SpinW factor 2 problem

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1 The problem

SpinW [1] results does not reproduce the test case of 1D ferromagnetic chain, neither 3D ferromagnetic cubic crystal. The magnon dispersion for such systems plotted with SpinW is twice as small as the result from textbooks [7, 2, 5, 9, 3, 6] (conversion from textbook's notations are discussed in Appendix I).

Since there are various notations for the Spin Hamiltonian, which is the starting point for the magnon dispersion calculation, in this paper all results are presents with respect to the notation of SpinW paper [10]:

$$H = \sum_{mi,nj} \boldsymbol{S}_{mi}^T \boldsymbol{J}_{mi,nj} \boldsymbol{S}_{nj} + \sum_{mi} \boldsymbol{S}_{mi}^T \boldsymbol{A}_{mi} \boldsymbol{S}_{mi} + \mu_B \boldsymbol{H}^T \sum_{mi} g_i \boldsymbol{S}_{mi},$$

where double counting is present in the sum and negative J means ferromagnetic alignment. First term descries exchange interaction, second – single ion anisotropy, third – external magnetic field. The indices m, n are indexing the crystallographic unit cell (running from 1 to L), while i and j label the magnetic atoms inside unit cell (running from 1 to N). $\boldsymbol{S}_i$ is a 3×1 column vector of spin operators $\{S_{mi}^x, S_{mi}^y, S_{mi}^z\}$, $\boldsymbol{J}_{mi,nj}$ is a matrix of exchange parameters, $\boldsymbol{A}_{mi}$ - matrix of single ion anisotropy, $\boldsymbol{H}$ - column vector of external magnetic field.

For the ferromagnetic 3D crystal with one magnetic center in unit cell the solution of SpinW gives:

$$E(\boldsymbol{k}) = \hbar\omega(\boldsymbol{k}) = SJn\left(\frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right) - 1\right),$$

where l is the length of lattice parameters. While the textbook's results gives for the same system:

$$E(\boldsymbol{k}) = \hbar\omega(\boldsymbol{k}) = 2SJn\left(\frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right) - 1\right). \quad (1)$$

In the Fig. 1 The magnon dispersion is plotted for both solutions along the k-path specified in [8], $J = 1$, $S = 1$, $n = 6$.

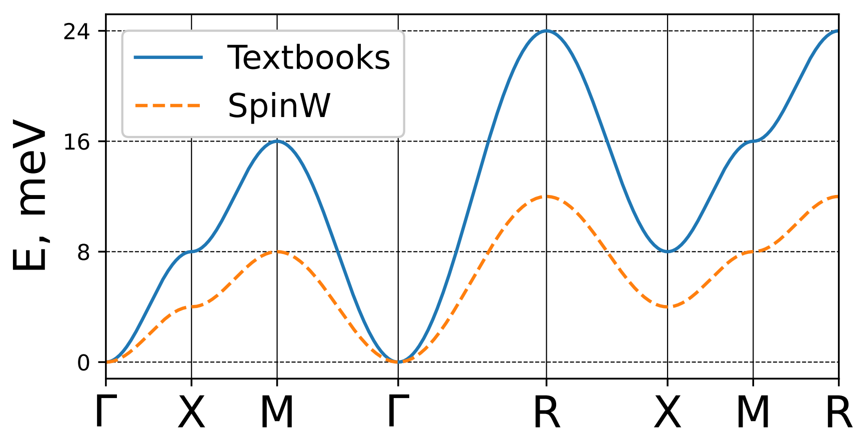


Figure 1: Magnon dispersion comparison between SpinW and textbooks ($J = 1$, $S = 1$).

In the SpinW paper [10] the solution starts by the two consecutive rotations, which results in the rotation of the exchange matrix $\boldsymbol{J}'_{mi,nj} = \boldsymbol{J}_{mi,nj}\boldsymbol{R}_{n-m}$ the definition of the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$. This rotation does not affect the following discussion, therefore we drop the $'$ sign in the $\boldsymbol{J}_{mi,nj}$ and use the complex valued vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, without recalling their definition here. The unique comment that is important here is that for ferromagnetic case (oriented along z axis) the values of the vectors are:

$$\boldsymbol{u} = (1, i, 0)^T$$

$$\boldsymbol{v} = (0, 0, 1)^T$$

The single-ion anisotropy term and magnetic field term can be merged into the exchange term as explained in the SpinW paper [10].

2 The solution

Starting point for the following discussion is equation (20) from the SpinW paper [10] (adjusted with respect to the comment at the end of the previous section):

$$H = \sum_{mi,nj} \left\{ \sqrt{\frac{S_i}{2}} \left(\overline{\boldsymbol{u}}_i^T b_{mi} + \boldsymbol{u}_i^T b_{mi}^\dagger \right) + \boldsymbol{v}_i^T (S_i - b_{mi}^\dagger b_{mi}) \right\} \cdot \boldsymbol{J}_{mi,nj} \cdot \left\{ \sqrt{\frac{S_j}{2}} \left(\overline{\boldsymbol{u}}_j b_{nj} + \boldsymbol{u}_j b_{nj}^\dagger \right) + \boldsymbol{v}_j (S_j - b_{nj}^\dagger b_{nj}) \right\},$$

where $b_{mi}^\dagger$ and b_{mi} are the creation and annihilation operators of the local quantum spin deviations. Overline denotes complex conjugate.

