1 Definition of the Hamiltonian

There is a number of details in the definition of the Heisenberg Hamiltonians, which may cause an incompatibility of the direct results. In this paper the main definition is as follows:

$$\hat{H} = -J \sum_{ij} \hat{\mathbf{S}}_i^T \hat{\mathbf{S}}_j, \tag{1}$$

where J is an isotropic exchange parameter. The double counting is present in the Hamiltonian, i.e. both terms $i \to j$ and $j \to i$ are present in the sum. $\hat{\mathbf{S}}_i$ is a 3×1 column vector of the spin operators $(\hat{\mathbf{S}}_i^x, \hat{\mathbf{S}}_i^y, \hat{\mathbf{S}}_i^z)$. Index i run over all N sites in the system and index j runs over neighbors for the site i.

Bold mathematical symbols in this paper represent vectors or matrices and usual symbols – scalars. For instance, J is a scalar exchange parameter, while $\mathbf{J}$ is a matrix of exchange, for the isotropic case it is defined as

$$\mathbf{J} = \begin{pmatrix} J & 0 & 0 \\ 0 & J & 0 \\ 0 & 0 & J \end{pmatrix}$$

Several comparisons of the exchange Hamiltonians and consecutive spin wave Hamiltonians are done in this paper and for each one the details of the convergence are discussed. The results are present in both ways: the original source and in the definition of this paper, when possible.

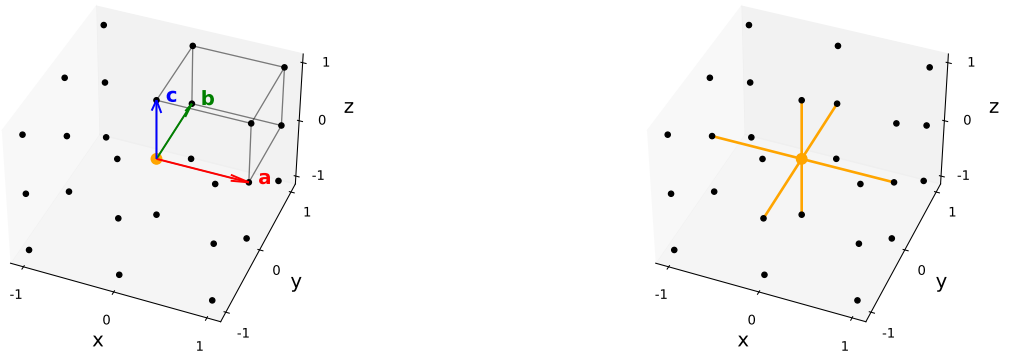
2 Ferromagnetic cubic system

Parameters and they values for the case study system – cubic lattice of ferromagnetic spins oriented along the direction of z axis are defined in this section.

Lattice (see Fig. 1a) in cartesian coordinate system is defined by the lattice parameters and angles:

$$\begin{array}{ccc} \mathbf{a} = (l, 0, 0) & \mathbf{b} = (0, l, 0) & \mathbf{c} = (0, 0, l) \\ \alpha = 90^\circ & \beta = 90^\circ & \gamma = 90^\circ \end{array}$$

In each unit cell one spin $\mathbf{S}$ at the position $(0, 0, 0)$ (in relative coordinates) is oriented along z axis. Each spin has 6 neighbors as shown in Fig. 1b for the $(0, 0, 0)$ unit cell.



(a) (b)

Figure 1: (a) Lattice and (b) 6 neighbors for the spin in $(0, 0, 0)$ unit cell.

The reciprocal lattice is defined as:

$$\mathbf{b_1} = (\frac{2\pi}{l}, 0, 0) \quad \mathbf{b_2} = (0, \frac{2\pi}{l}, 0) \quad \mathbf{b_3} = (0, 0, \frac{2\pi}{l})$$
$$k_\alpha = 90^\circ \qquad k_\beta = 90^\circ \qquad k_\gamma = 90^\circ$$

Y-Γ-X-M-Γ-R-X-M-R path (see Fig. 2) is used for magnon dispersion plots.

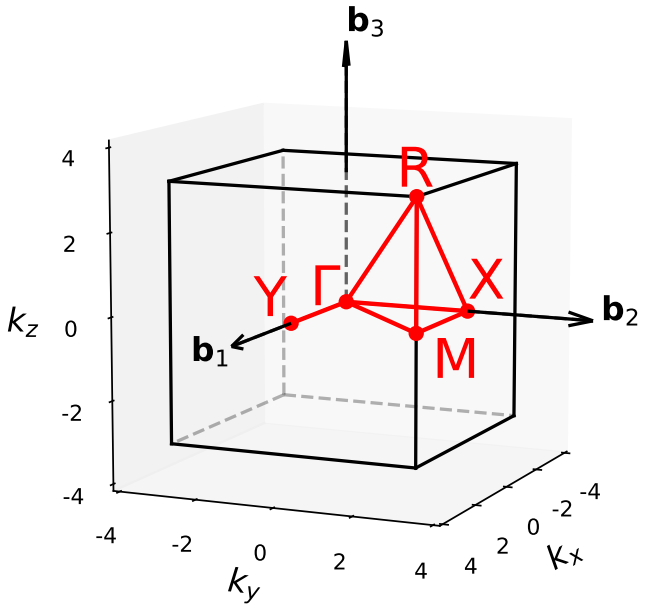


Figure 2: Path for the magnon dispersion plots in reciprocal space: Y-Γ-X-M-Γ-R-X-M-R.

