldsymbol{\delta})\right]\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}}\,,\end{aligned}$$

where N is the number of sites on the lattice. Finally, defining

$$\gamma_{\mathbf{k}} \equiv \frac{1}{q}\sum_{\boldsymbol{\delta}}\cos(\mathbf{k}\cdot\boldsymbol{\delta})\,,\tag{17}$$

[2] This is shown in Section 4.3.

we can write $\hat{H}_1$ as

$$\hat{H}_1 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} \,, \tag{18}$$

where

$$\epsilon_{\mathbf{k}} \equiv qJS(1-\gamma_{\mathbf{k}}) \tag{19}$$

is the ferromagnetic magnon dispersion relation.

2.1 1D chain

For a 1D ferromagnetic Heisenberg chain, the nearest-neighbor vectors are

$$\delta_1 = a \,, \qquad \delta_2 = -a \,, \tag{20}$$

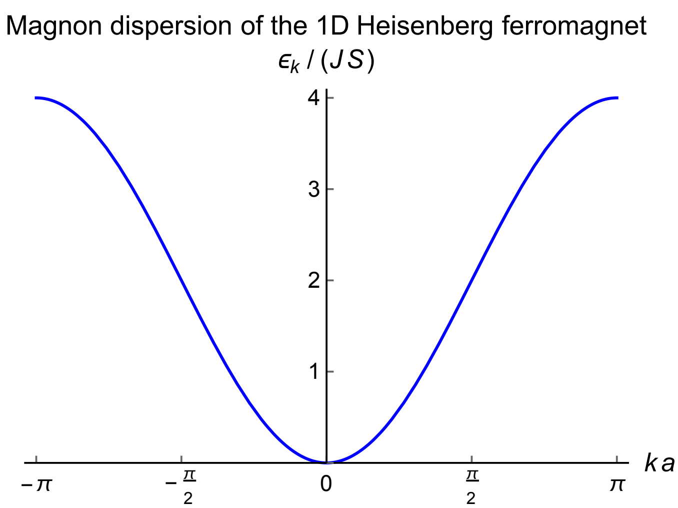
where a is the lattice constant, so

$$\gamma_k = \frac{1}{2}[\cos(ka) + \cos(-ka)] = \cos(ka) \tag{21}$$

and thus the magnon dispersion is

$$\epsilon_k = 2JS[1-\cos(ka)] \,. \tag{22}$$

A plot of this is shown below.



At low temperatures,[3] the Hamiltonian thus reads

$$\hat{H} = -NJS^2 + 2JS \sum_k [1-\cos(ka)] \hat{b}^\dagger_k \hat{b}_k \,. \tag{23}$$

[3]Keeping only the ground-state energy term and $\hat{H}_1$.

3 Heisenberg antiferromagnet

Let's use the Holstein–Primakoff transformation to rewrite the antiferromagnetic Heisenberg Hamiltonian,

$$\hat{H} = J\sum_{\langle ij\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \tag{24}$$

$$= J\sum_{\langle ij\rangle} [\hat{S}_i^z \hat{S}_j^z + \tfrac{1}{2}(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+)]\,, \tag{25}$$

where $J > 0$, up to order $\mathcal{O}(S^1)$ for a system with no geometrical frustration whose spins reside on two sublattices, which we will refer to as A and B. We will use i (j) to index the spins on sublattice A (B). We will map the spin operators for both sublattices as

$$\text{Sublattice } A: \quad \begin{cases} \hat{S}_i^z = S - \hat{a}_i^\dagger \hat{a}_i \\ \hat{S}_i^+ = \sqrt{2S - \hat{a}_i^\dagger \hat{a}_i}\, \hat{a}_i \\ \hat{S}_i^- = \hat{a}_i^\dagger \sqrt{2S - \hat{a}_i^\dagger \hat{a}_i} \end{cases}, \tag{26}$$

$$\text{Sublattice } B: \quad \begin{cases} \hat{S}_j^z = \hat{b}_j^\dagger \hat{b}_j - S \\ \hat{S}_j^+ = \hat{b}_j^\dagger \sqrt{2S - \hat{b}_j^\dagger \hat{b}_j} \\ \hat{S}_j^- = \sqrt{2S - \hat{b}_j^\dagger \hat{b}_j}\, \hat{b}_j \end{cases}, \tag{27}$$