After the expansion the Hamiltonian Has the zero energy term E_0, the term with one-operator terms, expectation value of which vanishes. And the two-operator term $H^{(2)}$, which is the center of attention in linearised spin-wave theory. We focus on this term, taking into account the property of the exchange matrix $\boldsymbol{J}_{mi,nj} = \boldsymbol{J}_{i,j}(d)$, $\boldsymbol{d} = \boldsymbol{r}_n - \boldsymbol{r}_m$:

$$\begin{aligned} H^{(2)} = \frac{\sqrt{S_i S_j}}{2} \Big(&\overline{\boldsymbol{u}}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{d}) \overline{\boldsymbol{u}}_j b_{mi} b_{nj} + \overline{\boldsymbol{u}}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{d}) \boldsymbol{u}_j b_{mi} b_{nj}^\dagger \\ &+ \boldsymbol{u}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{d}) \overline{\boldsymbol{u}}_j b_{mi}^\dagger b_{nj} + \boldsymbol{u}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{d}) \boldsymbol{u}_j b_{mi}^\dagger b_{nj}^\dagger \Big) \\ &- \boldsymbol{v}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{d}) \boldsymbol{v}_j \left(S_i b_{nj}^\dagger b_{nj} + S_j b_{mi}^\dagger b_{mi} \right) \end{aligned}$$

The next step of the solution is to apply Fourier transformation in order to move from the creation and annihilation operators of the local quantum spin deviations ($b_{mi}^\dagger$ and b_{mi}) to the creation and annihilation operators of collective quantum excitations ($b^\dagger(k)$ and $b(k)$).

$$b_{mi} = \frac{1}{\sqrt{L}} \sum_{\boldsymbol{k} \in \text{B.Z.}} b_i(\boldsymbol{k}) e^{\boldsymbol{i}\boldsymbol{k}\boldsymbol{r}_m},$$

$$b_{mi}^\dagger = \frac{1}{\sqrt{L}} \sum_{\boldsymbol{k} \in \text{B.Z.}} b_i^\dagger(\boldsymbol{k}) e^{-\boldsymbol{i}\boldsymbol{k}\boldsymbol{r}_m},$$

After the Fourier transformation the Hamiltonian has the form:

$$
\begin{aligned}
H^{(2)} = \sum_{ij}\sum_{\boldsymbol{k}} \Bigg[& \frac{\sqrt{S_iS_j}}{2}\overline{\boldsymbol{u}}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{k})\overline{\boldsymbol{u}}_j b_i(\boldsymbol{k})b_j(-\boldsymbol{k}) + \frac{\sqrt{S_iS_j}}{2}\overline{\boldsymbol{u}}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{k})\boldsymbol{u}_j b_i(\boldsymbol{k})b_j^\dagger(\boldsymbol{k}) \\
& + \frac{\sqrt{S_iS_j}}{2}\boldsymbol{u}_i^T \boldsymbol{J}_{i,j}(-\boldsymbol{k})\overline{\boldsymbol{u}}_j b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k}) + \frac{\sqrt{S_iS_j}}{2}\boldsymbol{u}_i^T \boldsymbol{J}_{i,j}(-\boldsymbol{k})\boldsymbol{u}_j b_i^\dagger(\boldsymbol{k})b_j^\dagger(-\boldsymbol{k}) \\
& - S_i\boldsymbol{v}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{0})\boldsymbol{v}_j b_j^\dagger(\boldsymbol{k})b_j(\boldsymbol{k}) + S_j\boldsymbol{v}_i^T \boldsymbol{J}_{i,j}(\boldsymbol{0})\boldsymbol{v}_j b_i^\dagger(\boldsymbol{k})b_i(\boldsymbol{k}) \Bigg]
\end{aligned}
$$

We follow the definitions from the equation (26) of the SpinW paper [10]:

$$
\boldsymbol{J}_{i,j}(\boldsymbol{k}) = \sum_{\boldsymbol{d}} \boldsymbol{J}_{i,j}(\boldsymbol{d})e^{-i\boldsymbol{kd}}
$$

$$
\begin{aligned}
A(\boldsymbol{k})^{i,j} &= \frac{\sqrt{S_i, S_j}}{2}\boldsymbol{u}_i^T \boldsymbol{J}_{i,j}(-\boldsymbol{k})\overline{\boldsymbol{u}}_j, \\
B(\boldsymbol{k})^{i,j} &= \frac{\sqrt{S_i, S_j}}{2}\boldsymbol{u}_i^T \boldsymbol{J}_{i,j}(-\boldsymbol{k})\boldsymbol{u}_j, \\
C(\boldsymbol{k})^{i,j} = C^{i,j} &= \delta_{i,j}\sum_l S_l\boldsymbol{v}_i^T \boldsymbol{J}_{i,l}(\boldsymbol{0})\boldsymbol{v}_l.
\end{aligned}
$$

With this notation Hamiltonian has the form:

$$
\begin{aligned}
H^{(2)} = \sum_{ij}\sum_{\boldsymbol{k}} \Big[& \overline{B^{i,j}(\boldsymbol{k})} b_i(\boldsymbol{k})b_j(-\boldsymbol{k}) + \overline{A^{i,j}(\boldsymbol{k})} b_i(\boldsymbol{k})b_j^\dagger(\boldsymbol{k}) \\
& + A^{i,j}(\boldsymbol{k})b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k}) + B^{i,j}(\boldsymbol{k})b_i^\dagger(\boldsymbol{k})b_j^\dagger(-\boldsymbol{k}) \\
& - 2C^{i,j}b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k}) \Big]
\end{aligned} \tag{2}
$$