For the final results and for the Figs. 1 and 2 the following numerical values are used:

$$J = 1 \text{ meV}, \quad S = 1, \quad l = 1, \quad n = 6$$

For the 1D chain the values are the same, but $n = 2$.

3 Main magnon dispersion

In Appendix I magnon dispersion is derived from the Hamiltonian in eq. (1). The final result for the cubic system is present in eq. 2 ($n = 6$).

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

For the 1D chain dispersion law is ($n = 2$)

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

It is plotted in Fig. 3 for the path Y-Γ-X-M-Γ-R-X-M-R. The picture is produced with the script «codes/dispersion.py» using «main_dispersion» function.

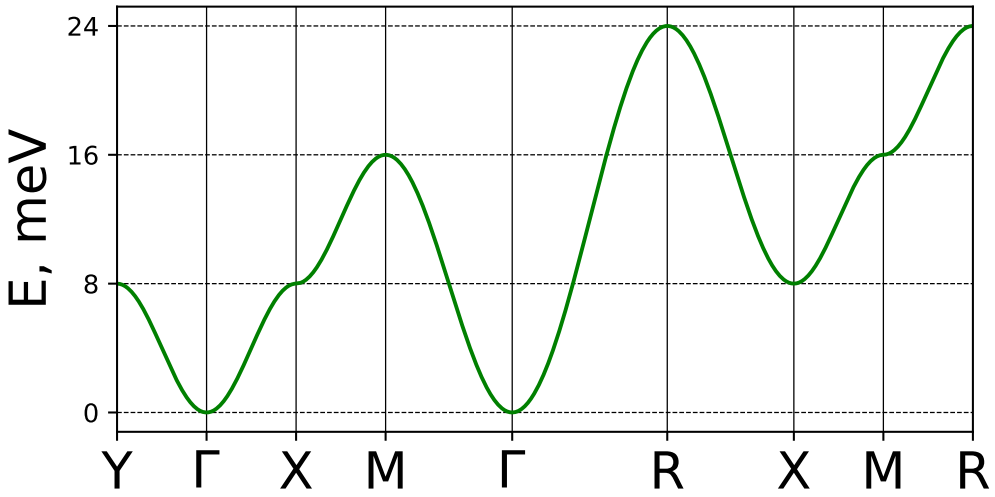


Figure 3: Magnon dispersion plotted with equation (2).

4 Literature check

In this section the result from eq. (2) is compared with the textbook results. Hamiltonian definitions are compared with the equation (1) and conversions are made if necessary, for each source. Detailed analysis of each source is provided in Appendix II. In Table 1 the summary of textbook's review is provided.

Table 1: Comparison of magnon dispersion formulas with textbooks (converted to the notation of this paper).

Source	Formula
This paper	$\hbar\omega(\mathbf{k}) = 2JSn\left(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right)\right)$
[6]	$\hbar\omega(\mathbf{k}) = 2nJS\left(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right)\right)$
[2]	$\hbar\omega(\mathbf{k}) = 2nJS\left(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right)\right)$
[4]	$\hbar\omega(\mathbf{k}) = 2SJn\left(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right)\right)$
[8]	$\hbar\omega(\mathbf{k}) = 2JSn\left(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right)\right)$
[3]	$\hbar\omega(\mathbf{k}) = 2JSn\left(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right)\right)$
[5]	$\hbar\omega(\mathbf{k}) = Sn2J\left(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right)\right)$

5 SpinW

In this section the method from SpinW paper [9] and the results plotted by the code [1] itself are discussed.

First of all, one has to look at the definition of the spin Hamiltonian, which is provided in eq. (1) of [9]:

> We would like to solve the most general magnetic Hamiltonian of interacting localized magnetic moments on a periodic lattice using LSWT. To accomplish this, a method is necessary that can deal with Hamiltonians where the quadratic spin exchange interactions are expressed with 3×3 matrices. In this case the exchange energy of two spins will be a matrix product $\mathbf{S}_i^T \mathbf{J} \mathbf{S}_j$, where $\mathbf{S}_i$ is a 3×1 column vector of the spin operators $\{S_i^x, S_i^y, S_i^z\}$ of site i and $\mathbf{J}$ is the exchange matrix coupling the two sites. $\langle ... \rangle$ Including the external magnetic field and g-tensor, we propose to solve the following Hamiltonian:
>
> $$H = \sum_{mi,nj} \mathbf{S}_{mi}^T \mathbf{J}_{mi,nj} \mathbf{S}_{nj} + \sum_{mi} \mathbf{S}_{mi}^T \mathbf{A}_{mi} \mathbf{S}_{mi} + \mu_B \mathbf{H}^T \sum_{mi} g_i \mathbf{S}_{mi}.$$
>
> The indices m, n are indexing the crystallographic unit cell (running from 1 to L), while i and j label the magnetic atoms inside the unit cell (running from 1 to N), $\mathbf{H}$ is the external magnetic field column vector, μ_B is the Bohr magneton.