where the bosonic operators of sublattice A commute with those sublattice B. Since we are only interested in terms up to order $\mathcal{O}(S^1)$, we will use the linear approximation ($\langle \hat{a}_j^\dagger \hat{a}_j\rangle \ll S$ and $\langle \hat{b}_j^\dagger \hat{b}_j\rangle \ll S$) and rewrite the Hamiltonian as

$$\begin{aligned}
\hat{H} &\approx J\sum_{\langle ij\rangle} [(S - \hat{a}_i^\dagger \hat{a}_i)(\hat{b}_j^\dagger \hat{b}_j - S) + \tfrac{1}{2}(\hat{a}_i \sqrt{2S}\, \hat{b}_j \sqrt{2S} + \hat{a}_i^\dagger \sqrt{2S}\, \hat{b}_j^\dagger \sqrt{2S})] \\
&= -\frac{NqJS^2}{2} + J\sum_{\langle ij\rangle} [S(\hat{a}_i^\dagger \hat{a}_i + \hat{b}_j^\dagger \hat{b}_j) - \underbrace{\hat{a}_i^\dagger \hat{a}_i \hat{b}_j^\dagger \hat{b}_j}_{=\mathcal{O}(S^0)\approx 0} + S(\hat{a}_i \hat{b}_j + \hat{a}_i^\dagger \hat{b}_j^\dagger)] \\
&\approx -\frac{NqJS^2}{2} + JS\sum_{\langle ij\rangle} (\hat{a}_i^\dagger \hat{a}_i + \hat{b}_j^\dagger \hat{b}_j + \hat{a}_i \hat{b}_j + \hat{a}_i^\dagger \hat{b}_j^\dagger) \\
&= -\frac{NqJS^2}{2} + \left[JS\sum_{\langle ij\rangle} (\hat{a}_i \hat{b}_j + \hat{a}_i^\dagger \hat{b}_j^\dagger) + qJS\sum_{i\in A} \hat{a}_i^\dagger \hat{a}_i + qJS\sum_{j\in B} \hat{b}_j^\dagger \hat{b}_j \right],
\end{aligned}$$

where N is the number of sites on the lattice and q is the coordination number of the lattice. The Hamiltonian is therefore of the form

$$\hat{H} = -\frac{NqJS^2}{2} + \hat{H}_1 + \mathcal{O}\left(S^0\right)\,, \tag{28}$$

where the first term is the classical ground-state energy of the antiferromagnet and

$$\hat{H}_1 = JS \sum_{\langle ij \rangle} (\hat{a}_i \hat{b}_j + \hat{a}_i^\dagger \hat{b}_j^\dagger) + qJS \sum_{i \in A} \hat{a}_i^\dagger \hat{a}_i + qJS \sum_{j \in B} \hat{b}_j^\dagger \hat{b}_j \tag{29}$$

contains the antiferromagnetic magnon dispersion relation. We can rewrite the sum over nearest neighbors as

$$\sum_{\langle ij \rangle} (\hat{a}_i \hat{b}_j + \hat{a}_i^\dagger \hat{b}_j^\dagger) = \sum_{i \in A} \sum_{\boldsymbol{\delta}} (\hat{a}_i \hat{b}_{i+\boldsymbol{\delta}} + \hat{a}_i^\dagger \hat{b}_{i+\boldsymbol{\delta}}^\dagger) \,, \tag{30}$$

where the sum over $\boldsymbol{\delta}$ is carried out over the vectors $\boldsymbol{\delta}_1$, $\boldsymbol{\delta}_2$, ... , $\boldsymbol{\delta}_q$ (these vectors are the displacement vectors between neighboring spins *within the same sublattice*), and the operator $\hat{b}_{i+\boldsymbol{\delta}}$ annihilates a boson at the B site whose position is $\mathbf{r}_i + \boldsymbol{\delta}$. Let's now rewrite $\hat{H}_1$ in momentum space:

$$\begin{aligned}
\hat{H}_1 &= \frac{JS}{N/2} \sum_{i \in A} \sum_{\boldsymbol{\delta}, \mathbf{k}, \mathbf{k}'} (e^{i\mathbf{k}\cdot\mathbf{r}_i} e^{i\mathbf{k}'\cdot(\mathbf{r}_i + \boldsymbol{\delta})} \hat{a}_{\mathbf{k}} \hat{b}_{\mathbf{k}'} + e^{-i\mathbf{k}\cdot\mathbf{r}_i} e^{-i\mathbf{k}'\cdot(\mathbf{r}_i + \boldsymbol{\delta})} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'}^\dagger) + qJS \sum_{\mathbf{k}} (\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}) \\
&= JS \sum_{\boldsymbol{\delta}, \mathbf{k}} (e^{-i\mathbf{k}\cdot\boldsymbol{\delta}} \hat{a}_{\mathbf{k}} \hat{b}_{-\mathbf{k}} + e^{i\mathbf{k}\cdot\boldsymbol{\delta}} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{-\mathbf{k}}^\dagger) + qJS \sum_{\mathbf{k}} (\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}) \,,
\end{aligned}$$

where $N/2$ is the number of sublattice A (and sublattice B) sites, and in the second line we have used

$$\sum_{i \in A} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}_i} = \frac{N}{2} \delta_{\mathbf{k}', -\mathbf{k}} \,. \tag{31}$$

Defining

$$\gamma_{\mathbf{k}} \equiv \frac{1}{q} \sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}} \tag{32}$$

and assuming $\gamma_{\mathbf{k}} = \gamma_{-\mathbf{k}}$,[4] as is often the case due to symmetry, $\hat{H}_1$ reads

$$\hat{H}_1 = qJS \sum_{\mathbf{k}} [\gamma_{\mathbf{k}} (\hat{a}_{\mathbf{k}} \hat{b}_{-\mathbf{k}} + \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{-\mathbf{k}}^\dagger) + \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{b}_{-\mathbf{k}}^\dagger \hat{b}_{-\mathbf{k}}] \,, \tag{33}$$

where we have rewritten $\sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} = \sum_{\mathbf{k}} \hat{b}_{-\mathbf{k}}^\dagger \hat{b}_{-\mathbf{k}}$ so that every bosonic operator for sublattice B is in terms of the same momentum, namely $-\mathbf{k}$. In order to diagonalize this Hamiltonian, let's perform the Bogoliubov transformation

$$\begin{pmatrix} \hat{\alpha}_{\mathbf{k}} \\ \hat{\beta}_{\mathbf{k}}^\dagger \end{pmatrix} \equiv \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ -v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}_{-\mathbf{k}}^\dagger \end{pmatrix} \,, \tag{34}$$

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are real and must satisfy

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1 \tag{35}$$

[4] Or equivalently, assuming $\gamma_{\mathbf{k}}$ is real.

in order to preserve the bosonic commutation relations:

$$\begin{aligned}
[\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}^\dagger_{\mathbf{k}'}] = [\hat{\beta}_{\mathbf{k}}, \hat{\beta}^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'}\,, \\
[\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}_{\mathbf{k}'}] = [\hat{\beta}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}'}] = [\hat{\alpha}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}'}] = [\hat{\alpha}_{\mathbf{k}}, \hat{\beta}^\dagger_{\mathbf{k}'}] = 0\,.
\end{aligned} \tag{36}$$

The inverse transformation is therefore given by

$$\begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}^\dagger_{-\mathbf{k}} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{\alpha}_{\mathbf{k}} \\ \hat{\beta}^\dagger_{\mathbf{k}} \end{pmatrix}\,. \tag{37}$$

In terms of these new bosonic operators, $\hat{H}_1$ now reads

$$\begin{aligned}
\hat{H}_1 = qJS \sum_{\mathbf{k}} \Big\{ &\gamma_{\mathbf{k}} \big[(u_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + v_{\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}})(v_{\mathbf{k}}\hat{\alpha}^\dagger_{\mathbf{k}} + u_{\mathbf{k}}\hat{\beta}_{\mathbf{k}}) + (u_{\mathbf{k}}\hat{\alpha}^\dagger_{\mathbf{k}} + v_{\mathbf{k}}\hat{\beta}_{\mathbf{k}})(v_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + u_{\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}}) \big] \\
&+ (u_{\mathbf{k}}\hat{\alpha}^\dagger_{\mathbf{k}} + v_{\mathbf{k}}\hat{\beta}_{\mathbf{k}})(u_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + v_{\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}}) + (v_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + u_{\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}})(v_{\mathbf{k}}\hat{\alpha}^\dagger_{\mathbf{k}} + u_{\mathbf{k}}\hat{\beta}_{\mathbf{k}}) \Big\} \\
= qJS \sum_{\mathbf{k}} \Big\{ &(u^2_{\mathbf{k}} + v^2_{\mathbf{k}} + 2\gamma_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}})(\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + \hat{\beta}^\dagger_{\mathbf{k}}\hat{\beta}_{\mathbf{k}}) + [\gamma_{\mathbf{k}}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) + 2u_{\mathbf{k}}v_{\mathbf{k}}](\hat{\alpha}_{\mathbf{k}}\hat{\beta}_{\mathbf{k}} + \hat{\alpha}^\dagger_{\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}}) \\
&+ 2v^2_{\mathbf{k}} + 2\gamma_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \Big\}\,.
\end{aligned} \tag{38}$$