Next step consist in the rewriting the Hamiltonian in the quadratic form:

$$
H = \sum_{\boldsymbol{k}?} \boldsymbol{x}^\dagger(\boldsymbol{k})h(\boldsymbol{k})\boldsymbol{x}(\boldsymbol{k}), \tag{3}
$$

where

$$
\boldsymbol{x}(\boldsymbol{k}) = \Big[b_1(\boldsymbol{k}), \dots, b_N(\boldsymbol{k}, b_1^\dagger(-\boldsymbol{k}), \dots, b_N^\dagger(-\boldsymbol{k}))\Big]^T
$$

and (in the SpinW paper)

$$
h(\boldsymbol{k}) = \begin{pmatrix} \boldsymbol{A}(\boldsymbol{k}) - \boldsymbol{C} & \boldsymbol{B}(\boldsymbol{k}) \\ \boldsymbol{B}^\dagger(\boldsymbol{k}) & \overline{\boldsymbol{A}(-\boldsymbol{k})} - \boldsymbol{C} \end{pmatrix}
$$

where † means hermitian conjugate.

There is a question mark near the $\boldsymbol{k}$ under the sum, since that is the place where SpinW solution and what we are going to do next differ. In the article of Colpa [4], in the textbook by Rezende [7] (page 83) and indirectly in the article of White [12], textbook [6] the restriction $\boldsymbol{k} > 0$ is implied, which means that for each $\boldsymbol{k}$ in the sum $-\boldsymbol{k}$ is not in the sum. In addition in the textbook by White [13] the factor 1/2 added in front of the quadratic Hamiltonian (3) with no restriction to $\boldsymbol{k}$, which is equivalent to the restriction on $\boldsymbol{k}$ mentioned above.

However, SpinW paper proceed to cast the Hamiltonian (2) into quadratic form (3) without any restriction on $\boldsymbol{k}$, moreover, it is specifically noted under the sum in equation 23 that $\boldsymbol{k} \in$ B.Z.. That fact directly leads to the doubling of each two-operator term, since in eq. (3)

for each $\boldsymbol{k}$ there are terms $b_i^\dagger(\boldsymbol{k})b_i(\boldsymbol{k})$ and $b_i^\dagger(-\boldsymbol{k})b_i(-\boldsymbol{k})$, while for corresponding $-\boldsymbol{k}$ there are terms $b_i^\dagger(-\boldsymbol{k})b_i(-\boldsymbol{k})$ and $b_i^\dagger(\boldsymbol{k})b_i(\boldsymbol{k})$. Meanwhile, in eq. (2) for each $\boldsymbol{k}$ there is only one term $b_i^\dagger(\boldsymbol{k})b_i(\boldsymbol{k})$ and for corresponding $-\boldsymbol{k}$ there is term $b_i^\dagger(-\boldsymbol{k})b_i(-\boldsymbol{k})$. After the diagonalization the Hamiltonian has the form:

$$H = \sum_i \sum_{\boldsymbol{k}} \left[\hbar\omega_i^{(1)}(\boldsymbol{k})\beta_i^\dagger(\boldsymbol{k})\beta_i(\boldsymbol{k}) + \hbar\omega_i^{(2)}(\boldsymbol{k})\beta_i^\dagger(-\boldsymbol{k})\beta_i(-\boldsymbol{k})\right]$$

After the diagonalization SpinW takes only first ($\omega_i^{(1)}(\boldsymbol{k})$) N frequencies as magnon modes and loses part of the solution for $\boldsymbol{k}$, which comes from corresponding $-\boldsymbol{k}$ term. The correct way to proceed with the result from the paper is to take combination of first N and second N frequencies:

$$E_i(\boldsymbol{k}) = \hbar(\omega_i^{(1)}(\boldsymbol{k}) + \omega_i^{(2)}(-\boldsymbol{k}))$$

For the ferromagnetic case of 3D cubic crystal:

$$\omega^{(1)}(\boldsymbol{k}) = \omega^{(2)}(\boldsymbol{k}) = \hbar\omega(\boldsymbol{k}) = \frac{SJn}{\hbar}\left(\frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right) - 1\right)$$

and

$$E(\boldsymbol{k}) = 2SJn\left(\frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right) - 1\right),$$

which now matches with the textbook's result.

3 Another view on the source of the problem

In the SpinW paper the diagonalization of the quadratic form (3) follows the method by Colpa [4]. In the code itself the diagonalization method by White [13] is mentioned. Let us compare the starting points of Colpa and White with SpinW before diagonalization.

3.1 Colpa

Colpa discusses the diagonalization of the Bogolubov Hamiltonian of the form:

$$H = \sum_{r',r=1}^{m} \left(\alpha_{r'}^\dagger\Delta_{1r'r}\alpha_r + \alpha_{r'}^\dagger\Delta_{2r'r}\alpha_{m+r}^\dagger + \alpha_{m+r'}\Delta_{3r'r}\alpha_r + \alpha_{m+r'}\Delta_{4r'r}\alpha_{m+r}^\dagger\right), \tag{4}$$

with the following comment on the possible nature of the indices r and $m+r$:

> The reason why we consider first eq (2.1) is that it often occurs in practice [in solid-state physics e.g. all operators with indes r correspond to the same wave vector $\boldsymbol{k}$, those with $m+r$ to $-\boldsymbol{k}$; m denotes the number of degrees of freedom in the unit cell (or less)]