This definition includes double counting and is the same as in eq. (1) with an opposite sign of the exchange constant. In order to move to the definition of this paper one needs to introduce the following substitution:

$$J \to -J \tag{5}$$

In the case of the cubic system $N = 1$. On the way of the solution two vectors are introduced: $\mathbf{u}_j$ and $\mathbf{v}_j$, which are defined from the matrix of local rotations $\mathbf{R}'_j$. In the case of the ferromagnetic system no rotation is needed and the local rotation matrix and vectors are (index j is dropped because there is only one magnetic site in unit cell in cubic ferromagnetic system)

$$\mathbf{R}_j = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad \mathbf{u}_j = \begin{pmatrix} 1 \\ \mathrm{i} \\ 0 \end{pmatrix}; \quad \mathbf{v}_j = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

As the next step in the paper Hamiltonian is written with the collective creation and annihilation operators in a matrix form (eq.(23) in [9]):

$$H = \sum_{k \in B.Z.} \mathbf{x}^\dagger(\mathbf{k}) \mathbf{h}(\mathbf{k}) \mathbf{x}(\mathbf{k})$$

where $\mathbf{x}(\mathbf{k}) = [b(\mathbf{k}), b^\dagger(-\mathbf{k})]^T$ for the cubic system. And matrix $\mathbf{h}(\mathbf{k})$ for the cubic system is (definitions in the eqs. (25) and (26) and(14) of [9] are used)

$$\mathbf{h}(\mathbf{k}) = \begin{bmatrix} \hbar\omega_1(\mathbf{k}) & 0 \\ 0 & \hbar\omega_1(-\mathbf{k}) \end{bmatrix}$$

with $(n = 6)$

$$\hbar\omega_1(\mathbf{k}) = SJn \left(\frac{1}{3} \left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l) \right) - 1 \right)$$

or in the notation of this paper (substitution (5))

$$\hbar\omega_1(\mathbf{k}) = SJn\left(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right)\right)$$

which is exactly twice smaller than the result in eq. (2). For the general case $\mathbf{h}(\mathbf{k})$ requires further diagonalization, which is discussed in the section 7 of [9], in the case of a simple cubic system diagonalization procedure is not necessary. The final «diagonalized» Hamiltonian is

$$H = \sum_{\mathbf{k}\in B.Z.}\left(\hbar\omega_1(\mathbf{k})\hat{b}^\dagger(\mathbf{k})\hat{b}(\mathbf{k}) + \hbar\omega_1(-\mathbf{k})\hat{b}(-\mathbf{k})\hat{b}^\dagger(-\mathbf{k})\right)$$

Since $[\hat{b}(\mathbf{k})\hat{b}^\dagger(\mathbf{k})] = 1$

$$H = \sum_{\mathbf{k}\in B.Z.}\left(\hbar\omega_1(\mathbf{k})\hat{b}^\dagger(\mathbf{k})\hat{b}(\mathbf{k}) + \hbar\omega_1(-\mathbf{k})\hat{b}^\dagger(-\mathbf{k})\hat{b}(-\mathbf{k}) + \hbar\omega_1(\mathbf{k})\right) \tag{6}$$

which does not have the desired form of the Hamiltonian of the collection of independent quasiparticles (magnons)

$$\hat{H} = E_0 + \sum_{\mathbf{k}}\hbar\omega(\mathbf{k})\hat{b}^\dagger(\mathbf{k})\hat{b}(\mathbf{k}) \tag{7}$$

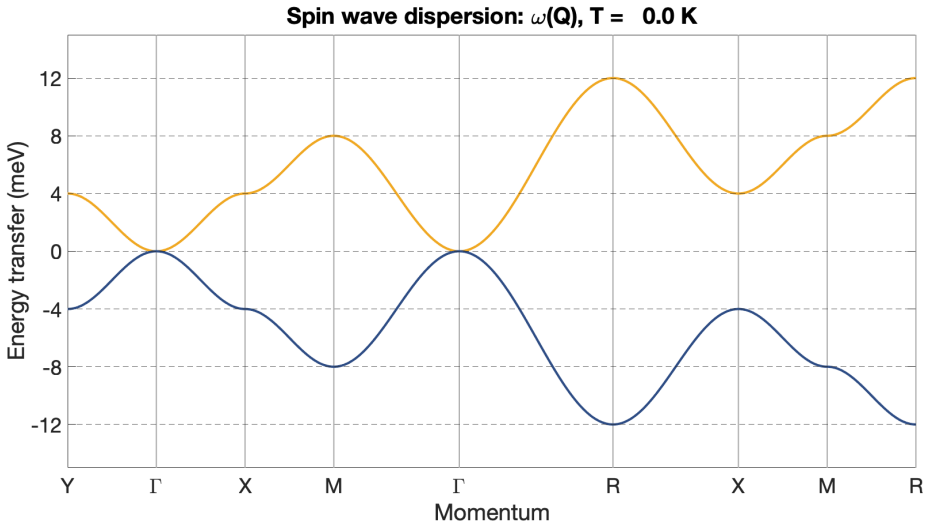


Figure 4: Magnon dispersion plotted with SpinW.

The sum over the Brillouin zone contains the $-\mathbf{k}$ vector for each $\mathbf{k}$ vector, therefore the eq.(6) can be transformed to the desired form of the eq. (7) (the constant energy shift is ignored here):

$$\begin{aligned} H &= \sum_{\mathbf{k}\in B.Z.}\left(\hbar\omega_1(\mathbf{k})\hat{b}^\dagger(\mathbf{k})\hat{b}(\mathbf{k}) + \hbar\omega_1(-\mathbf{k})\hat{b}^\dagger(-\mathbf{k})\hat{b}(-\mathbf{k})\right) \\ &= \sum_{\mathbf{k}\in B.Z.}\left(\hbar(\omega_1(\mathbf{k}) + \omega_1(\mathbf{k}))\hat{b}^\dagger(\mathbf{k})\hat{b}(\mathbf{k})\right) \end{aligned}$$

Which in the case of the cubic system leads to the same result as in eq. (2) in the desired form of eq. (7):

$$H = \sum_{\mathbf{k}\in B.Z.}\left(\hbar\omega(\mathbf{k})\hat{b}^\dagger(\mathbf{k})\hat{b}(\mathbf{k})\right)$$

where (in notation of SpinW)

$$\hbar\omega(\mathbf{k}) = 2\hbar\omega_1(\mathbf{k}) = 2SJn\left(\frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right) - 1\right)$$

However the SpinW code does plot the energies from eq. (6), but multiply the $\hbar\omega_1$ from the second term by -1. In Fig. 4 the dispersion for the same path as in Fig. 3 is plotted. The picture is produces with the script «codes/spinw3D.m», which is based on the Tutorial 1 from the SpinW website (`https://www.spinw.org/tutorials/01tutorial`)

6 «Spin Waves and Magnetic Exchange Hamiltonian in CrSBr»[7]

In this section the fitting of the experimental measurements for magnon dispersion of CrSBr are discussed.