In order for this Hamiltonian to be diagonal, we must explicitly find $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ such that the coefficient of the term $(\hat{\alpha}_{\mathbf{k}}\hat{\beta}_{\mathbf{k}} + \hat{\alpha}^\dagger_{\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}})$ is zero:

$$\gamma_{\mathbf{k}}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) + 2u_{\mathbf{k}}v_{\mathbf{k}} = 0\,. \tag{39}$$

Inserting the condition from Eq. 35, we can solve for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$:

$$u^2_{\mathbf{k}} = \frac{1}{2}\left(\frac{1}{\sqrt{1-\gamma^2_{\mathbf{k}}}} + 1 \right)\,, \tag{40}$$

$$v^2_{\mathbf{k}} = \frac{1}{2}\left(\frac{1}{\sqrt{1-\gamma^2_{\mathbf{k}}}} - 1 \right)\,, \tag{41}$$

$$u_{\mathbf{k}}v_{\mathbf{k}} = -\frac{1}{2}\frac{\gamma_{\mathbf{k}}}{\sqrt{1-\gamma^2_{\mathbf{k}}}}\,. \tag{42}$$

$\hat{H}_1$ is therefore diagonalized:

$$\hat{H}_1 = qJS \sum_{\mathbf{k}} [(u^2_{\mathbf{k}} + v^2_{\mathbf{k}} + 2\gamma_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}})(\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + \hat{\beta}^\dagger_{\mathbf{k}}\hat{\beta}_{\mathbf{k}}) + 2v^2_{\mathbf{k}} + 2\gamma_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}]\,. \tag{43}$$

Using the expressions for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ we just found, we can simplify this further to

$$\hat{H}_1 = qJS \sum_{\mathbf{k}} \sqrt{1-\gamma^2_{\mathbf{k}}}\,(\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}} + \hat{\beta}^\dagger_{\mathbf{k}}\hat{\beta}_{\mathbf{k}}) - qJS \sum_{\mathbf{k}} \left(1 - \sqrt{1-\gamma^2_{\mathbf{k}}}\right)\,. \tag{44}$$

This term contains a constant term, which *lowers* the ground-state energy of the antiferromagnet. This can be understood as quantum fluctuations lowering the ground-state energy of the system and tells us that the classical Néel state is not the ground state of this quantum antiferromagnet. We thus find that up to $\mathcal{O}(S^1)$, the Hamiltonian for a Heisenberg antiferromagnet is

$$\hat{H} = -\frac{NqJS(S+\sigma)}{2} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (\hat{\alpha}^\dagger_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + \hat{\beta}^\dagger_{\mathbf{k}} \hat{\beta}_{\mathbf{k}}) \,, \tag{45}$$

where

$$\epsilon_{\mathbf{k}} \equiv qJS\sqrt{1-\gamma_{\mathbf{k}}^2} \tag{46}$$

is the antiferromagnetic magnon dispersion relation and

$$\sigma \equiv \frac{2}{N} \sum_{\mathbf{k}} \left(1 - \sqrt{1-\gamma_{\mathbf{k}}^2}\right) \,. \tag{47}$$

For reference, for a system with simple cubic sublattices, $\sigma \approx 0.194$.

3.1 1D chain

For a 1D antiferromagnetic Heisenberg chain, the two $\boldsymbol{\delta}$ vectors (which are just scalars in 1D) are