Good for us! We have just the case of the solid-state physics. Note, that in the Hamiltonian (4) the sum is carried over m and not $2m$, which means that under the sum the terms with $\boldsymbol{k}$ and $-\boldsymbol{k}$ are written explicitly. Now lets recall the Hamiltonian (2):

$$\begin{aligned} H^{(2)} = \sum_{ij}\sum_{\boldsymbol{k}} \Big[&\overline{B^{i,j}(\boldsymbol{k})}b_i(\boldsymbol{k})b_j(-\boldsymbol{k}) + \overline{A^{i,j}(\boldsymbol{k})}b_i(\boldsymbol{k})b_j^\dagger(\boldsymbol{k}) \\ &+ A^{i,j}(\boldsymbol{k})b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k}) + B^{i,j}(\boldsymbol{k})b_i^\dagger(\boldsymbol{k})b_j^\dagger(-\boldsymbol{k}) \\ &- 2C^{i,j}b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k})\Big] \end{aligned}$$

Here only the part for the $\boldsymbol{k}$ is written explicitly for each $\boldsymbol{k}$ under the sum. Therefore one need to add terms for $-\boldsymbol{k}$ in order to construct the form (4). There are two ways to do that:

- To restrict ourselves to the $\boldsymbol{k} > 0$ and rewrite the Hamiltonian.
- To keep the whole set of $\boldsymbol{k}$ and add $\sum_{-\boldsymbol{k}}$ to the Hamiltonian.

Lets focus on the first way here, since it is the one that is implied in the article of Colpa. We will discuss the second approach in the next subsection. First of all, let write the Hamiltonian in a more compact form:

$$
\begin{aligned}
H^{(2)} = \sum_{ij}\sum_{\boldsymbol{k}} \Big[2(A^{i,j}(\boldsymbol{k}) - C^{i,j})b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k}) + \overline{B^{i,j}(\boldsymbol{k})}b_i(\boldsymbol{k})b_j(-\boldsymbol{k}) + B^{i,j}(\boldsymbol{k})b_i^\dagger(\boldsymbol{k})b_j^\dagger(-\boldsymbol{k})\Big] \\
+ \sum_i\sum_{\boldsymbol{k}} A^{i,i}(\boldsymbol{k}) \\
= \sum_{ij}\sum_{\boldsymbol{k}} H^{i,j}(\boldsymbol{k}) + const,
\end{aligned}
$$

where we used the fact that $\boldsymbol{A}(\boldsymbol{k})$ is Hermitian (see Appendix II) and the commutator $[b_i(\boldsymbol{k})b_j^\dagger(\boldsymbol{k})] = \delta_{i,j}$. In the following we omit the constant term of the energy shift.

$$
\begin{aligned}
H^{(2)} &= \sum_{ij}\sum_{\boldsymbol{k}>0} \big(H^{i,j}(\boldsymbol{k}) + H^{i,j}(-\boldsymbol{k})\big) \\
&= \sum_{ij}\sum_{\boldsymbol{k}>0} \Big[2(A^{i,j}(\boldsymbol{k}) - C^{i,j})b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k}) + \overline{B^{i,j}(\boldsymbol{k})}b_i(\boldsymbol{k})b_j(-\boldsymbol{k}) + B^{i,j}(\boldsymbol{k})b_i^\dagger(\boldsymbol{k})b_j^\dagger(-\boldsymbol{k}) \\
&\quad + 2(A^{i,j}(-\boldsymbol{k}) - C^{i,j})b_i^\dagger(-\boldsymbol{k})b_j(-\boldsymbol{k}) + \overline{B^{i,j}(-\boldsymbol{k})}b_i(-\boldsymbol{k})b_j(\boldsymbol{k}) + B^{i,j}(-\boldsymbol{k})b_i^\dagger(-\boldsymbol{k})b_j^\dagger(\boldsymbol{k})\Big]
\end{aligned}
$$

Let us rewrite this Hamiltonian in the form directly comparable with the quadratic form (3) (here we used $B^{i,j}(\boldsymbol{k}) + B^{j,i}(-\boldsymbol{k}) = 2B^{i,j}(\boldsymbol{k})$, see Appendix II):

$$
\begin{aligned}
H^{(2)} = \sum_{ij}\sum_{\boldsymbol{k}} \Big[2(A^{i,j}(\boldsymbol{k}) - C^{i,j})b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k})\Big] \\
+ (\overline{B^{j,i}(\boldsymbol{k})} + \overline{B^{i,j}(-\boldsymbol{k})})b_i(\boldsymbol{k})b_j(-\boldsymbol{k}) \\
+ (B^{i,j}(\boldsymbol{k}) + B^{j,i}(-\boldsymbol{k}))b_i^\dagger(\boldsymbol{k})b_j^\dagger(-\boldsymbol{k}) \\
+ 2(A^{j,i}(\boldsymbol{k}) - C^{j,i})b_i(\boldsymbol{k})b_j^\dagger(\boldsymbol{k})\Big] \\
= \sum_{ij}\sum_{\boldsymbol{k}} \Big[2(A^{i,j}(\boldsymbol{k}) - C^{i,j})b_i^\dagger(\boldsymbol{k})b_j(\boldsymbol{k})\Big] \\
+ 2\overline{B^{j,i}(\boldsymbol{k})}b_i(\boldsymbol{k})b_j(-\boldsymbol{k}) \\
+ 2B^{i,j}(\boldsymbol{k})b_i^\dagger(\boldsymbol{k})b_j^\dagger(-\boldsymbol{k}) \\
+ 2(A^{j,i}(\boldsymbol{k}) - C^{j,i})b_i(\boldsymbol{k})b_j^\dagger(\boldsymbol{k})\Big]
\end{aligned}
$$