First of all one has to look at the definition of the Hamiltonian in eq. (1) of [7]:

$$H = \sum_{i,j} J_{\langle ij\rangle}\vec{S}_i \cdot \vec{S}_j \tag{8}$$

Double counting is present in this definition (I asked Allen Scheie directly and the answer was yes), therefore the Hamiltonian is defined in the same way as in eq. (1) with the substitution $J \to -J$ (and in the same way as in SpinW).

There are two processes in the experimental paper, which we are interested in:

1. Fitting of experimental data to obtain J values.
2. Plotting of magnon dispersion with SpinW using fitted J values.

6.1 Fit of experimental data

The codes of the paper are public (`doi.org/10.13139/ORNLNCCS/1869252`) and could be examined. Codes of our interest are located in the «CrSB_Data&SpinWaveFits» folder. The script «FitSpinWaves.ipynb» fits the spin-wave energies. In this script several functions from the «pylib.HeisenbergFMSpinWave» are used for plotting of magnon branches. Those functions are written in the file «pylib/HeisenbergFMSpinWave.py». Computation of acoustic and optical branches traces down to the functions «hw_ac» and «hw_op» form this file. Those two functions depend on the function «scriptJs» and global variables «Jz» and «qzero». Finally, there is a piece of code from which one could extract dispersion law used for the fit:

```
@njit
def scriptJs(qvec, J):
    '''create J1 and J2'''

    # Define the q vectors and the energies
    qvrlu = qvec*2*np.pi
    en1 = np.zeros_like(qvec[:,0], dtype=np.complex128)
    en2 = np.zeros_like(qvec[:,0], dtype=np.complex128)

    # Loop through all neighbors
    for i in range(len(dists)):
        d = dists[i]
        if d[-2] >= len(J):  #we got to highest J defined
```

```
                break

            rmr = d[:3] #distance between sites
            Ji = J[int(d[-2])]  #exchange constant

            ### Removed factor of 2 compared to Gd.
            if d[-3] == 1: #It's a site-1 to site-1 exchange
                en1 += Ji*np.exp(-1j*np.dot(qvrlu,rmr))
            elif d[-3] == 2: #It's a site-1 to site-2 exchange
                en2 += Ji*np.exp(-1j*np.dot(qvrlu,rmr))

    return en1, en2

qzero = np.array([[0,0,0]], dtype=np.float64)
Jz = 3/2
Anisotropy = 0.0

@njit
def hw_ac(qvec, J):
    '''accoustic magnon branch. J is a list of exchange
                                                values
    from nearest neighbor to further neighbor'''
    j10, j20 = scriptJs(qzero, J)
    j1, j2 = scriptJs(qvec, J)
    return -Jz*(j10 + j20 - j1 - np.abs(j2)) + Anisotropy

@njit
def hw_op(qvec, J):
    '''optical magnon branch. J is a list of exchange values
    from nearest neighbor to further neighbor'''
    j10, j20 = scriptJs(qzero, J)
    j1, j2 = scriptJs(qvec, J)
    return -Jz*(j10 + j20 - j1 + np.abs(j2)) + Anisotropy
```

The function «scriptJs» prepare $\mathcal{J}(\mathbf{k})$ sum:

$$\mathcal{J}(\mathbf{k}) = \sum_{\delta_i} J_i e^{-\mathrm{i}\mathbf{k}\boldsymbol{\delta}_i}$$

Then functions «hw_ac» and «hw_op» compute dispersion law for the 2 branches, with the equation (for acoustic branch) (J_z in the code is S here):

$$\hbar\omega(\mathbf{k}) = -S(\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{k})) \tag{9}$$

which is the same as the formula from «Rare earth magnetism»[5] (section 8.6) with an additional «−» sign, but the definition of the Hamiltonian in this book is different from the one stated in experimental paper, thus the factor 2 is missing in the eq. (9). Therefore with respect to the definition of the Hamiltonian in eq. (8) the J values in the experimental paper may be overestimated by the factor of 2.

6.2 Plot with SpinW

Plots with SpinW (scripts and input data) are located in «CrSB_Data&SpinWaveFits/SpinW_code» folder. The script, which plots the dispersion of CrSBr is «CSB_dispersions.m». It produces the following pictures for the dispersion:

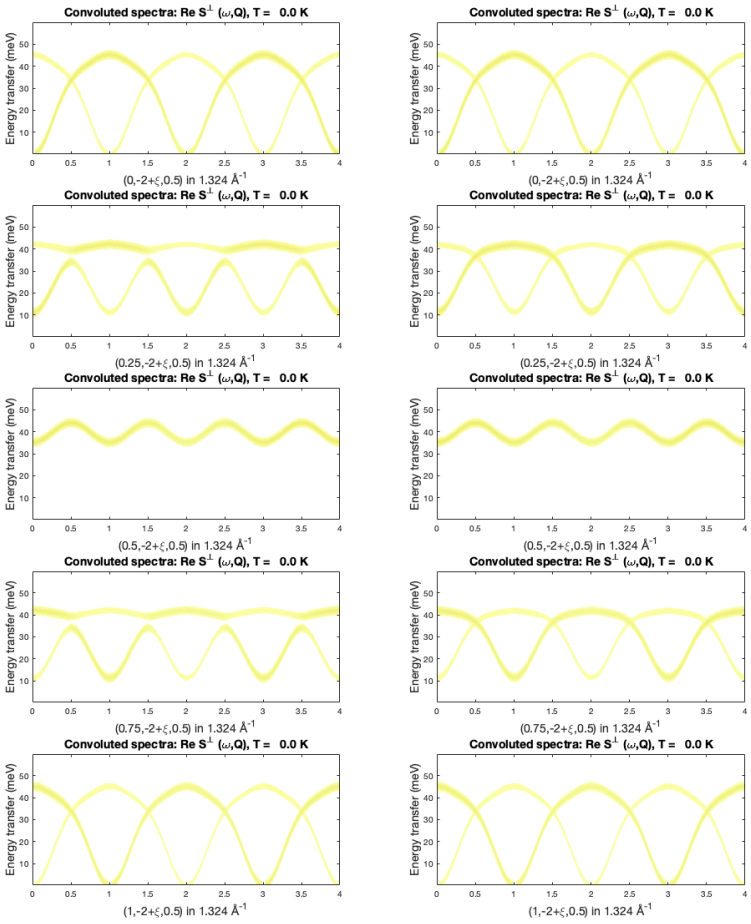


Figure 5: Magnon dispersion from experimental paper plotted with SpinW.

In order to see the second set of branches as in the example of ferromagnetic cubic system (section 5) The code is slightly modified: line

```
sw_plotspec(csbSpec,'axLim',[0 50],'mode',3,'dE',2,'colorbar
                                                    ',false,'legend',false
                                                    )
```

is substituted with

```
sw_plotspec(csbSpec,'mode',1,'colorbar',false,'legend',false
                                                    )
```

which produces the following picture:

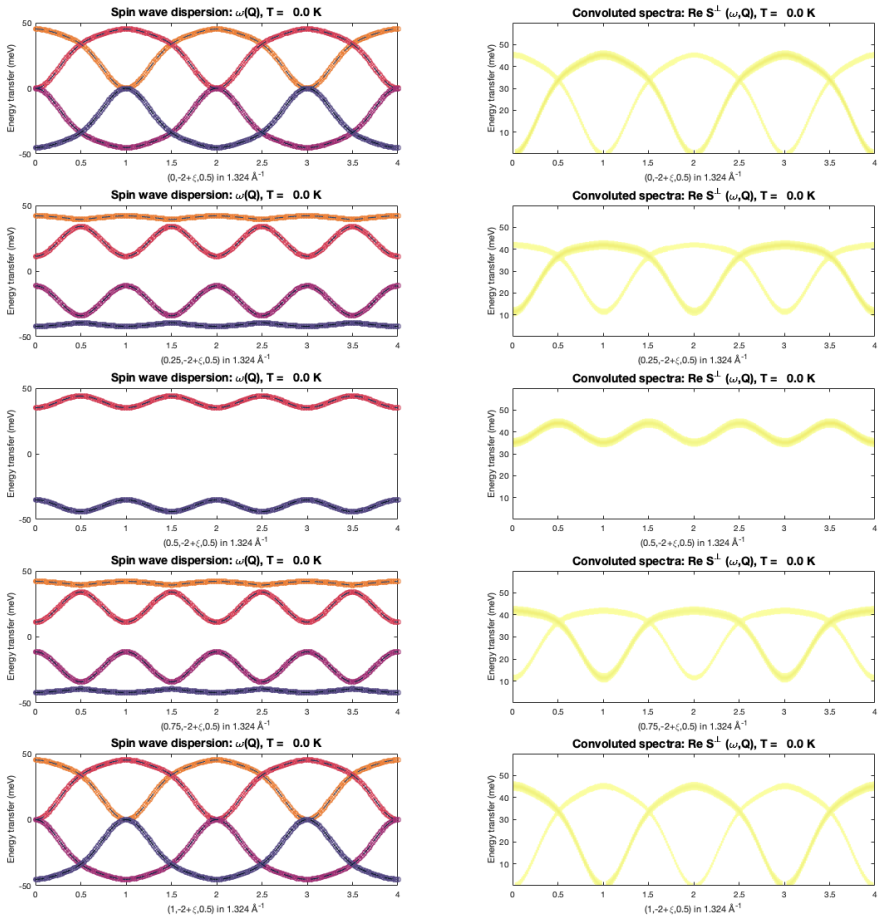


Figure 6: Magnon dispersion from experimental paper plotted with SpinW (with code modification).

One could see that the magnon dispersion (left column) has two sets of branches, which are equal to each other with one being multiply by -1, as it happens with the example of ferromagnetic cubic system. In both cases the values of magnon dispersion are the half of the one from the method of this paper and J values from experimental paper.

In conclusion: The SpinW plots are underestimated by the factor $1/2$.

The final conclusion is that since exchange values are overestimated by the factor of 2 and magnon dispersion from SpinW in underestimated by the factor of $1/2$ the results in the experimental paper are consistent with each other ($2 \cdot 1/2 = 1$), but when one wants to use the J values from experimental paper independently of SpinW code the mismatch of the factor 2 happens.