$$\delta_1 = a \,, \qquad \delta_2 = -a \,, \tag{48}$$

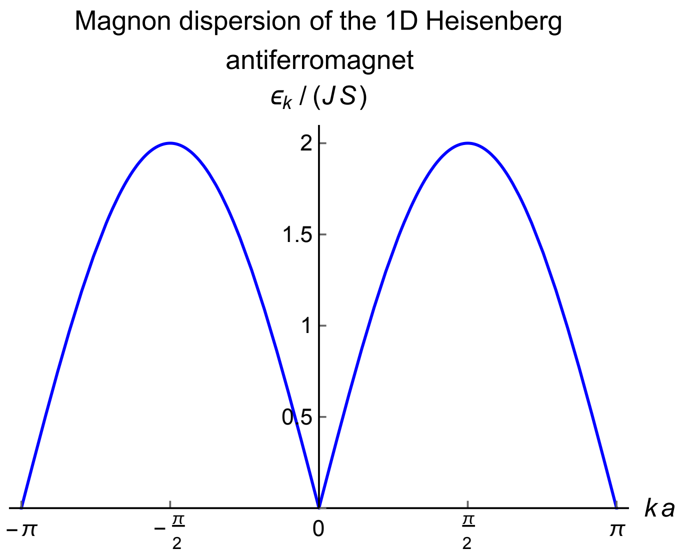
where a is the lattice constant, equal to the distance between neighboring spins *within the same sublattice*, so

$$\begin{aligned} \gamma_k &= \frac{1}{2} \sum_{\delta} e^{ik\delta} \\ &= \frac{1}{2}(e^{ik\delta_1} + e^{ik\delta_2}) \\ &= \frac{1}{2}(e^{ika} + e^{-ika}) \\ &= \cos(ka) \,. \end{aligned} \tag{49}$$

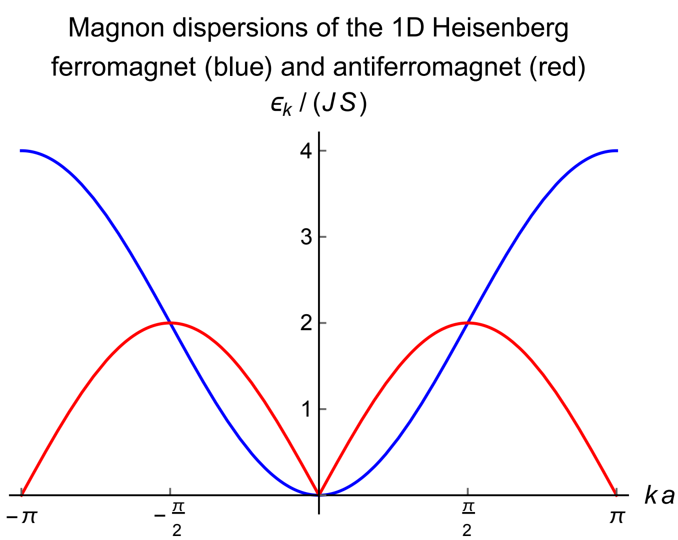
The antiferromagnetic magnon dispersion is therefore

$$\epsilon_k = 2JS|\sin(ka)| \,. \tag{50}$$

A plot of this is shown below.



For comparison, a plot of both the ferromagnetic (blue) and antiferromagnetic (red) magnon dispersions are shown below.



At low temperatures,[5] the Hamiltonian thus reads

$$\hat{H} = -NJS(S+\sigma) + 2JS\sum_k |\sin(ka)|(\hat{\alpha}_k^\dagger\hat{\alpha}_k + \hat{\beta}_k^\dagger\hat{\beta}_k)\,. \tag{51}$$

[5]Keeping only the ground-state energy term and $\hat{H}_1$.

4 Proofs

4.1 $[\hat{S}^z_j, \hat{S}^\pm_j] = \pm\hat{S}^\pm_j$ in the Holstein–Primakoff formalism

In order to avoid clutter we will omit the j subscript on the operators.

Proof.

$$\begin{aligned}
[\hat{S}^z, \hat{S}^+] &= [S - \hat{n}, \sqrt{2S - \hat{n}}\,\hat{b}] \\
&= -[\hat{n}, \sqrt{2S - \hat{n}}\,\hat{b}] \\
&= -(\sqrt{2S - \hat{n}}[\hat{n}, \hat{b}] + [\hat{n}, \sqrt{2S - \hat{n}}]\hat{b}) \\
&= -\sqrt{2S - \hat{n}}[\hat{n}, \hat{b}] \\
&= \sqrt{2S - \hat{n}}\,\hat{b} \\
&= \hat{S}^+\,, \\
[\hat{S}^z, \hat{S}^-] &= [S - \hat{n}, \hat{b}^\dagger\sqrt{2S - \hat{n}}] \\
&= -[\hat{n}, \hat{b}^\dagger\sqrt{2S - \hat{n}}] \\
&= -(\hat{b}^\dagger[\hat{n}, \sqrt{2S - \hat{n}}] + [\hat{n}, \hat{b}^\dagger]\sqrt{2S - \hat{n}}) \\
&= -[\hat{n}, \hat{b}^\dagger]\sqrt{2S - \hat{n}} \\
&= -\hat{b}^\dagger\sqrt{2S - \hat{n}} \\
&= -\hat{S}^-\,.
\end{aligned}$$