Thus, the matrix $h(\boldsymbol{k})$ is:

$$
h(\boldsymbol{k}) = \begin{pmatrix} 2(\boldsymbol{A}(\boldsymbol{k}) - \boldsymbol{C}) & 2\boldsymbol{B}(\boldsymbol{k}) \\ 2\boldsymbol{B}^\dagger(\boldsymbol{k}) & 2(\overline{\boldsymbol{A}(-\boldsymbol{k})} - \boldsymbol{C}) \end{pmatrix},
$$

solution of which are the same as in SpinW, but multiplied by the factor 2 and matches the textbook results.

Note that in that case we take only the first N energies out of the $2N$ energies from the diagonalization of the $2N \times 2N$ matrix. The reasoning is the same as in SpinW paper [10], or in the book of White [13], or in book of Tyablikov [11]: We are solving the matrix, which contains the terms both for $\boldsymbol{k}$ and $-\boldsymbol{k}$, therefore first N eigenvalues are positive and describe the creation of magnons, and the second N are negative and describe annihilation of magnons. After the diagonalization the matrix is:

$$h(\boldsymbol{k}) = \begin{pmatrix} \boldsymbol{\omega}^{(1)}(\boldsymbol{k}) & 0 \\ 0 & \boldsymbol{\omega}^{(2)}(\boldsymbol{k}) \end{pmatrix},$$

where $\boldsymbol{\omega}$ is an $N \times N$ diagonal matrix. And the diagonalized Hamiltonian looks like (up to a constant term):

$$H^{(2)} = \sum_{i,j}\sum_{\boldsymbol{k}>0}\left(\omega^{(1)}(\boldsymbol{k})\beta_i^\dagger(\boldsymbol{k})\beta_i(-\boldsymbol{k}) + \omega^{(2)}(\boldsymbol{k})\beta_i^\dagger(-\boldsymbol{k})\beta_i(-\boldsymbol{k})\right)$$

Here the magnon dispersion is $E_i(\boldsymbol{k}) = \hbar\omega_i^{(1)}(\boldsymbol{k})$, which gives the actual solution for the $\boldsymbol{k} > 0$, while $\omega^{(2)}(\boldsymbol{k})$ describes corresponding solutions for the $-\boldsymbol{k}$, which could be viewed as the creation of magnon with $-\boldsymbol{k}$ or annihilation of magnon with $\boldsymbol{k}$, which is effectively the same.

For the ferromagnetic cubic lattice:

$$E(\boldsymbol{k}) = 2SJn\left(\frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right) - 1\right),$$

which is the same as textbooks result.

3.2 White

White discusses the diagonalization of the Hamiltonian with dipole-dipole interaction in the book [13]. It includes the same math and ideas as the one we need to use for the solution of the Hamiltonian (2).

The quadratic form in his case is (page 246, equation (8.41)):

$$H = \frac{1}{2}\sum_{\boldsymbol{k}} \boldsymbol{x}_{\boldsymbol{k}}^\dagger H_{\boldsymbol{k}} \boldsymbol{x}_{\boldsymbol{k}}$$

And the Hamiltonian, which requires diagonalization (page 246, equation (8.40)):

$$H = E_0 + \sum_{\boldsymbol{k}}\left(A_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + B_{\boldsymbol{k}} a_{\boldsymbol{k}} a_{-\boldsymbol{k}} + \overline{B_{\boldsymbol{k}}} a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger\right)$$

From those two equations one can deduct the following. The terms with $a_{\boldsymbol{k}} a_{-\boldsymbol{k}}$ and $a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger$ are introducing the coupling between $+\boldsymbol{k}$ and $-\boldsymbol{k}$, therefore in order to solve the Hamiltonian one has to consider the Hamiltonian for positive and negative value of **each** $\boldsymbol{k}$.

4 Appendix I

4.1 Fundamentals of Magnonics [7]

In «Fundamentals of Magnonics» the derivation of magnon dispersion is done in chapter 3 «Quantum Theory of Spin Waves: Magnons».

The Hamiltonian is defined on page 72, eq. 3.6 as follows:

$$H = -g\mu_B \sum_i H_z S_i^z - J \sum_{i,\delta} \vec{S}_i \cdot \vec{S}_{i+\delta},$$

> where $\vec{S}_i$ is spin angular momentum operator as site i, <...> and $\vec{\delta}$ is the vector connecting site i with its nearest neighbors. <...> Notice also that the factor 2 in the exchange energy does not appear explicitly because each pair of spins is counted twice in the sum over lattice sites.

The definition of the Hamiltonian differs from SpinW with the sign, the following notation change is necessary at the end:

$$J \to -J$$

Magnon dispersion is provided on page 78 in eqs. 3.35 and 3.36

$$E_k = A_k = g\mu_B H_z + 2zJS(1 - \gamma_k),$$

> where γ_k is the structure factor given by
>
> $$\gamma_k = \frac{1}{z} \sum_{\vec{\delta}} e^{\mathrm{i}\vec{k}\cdot\vec{\delta}}$$

where z is the number of neighbors (n in the notation of this paper). γ_k for the cubic system is (it is provided on page 79 in eq. 3.37):

$$\gamma_k = \frac{1}{3}(\cos(k_x a) + \cos(k_y a) + \cos(k_z a))$$

where a is a lattice parameter (l in the notation of this paper). The final equation from the [7] in the notation of SpinW is

$$\hbar\omega(\mathbf{k}) = 2nJS\left(\frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right) - 1\right)$$

4.2 Magnetism in condensed matter [2]

The derivation of magnon dispersion for the ferromagnetic 1D chain is discussed in the section 6.6.6 «Magnons».