7 Appendix I

In this section the magnon dispersion law is derived from the Hamiltonian in eq. (1). First of all, the Hamiltonian is rewritten with the raising and lowering spin operators:

$$\hat{S}_i^{\pm} = \hat{S}_i^x \pm \mathrm{i}\hat{S}_i^y$$

$$\hat{\mathbf{S}}_i^T \hat{\mathbf{S}}_j = \hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_j^z; \quad \hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y = \frac{1}{2}\left(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+\right)$$

$$\hat{H} = -J \sum_{ij} \left(\frac{1}{2}\left(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+\right) + \hat{S}_i^z \hat{S}_j^z \right)$$

Since the commutator is

$$\left[\hat{S}_i^+ \hat{S}_j^-\right] = 2\hat{S}_i^z \delta_{ij}$$

and $i \neq j$ in the sum, the Hamiltonian becomes:

$$\hat{H} = -J \sum_{ij} \left(\frac{1}{2}\left(\hat{S}_j^- \hat{S}_i^+ + \hat{S}_i^- \hat{S}_j^+\right) + \hat{S}_i^z \hat{S}_j^z \right)$$

The spin-wave Hamiltonian is obtained with the linearised Holstein–Primakoff formalism.

$$\begin{gathered} \hat{S}_i^+ = \sqrt{2S}\hat{a}_i \\ \hat{S}_i^- = \sqrt{2S}\hat{a}_i^\dagger \\ \hat{S}_i^z = S - \hat{a}_i^\dagger \hat{a}_i \end{gathered}$$

$$\hat{H} = -J \sum_{ij} \left(\frac{1}{2}\left(2S\hat{a}_j^\dagger \hat{a}_i + 2S\hat{a}_i^\dagger \hat{a}_j\right) + \left(S - \hat{a}_i^\dagger \hat{a}_i\right)\left(S - \hat{a}_j^\dagger \hat{a}_j\right) \right)$$

$$\begin{gathered} \hat{H} = E_0 + \hat{H}^{(2)} + \ldots \\ E_0 = -JS^2 Nn \\ \hat{H}^{(2)} = -JS \sum_{ij} \left(\hat{a}_j^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{a}_j - \hat{a}_i^\dagger \hat{a}_i - \hat{a}_j^\dagger \hat{a}_j \right) \end{gathered} \tag{10}$$

where N is the number of spins in the system, n - number of neighbors for each spin (6 in the case of cubic system). From this point the quadratic part of the Hamiltonian $\hat{H}^{(2)}$ is considered.

The Fourier transform is introduced to move from the local operators $\hat{a}_i^\dagger$ and $\hat{a}_i$ to the collective creation and annihilation operators $\hat{a}_k^\dagger$ and $\hat{a}_k$:

$$\hat{a}_i = \frac{1}{\sqrt{N}} \sum_k e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} \hat{a}_k$$

$$\hat{a}_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} \hat{a}_k^\dagger$$

$$\frac{1}{N} \sum_i e^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\mathbf{r}_i} = \delta_{kk'}$$

$$\hat{H}^{(2)} = -JS \sum_i \sum_j \frac{1}{N} \left[\left(\sum_k e^{-\mathrm{i}\mathbf{k}\mathbf{r}_j} \hat{a}_k^\dagger \right) \left(\sum_{k'} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} \hat{a}_{k'} \right) + \left(\sum_k e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} \hat{a}_k^\dagger \right) \left(\sum_{k'} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_j} \hat{a}_{k'} \right) - \left(\sum_k e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} \hat{a}_k^\dagger \right) \left(\sum_{k'} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} \hat{a}_{k'} \right) - \left(\sum_k e^{-\mathrm{i}\mathbf{k}\mathbf{r}_j} \hat{a}_k^\dagger \right) \left(\sum_{k'} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_j} \hat{a}_{k'} \right) \right]$$

Since for each i there is the same pattern of neighbors, sum over j does not depend on i and it can be moved freely. Lets define $\boldsymbol{\delta}_j = \mathbf{r}_j - \mathbf{r}_i$ and rewrite the equation:

$$\hat{H}^{(2)} = -JS \sum_k \sum_{k'} \sum_j \left[e^{-\mathrm{i}\boldsymbol{\delta}_j\mathbf{k}} \left(\frac{1}{N} \sum_i e^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\mathbf{r}_i} \right) \hat{a}_k^\dagger \hat{a}_{k'} + e^{\mathrm{i}\boldsymbol{\delta}_j\mathbf{k}} \left(\frac{1}{N} \sum_i e^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\mathbf{r}_i} \right) \hat{a}_k^\dagger \hat{a}_{k'} - \left(\frac{1}{N} \sum_i e^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\mathbf{r}_i} \right) \hat{a}_k^\dagger \hat{a}_{k'} - e^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\boldsymbol{\delta}_j} \left(\frac{1}{N} \sum_i e^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\mathbf{r}_i} \right) \hat{a}_k^\dagger \hat{a}_{k'} \right]$$

every equation in round parenthesis is equal to $\delta_{kk'}$ and the Hamiltonian becomes

$$\hat{H}^{(2)} = -JS \sum_k \sum_j \left[e^{-\mathrm{i}\boldsymbol{\delta}_j\mathbf{k}} \hat{a}_k^\dagger \hat{a}_k + e^{\mathrm{i}\boldsymbol{\delta}_j\mathbf{k}} \hat{a}_k^\dagger \hat{a}_k - \hat{a}_k^\dagger \hat{a}_k - e^{\mathrm{i}(\mathbf{k}-\mathbf{k})\boldsymbol{\delta}_j} \hat{a}_k^\dagger \hat{a}_k \right] = 2JS \sum_k \sum_j (1 - \cos(\boldsymbol{\delta}_j\mathbf{k})) \hat{a}_k^\dagger \hat{a}_k$$

j runs from 1 to n, therefore:

$$\hat{H}^{(2)} = 2JSn \sum_k \left(1 - \frac{1}{n} \sum_j \cos(\boldsymbol{\delta}_j\mathbf{k}) \right) \hat{a}_k^\dagger \hat{a}_k = \sum_k \hbar\omega(\mathbf{k}) \hat{a}_k^\dagger \hat{a}_k$$