□

4.2 $[\hat{S}^+_j, \hat{S}^-_j] = 2\hat{S}^z_j$ in the Holstein–Primakoff formalism

In order to avoid clutter we will omit the j subscript on the operators.

Proof.

$$\begin{aligned}
[\hat{S}^+, \hat{S}^-] &= [\sqrt{2S - \hat{n}}\,\hat{b}, \hat{b}^\dagger\sqrt{2S - \hat{n}}] \\
&= \sqrt{2S - \hat{n}}[\hat{b}, \hat{b}^\dagger\sqrt{2S - \hat{n}}] + [\sqrt{2S - \hat{n}}, \hat{b}^\dagger\sqrt{2S - \hat{n}}]\hat{b} \\
&= \sqrt{2S - \hat{n}}\left(\hat{b}^\dagger[\hat{b}, \sqrt{2S - \hat{n}}] + \sqrt{2S - \hat{n}}\right) + [\sqrt{2S - \hat{n}}, \hat{b}^\dagger]\sqrt{2S - \hat{n}}\,\hat{b} \\
&= \sqrt{2S - \hat{n}}\left[\hat{b}^\dagger\left(\hat{b}\sqrt{2S - \hat{n}} - \sqrt{2S - \hat{n}}\,\hat{b}\right) + \sqrt{2S - \hat{n}}\right] \\
&\quad + \left(\sqrt{2S - \hat{n}}\,\hat{b}^\dagger - \hat{b}^\dagger\sqrt{2S - \hat{n}}\right)\sqrt{2S - \hat{n}}\,\hat{b} \\
&= (1 + \hat{n})(2S - \hat{n}) - \hat{b}^\dagger(2S - \hat{n})\,\hat{b} \\
&= (1 + \hat{n})(2S - \hat{n}) - \hat{b}^\dagger\hat{b}\big(2S - (\hat{n} - 1)\big)
\end{aligned}$$

$$
\begin{aligned}
&= (1+\hat{n})(2S-\hat{n}) - \hat{n}(2S-\hat{n}+1) \\
&= 2(S-\hat{n}) \\
&= 2\hat{S}^z\,. \qquad \square
\end{aligned}
$$

4.3 Obtaining the ferromagnetic Heisenberg Hamiltonian up to $\mathcal{O}(S^1)$ using the linear Holstein–Primakoff transformation from Eqs. 4

$$
\begin{aligned}
\hat{H} &\approx -J\sum_{\langle ij\rangle}[(S-\hat{n}_i)(S-\hat{n}_j) + \tfrac{1}{2}(\hat{b}_i\sqrt{2S}\,\hat{b}_j^\dagger\sqrt{2S} + \hat{b}_i^\dagger\sqrt{2S}\,\hat{b}_j\sqrt{2S})] \\
&= -J\sum_{\langle ij\rangle}[(S-\hat{n}_i)(S-\hat{n}_j) + S(\hat{b}_i\hat{b}_j^\dagger + \hat{b}_i^\dagger\hat{b}_j)] \\
&= -J\sum_{\langle ij\rangle}[S^2 - S(\hat{n}_i+\hat{n}_j) + \hat{n}_i\hat{n}_j + S(\hat{b}_i^\dagger\hat{b}_j + \hat{b}_j^\dagger\hat{b}_i)] \\
&= -\frac{NqJS^2}{2} + S\left[-J\sum_{\langle ij\rangle}(\hat{b}_i^\dagger\hat{b}_j + \hat{b}_j^\dagger\hat{b}_i) + qJ\sum_i\hat{n}_i\right] + \underbrace{J\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j}_{=\mathcal{O}(S^0)\approx 0} \\
&\approx -\frac{NqJS^2}{2} + S\left[-J\sum_{\langle ij\rangle}(\hat{b}_i^\dagger\hat{b}_j + \hat{b}_j^\dagger\hat{b}_i) + qJ\sum_i\hat{n}_i\right].
\end{aligned}
$$