The definition of the Hamiltonian is provided on page 122 in eqs. 6.9 and 6.10:

> (1) We begin with a semiclassical derivation of the spin wave dispersion. First, recall the Hamiltonian for the Heisenberg model,
>
> $$\hat{\mathcal{H}} = -\sum_{\langle ij\rangle} J\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$$
>
> (which is eqn. 6.4) In a one-dimensional chain each spin has two neighbours, so the Hamiltonian reduces to
>
> $$\hat{\mathcal{H}} = -2J\sum_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1}$$

with the comment to the equation (6.4) on the page 116 being:

where the constant J is the exchange integral and the symbol $\langle ij \rangle$ below the $\sum$ denotes a sum over nearest neighbours. The spins $\mathbf{S}_i$ are treated as three-dimensional vectors ...

The definition of the Heisenberg model is found for the first time in the section 4.2.1 on the page 76 in eqs. 4.7 and 4.8:

This motivates the Hamiltonian of the Heisenberg model:

$$\hat{\mathcal{H}} = -\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where J_{ij} is the exchange constant between the i^{th} and j^{th} spins. The factor of 2 is omitted because the summation includes each pair of spins twice. Another way of writing eqn 4.7 is

$$\hat{\mathcal{H}} = -2\sum_{i>j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where the $i > j$ avoids the «double-counting» and hence the factor of two returns. Often it is possible to take J_{ij} to be equal to a constant J for nearest neighbours spins and to be 0 otherwise.

The eq. 6.9 corresponds to the definition in eq. 4.7 and the eq. 6.10 corresponds to the definition in eq. 4.8. The definition in eq. 4.7 differs from SpinW with the sign, the following notation change is necessary at the end:

$$J \to -J$$

The Hamiltonian is solved specifically for the ferromagnetic 1D chain and not for the 3D cubic system with the final result (equation 6.20 on page 123 and equation -6.25 on page 124)

$$\hbar\omega = 4JS(1 - \cos(qa)),$$
$$E(q) = -2NS^2 J + 4JS(1 - \cos(qa)),$$

Magnon dispersion from eq. 6.20 is plotted in the book on page 123 in figure 6.12 (Fig. 2). Path from 0 to π/a is the same as the Γ-X path in Fig. 1. If the parameters J =1, S = 1 are substituted into the eq. 6.20 then those two graphs are exactly the same.

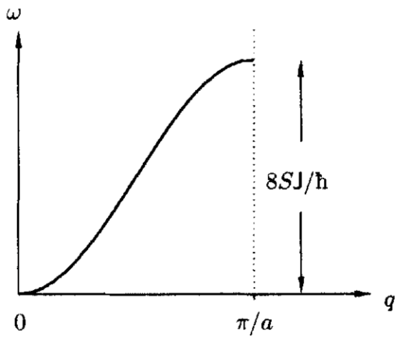


Fig. 6.12 **The spin wave dispersion relation for a one-dimensional chain of spins.**

Figure 2: Magnon dispersion plot from «Magnetism in condensed matter».

For the cubic system eq. 6.20 in SpinW notation looks like:

$$\hbar\omega(\boldsymbol{k}) = 2nJS(\frac{1}{3}(\cos(q_x a) + \cos(q_y a) + \cos(q_z a)) - 1)$$

4.3 Magnetisation oscillations and waves [5]

The derivation of magnon dispersion for the ferromagnet is discussed in the section 7.4 «Elements of microscopic spin-wave theory».

The definition of the Hamiltonian is provided on page 205 in eq. 7.82:

$$\hat{\mathcal{H}} = \gamma\hbar \sum_f \hat{S}_f^z - \sum_f \sum_{f' \neq f} I_{ff'} \mathbf{S}_f \mathbf{S}_{f'}$$

where $\mathbf{S}_f \mathbf{S}_{f'} = \hat{S}_f^x \hat{S}_{f'}^x + \hat{S}_f^y \hat{S}_{f'}^y + \hat{S}_f^z \hat{S}_{f'}^z$.

The double counting is present in this Hamiltonian, thus the definition of the Hamiltonian differs from SpinW with the sign, the following notation change is necessary at the end:

$$J \rightarrow -J$$

The dispersion law is provided in eq. 7.99 on page 209:

where $r_g = r_f - r_{f'}$, $I_g \equiv I_{ff'}$, and the last sum is over all lattice points except one, the initial. The Hamiltonian (7.98) has the desired form of (7.84), and

$$\varepsilon_k(k) = \gamma\hbar H + 2S \sum_g [1 - exp(\mathrm{i}\mathbf{k}\mathbf{r}_g)] I_g.$$

For the cubic ferromagnet the textbook provides the figure 7.13 (Fig. 3)