For the cubic system (l - length of the lattice vector):

$$\frac{1}{n} \sum_j \cos(\boldsymbol{\delta}_j\mathbf{k}) = \frac{1}{6} \left(\cos(k_x l) + \cos(-k_x l) + \cos(k_y l) + \cos(-k_y l) + \cos(k_z l) + \cos(-k_z l) \right) = \frac{1}{3} \left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l) \right)$$

and the final formula for the magnon dispersion is

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

8 Appendix II

8.1 «Fundamentals of Magnonics»[6]

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:

$$H = -g\mu_B \sum_i H_z S_i^z - J \sum_{i,\delta} \vec{S}_i \cdot \vec{S}_{i+\delta}, \tag{3.6}$$

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 (we ignore the Zeeman term) is the same as in eq. (1) with the following notation change:

$$\vec{S}_{i+\delta} \to \vec{S}_j, \quad \sum_{i,\delta} \to \sum_{i,j}$$

therefore, no conversion is needed for parameters of this textbook.

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

$$E_k = A_k = g\mu_B H_z + 2zJS(1 - \gamma_k), \tag{3.35}$$

where γ_k is the structure factor given by

$$\gamma_k = \frac{1}{z} \sum_{\vec{\delta}} e^{\mathrm{i}\vec{k}\cdot\vec{\delta}} \tag{3.36}$$

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)):

$$\gamma_k = \frac{1}{3}(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)) \tag{3.37}$$

where a is a lattice parameter (l in the notation of this paper). The final equation from the [6] in the notation of this paper is

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

This equation is the same as eq. (2) ($n = 6$).

8.2 «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,
>
> $$\hat{\mathcal{H}} = -\sum_{\langle ij \rangle} J \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \tag{6.9}$$
>
> (which is eqn. 6.4) In a one-dimensional chain each spin has two neighbours, so the Hamiltonian reduces to
>
> $$\hat{\mathcal{H}} = -2J \sum_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} \tag{6.10}$$

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:
>
> $$\hat{\mathcal{H}} = -\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{4.7}$$
>
> 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
>
> $$\hat{\mathcal{H}} = -2\sum_{i>j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{4.8}$$
>
> 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) is the same as in eq. (1), therefore, no conversion of parameters is needed for this textbook.

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)

$$\hbar\omega = 4JS(1 - \cos(qa)), \tag{6.20}$$
$$E(q) = -2NS^2J + 4JS(1 - \cos(qa)),$$

which matches with the eqs. (10) and (3) where 1D-chain is considered instead of 3D cubic system. Magnon dispersion from eq. (6.20) is plotted in the book on page 123 in figure 6.12 (Fig. 7). Path from 0 to π/a corresponds to the Γ-Y path in Fig. 3. If the parameters from this paper are substitute into the eq. (6.20) then those two graphs are exactly the same.

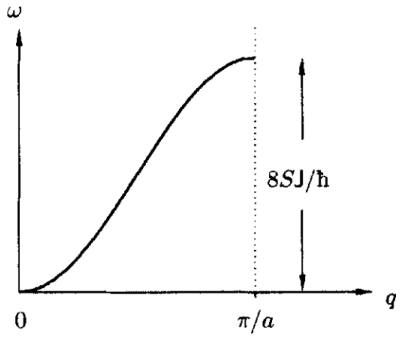


Fig. 6.12 The spin wave dispersion relation for a one-dimensional chain of spins.

Figure 7: Magnon dispersion plot from «Magnetism in condensed matter».

For the cubic system eq. 6.20 looks like:

$$\hbar\omega = 12JS(1 - \frac{1}{3}(\cos(q_x a) + \cos(q_y a) + \cos(q_z a)))$$

If it is to be rewritten with the notation of this paper it looks like ($n = 6$)

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

8.3 «Magnetisation oscillations and waves»[4]

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):

$$\hat{\mathcal{H}} = \gamma\hbar \sum_f \hat{S}_f^z - \sum_f \sum_{f' \neq f} I_{ff'} \mathbf{S}_f \mathbf{S}_{f'} \tag{7.82}$$

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, it is the same definition as in eq. (1) of this paper with the following notation change:

$$f \to i, \quad f' \neq f \to j, \quad I_{ff'} \to J, \quad \mathbf{S}_f \to \mathbf{S}_i, \quad \mathbf{S}_{f'} \to \mathbf{S}_j$$

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

$$\varepsilon_k(k) = \gamma\hbar H + 2S \sum_g [1 - exp(\mathrm{i}\mathbf{k}\mathbf{r}_g)] I_g. \tag{7.99}$$

For the cubic ferromagnet the textbook provides the figure 7.13 (Fig. 8)