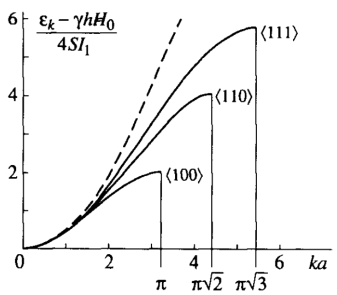
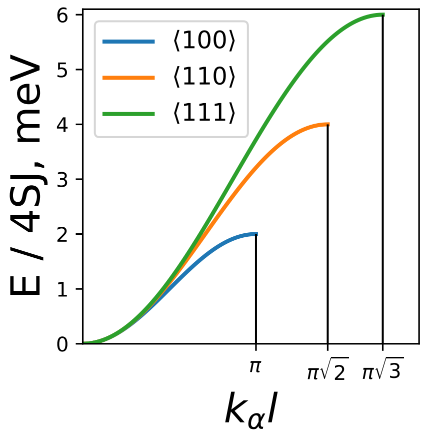


FIGURE 7.13
Dispersion characteristics of spin waves in a ferromagnet with simple cubic spin lattice for different directions of propagation calculated (solid curves) by formula (7.101), i.e., in the nearest-neighbor approximation and without allowance for dipole–dipole interaction. Dashed curve corresponds to the continuum despersion law.

(a) Original plot



(b) Same plot with use of eq. (1)

Figure 3: Magnon dispersion plot from «Magnetisation oscillations and waves».

In this picture curve ⟨100⟩ (from 0 to π) corresponds to the path Γ-X, curve ⟨110⟩ (from 0 to $\pi\sqrt{2}$) to the path Γ-M and curve ⟨111⟩ (from 0 to $\pi\sqrt{3}$) to the path Γ-R in the Fig. 1. In Fig. 3b the same graph is plotted by using the equation for magnon dispersion from this paper. The picture is produced with the script «codes/dispersion.py» using «custom_moaw» function.

The dispersion law from eq. 7.99 for the cubic system in the notation of SpinW is:

$$\hbar\omega(\mathbf{k}) = 2SIn\left(\frac{1}{3}\left(\cos(k_x r_x) + \cos(k_y r_y) + \cos(k_z r_z)\right) - 1\right)$$

4.4 The Oxford Solid State Basics [9]

The derivation of magnon dispersion for the ferromagnet is discussed in the exercise 20.3 for the Chapter 20 «Spontaneous Magnetic Order: Ferro-, Antiferro-, and Ferri-Magnetism».

The definition of the Hamiltonian is provided on page 229 in eqs. 20.6 and 20.2:

> Consider the Heisenberg Hamiltonian
>
> $$\hat{\mathcal{H}} = -\frac{1}{2}\sum_{\langle i,j\rangle} J\mathbf{S}_i \cdot \mathbf{S}_j + \sum_i g\mu_B \mathbf{B}\cdot\mathbf{S}_i$$
>
> and for this exercise set $\mathbf{B} = 0$.

For the first time Heisenberg Hamiltonian is defined on pages $225 - 226$ in eq. 20.2:

> Note that we have included a factor of 1/2 out front to avoid overcounting, since the sum actually counts both J_{ij} and J_{ji} (which are equal to each other).
>
> ⟨...⟩
>
> One can use brackets $\langle i, j\rangle$ to indicate that i and j are neighbors:
>
> $$\hat{\mathcal{H}} = -\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$$
>
> In a uniform system where each spin is coupled to its neighbors with the same strength, we can drop the indices from $J_{i,j}$ (since they all have the same value) and obtain the so-called *Heisenberg Hamiltonian*
>
> $$\hat{\mathcal{H}} = -\frac{1}{2}\sum_{\langle i,j\rangle} J\mathbf{S}_i \cdot \mathbf{S}_j$$

The double counting is present in this Hamiltonia as well as the additional factor of 1/2, thus the definition of the Hamiltonian differs from SpinW with the sign and factor 1/2, the following notation change is necessary at the end:

$$J \to -2J$$

The dispersion law for the cubic system is provided on page 230:

> ▷ Show that the dispersion curve for «spin-waves» of a ferromagnet is given by $\hbar\omega = |F(\mathbf{k})|$ where
>
> $$F(\mathbf{k}) = g\mu_b|B| + JS\left(6 - 2\left(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right)\right)$$
>
> where we assume a cubic lattice

In the notation of SpinW the dispersion law becomes:

$$\hbar\omega(\mathbf{k}) = 2JSn\left(\frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right) - 1\right)$$

4.5 Magnetism and magnetic materials [3]

The derivation of magnon dispersion for the ferromagnet is discussed in the section 5.4.1 «Spin waves».

The definition of the Hamiltonian is provided on page 137 in eq. 5.24:

> When there is a lattice, the Hamiltonian[1] is generalized to a sum over all pairs of atoms on lattice sites i, j:
> $$\hat{\mathcal{H}} = -2\sum_{i>j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$$

In this definition there is no double counting ($i > j$), but there is a factor of 2 present, thus the definition of the Hamiltonian differs from SpinW with the sign, the following notation change is necessary at the end:

$$J \to -J$$

The dispersion law for the cubic system is provided on page 163:

> The generalization to a three-dimensional cubic lattice with nearest-neighbour interactions is
> $$\hbar\omega_q = 2JS\left[Z - \sum_{\delta}\cos\mathbf{q}\cdot\delta\right],$$
> where the sum is over the Z vectors δ connecting the central atom to its nearest neighbours.

In case of the cubic system $Z = 6$ and there are 6 nearest-neighbours with the vectors

$$\begin{array}{ccc} (l,0,0), & (0,l,0), & (0,0,l), \\ (-l,0,0), & (0,-l,0), & (0,0,-l), \end{array}$$

And the dispersion in notation of SpinW law becomes:

$$\hbar\omega_q = 2JSZ\left(\frac{1}{3}\left(\cos(q_x l) + \cos(q_y l) + \cos(q_z l)\right) - 1\right),$$

4.6 Rare earth magnetism [6]

The derivation of magnon dispersion for the ferromagnet is discussed in the chapter 5 «Spin waves in the ferromagnetic heavy rare earths».

The definition of the Hamiltonian is provided on page 186 in eq. 5.2.1:

$$\hat{\mathcal{H}} = \sum_i\left[\sum_{l=2,4,6} B_l^0 Q_l^0(\mathbf{J}_i) + B_6^6 Q_6^6(\mathbf{J}_i) - g\mu_B \mathbf{J}_i \cdot \mathbf{H}\right] - \frac{1}{2}\sum_{i\neq j}\mathcal{J}(ij)\mathbf{J}_i \cdot \mathbf{J}_j$$

In the eq. 5.2.1 crystal field and magnetic field are considered in the first sum, while the second term represents Heisenberg Hamiltonian. There is a double counting in the sum as well as the factor 1/2, thus the definition of the Hamiltonian differs from SpinW with the sign and factor 1/2, the following notation change is necessary at the end:

$$J \to -2J$$

The spin-wave spectra is defined on the page 190 in the eq. 5.2.22:

The energy parameters are

$$U_1 = \frac{1}{2}\sum_{\mathbf{q}}(E_{\mathbf{q}} - A_{\mathbf{q}}); \quad E_{\mathbf{q}} = \sqrt{A_{\mathbf{q}}^2 - B^2}.$$

where $A_{\mathbf{q}}$, A and B are defined in the eqs. 5.2.18 and 5.2.15:

$$A = \frac{1}{J}\left\{3B_2^0 J^{(2)} - 21 B_6^6 J^{(6)} \cos 6\phi + g\mu_B J H \cos(\phi - \phi_H)\right\}$$
$$B = \frac{1}{J}\left\{3B_2^0 J^{(2)} + 15 B_6^6 J^{(6)} \cos 6\phi\right\}.$$

⟨...⟩

$$A_{\mathbf{q}} = A + J\left\{\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q})\right\}$$

$A = 0$ and $B = 0$ if no magnetic field nor anisotropic effects are considered. In the case of this paper $L = 0$, thus $J = S$ and the equation for the dispersion law is

$$E_{\mathbf{q}} = S\left(\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q})\right)$$

$\mathcal{J}(\mathbf{q})$ is defined in the eq. 5.1.1a:

$$\mathcal{J}_{ss'}(\mathbf{q}) = \sum_{j \in s'-subl.} \mathcal{J}(ij) e^{-\mathrm{i}\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}; \quad i \in s - sublattice,$$

And for the cubic lattice it becomes:

$$\mathcal{J}(\mathbf{q}) = J\left(e^{-\mathrm{i}q_x l} + e^{\mathrm{i}q_x l} + e^{-\mathrm{i}q_y l} + e^{\mathrm{i}q_y l} + e^{-\mathrm{i}q_z l} + e^{\mathrm{i}q_z l}\right) = 2J\left(\cos(q_x l) + \cos(q_y l) + \cos(q_z l)\right)$$

And the dispersion in the notation of SpinW law becomes:

$$E_{\mathbf{q}} = 2nSJ\left(\frac{1}{3}\left(\cos(q_x l) + \cos(q_y l) + \cos(q_z l)\right) - 1\right)$$

4.7 Quantum theory of magnetism [13]

The derivation of magnon dispersion is discussed in the section 8.2.1 «Spin-waves theory». The definition of the Hamiltonian is provided on page 238 in eq. 8.2:

> Let us begin by considering a lattice of spins whose interactions may be described by the Heisenberg exchange interaction (2.89). Suppose we apply a uniform static field which serves to define a z-axis. We now wich to determine how this system responds to the time- and space-dependent field $\boldsymbol{H}_1 c$. If this field is in the x direction, the total Hamiltonian becomes
>
> $$H = -\sum_i \sum_{j \neq i} J_{ij} S_i \cdot S_j + g\mu_B H_0 \sum_i S_i^z + g\mu_B H_1 \sum_i S_i^x \cos(\boldsymbol{q}\cdot\boldsymbol{r})\cos(\omega t).$$

There is a double counting in the sum as well as the factor, thus the definition of the Hamiltonian differs from SpinW with the sign, the following notation change is necessary at the end:

$$J \to -J$$

The spin-wave spectra is defined on the page 239 in the eq. 8.10:

$$\omega(\boldsymbol{k}) = \gamma H_0 + \frac{2NS}{\hbar}[J(0) - J(\boldsymbol{q})].$$

where $J(\boldsymbol{k})$ is defined on page 134 in the eq. 4.6:

$$J(-\boldsymbol{q}') \equiv \frac{1}{N}\sum_{i \neq j} J(\boldsymbol{R}_i - \boldsymbol{R}_j) e^{i\boldsymbol{q}'\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}$$

And the dispersion in the notation of SpinW law becomes:

$$\omega(\mathbf{q}) = \frac{2nSJ}{\hbar}\left(\frac{1}{3}\left(\cos(q_x l) + \cos(q_y l) + \cos(q_z l)\right) - 1\right)$$

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