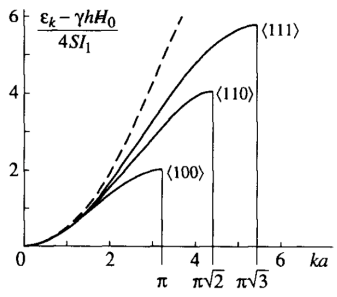
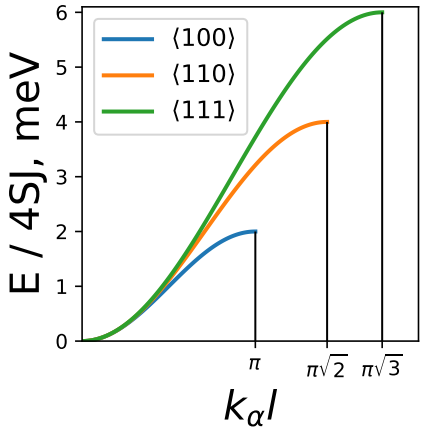


FIGURE 7.13
Dispersion characteristics of spin waves in a ferromagnet with simple cubic spin lattice for different directions of propagation calculated (solid curves) by formula (7.101), i.e., in the nearest-neighbor approximation and without allowance for dipole–dipole interaction. Dashed curve corresponds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

(a) Original plot



(b) Same plot with use of eq. (2)

Figure 8: Magnon dispersion plot from «Magnetisation oscillations and waves».

In this picture curve $\langle 100 \rangle$ (from 0 to π) corresponds to the path Γ-Y, curve $\langle 110 \rangle$ (from 0 to $\pi\sqrt{2}$) to the path Γ-M and curve $\langle 111 \rangle$ (from 0 to $\pi\sqrt{3}$) to the path Γ-R in the Fig. 3. In Fig. 8b 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 is

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

where g varies from 1 to 6, $r_g \in [r_x, -r_x, r_y, -r_y, r_z, -r_z]$ and $I_g = I$ for each g.

In the notation of this paper the dispersion law becomes ($n = 6$)

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

8.4 «The Oxford Solid State Basics»[8]

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
>
> $$\hat{\mathcal{H}} = -\frac{1}{2}\sum_{\langle i,j \rangle} J\mathbf{S}_i \cdot \mathbf{S}_j + \sum_i g\mu_B \mathbf{B} \cdot \mathbf{S}_i \qquad (20.6)$$
>
> 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).
>
> $\langle ... \rangle$

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*

$$\hat{\mathcal{H}} = -\frac{1}{2}\sum_{\langle i,j\rangle} J\mathbf{S}_i \cdot \mathbf{S}_j \tag{20.2}$$

The double counting is present in this Hamiltonian, thus, it is the same definition as in eq. (1) of this paper with the additional factor of 1/2, thus if we assume that definition of «The Oxford Solid State Basics» and this paper give the same Hamiltonian one have to introduce the following substitution of exchange parameter in order to move to the definition of this paper:

$$J \to 2J \tag{11}$$

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 this paper (with the substitution (11)) the dispersion law becomes ($n = 6$)

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

8.5 «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:

$$\hat{\mathcal{H}} = -2\sum_{i>j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j \tag{5.24}$$

In this definition there is no double counting ($i > j$), but there is a factor of 2 present, thus exchange constants of the Hamiltonian in eq. (5.24) are the same as in eq. (1) and final results for magnon dispersion are directly comparable.

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

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

And the dispersion law becomes:

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

which is the same as eq. (2).

8.6 «Rare earth magnetism»[5]

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):

$$\hat{\mathcal{H}} = \sum_i \left[\sum_{l=2,4,6} B_l^0 Q_l^0(\mathbf{J}_i) + B_6^6 Q_6^6(\mathbf{J}_i) - g\mu_B \mathbf{J}_i \cdot \mathbf{H}\right] - \frac{1}{2}\sum_{i\neq j} \mathcal{J}(ij)\mathbf{J}_i \cdot \mathbf{J}_j \quad (5.2.1)$$

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, thus, it is the same definition as in eq. (1) of this paper with the additional factor of 1/2, therefore, if we assume that definition of «Rare earth magnetism» and this paper give the same Hamiltonian one have to introduce the following substitution of exchange parameter in order to move to the definition of this paper:

$$\mathcal{J} \to 2J$$

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

The energy parameters are

$$U_1 = \frac{1}{2}\sum_{\mathbf{q}}(E_{\mathbf{q}} - A_{\mathbf{q}}); \quad E_{\mathbf{q}} = \sqrt{A_{\mathbf{q}}^2 - B^2}. \quad (5.2.22)$$

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

$$\begin{gathered} A = \frac{1}{J}\left\{3B_2^0 J^{(2)} - 21B_6^6 J^{(6)}\cos 6\phi + g\mu_B JH\cos(\phi - \phi_H)\right\} \\ B = \frac{1}{J}\left\{3B_2^0 J^{(2)} + 15B_6^6 J^{(6)}\cos 6\phi\right\}. \end{gathered} \quad (5.2.15)$$

$\langle ... \rangle$

$$A_{\mathbf{q}} = A + J\left\{\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q})\right\} \quad (5.2.18)$$

$A = 0$ 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. (**??**):

$$\mathcal{J}_{ss\prime}(\mathbf{q}) = \sum_{j \in s\prime - subl.} \mathcal{J}(ij) e^{-\mathrm{i}\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}; \quad i \in s - sublattice, \tag{5.1.1a}$$

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 law becomes:

$$E_{\mathbf{q}} = S(6J - 2J\left(\cos(q_x l) + \cos(q_y l) + \cos(q_z l)\right))$$

In the notation of this paper after the substitution (8.6) formula for the dispersion law is ($n = 6$)

$$E_{\mathbf{k}} = Sn2J(1 - \frac{1}{3}\left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l)\right))$$

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[1] Spinw. `https://www.spinw.org/`.

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