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 work 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 will be done in this paper and for each one the details of the convergence will be discussed. When possible the results will be present in both ways: the original source and in the definition of this paper.

2 Ferromagnetic cubic system

In this section I will define the parameters and they values for the case study system - cubic lattice of ferromagnetic spins oriented along the direction of z axis.

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

$$\mathbf{a} = (l, 0, 0) \quad \mathbf{b} = (0, l, 0) \quad \mathbf{c} = (0, 0, l)$$
$$\alpha = 90° \qquad \beta = 90° \qquad \gamma = 90°$$

In each unit cell there is one spin S at the position $(0, 0, 0)$ (in relative coordinates).

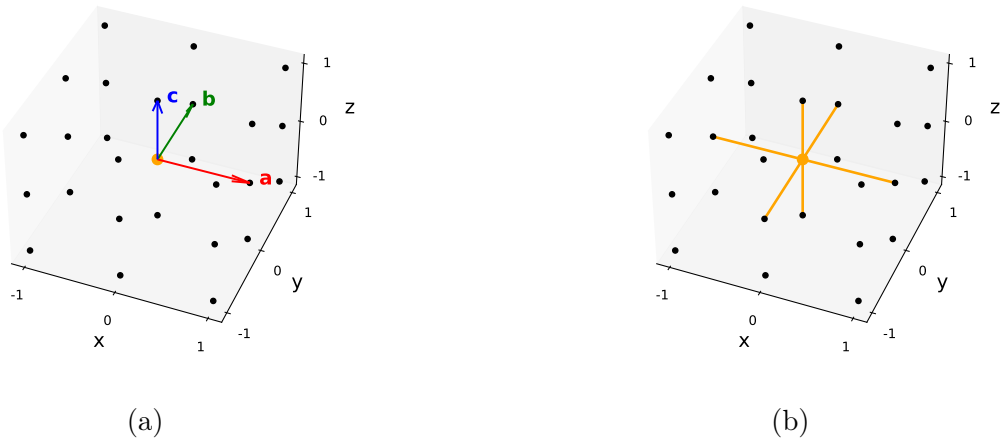Spin in the $(0, 0, 0)$ unit cell will have 6 neighbors as shown in Fig. 1b.

(a)   (b)

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

The reciprocal lattice will have the form of:

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

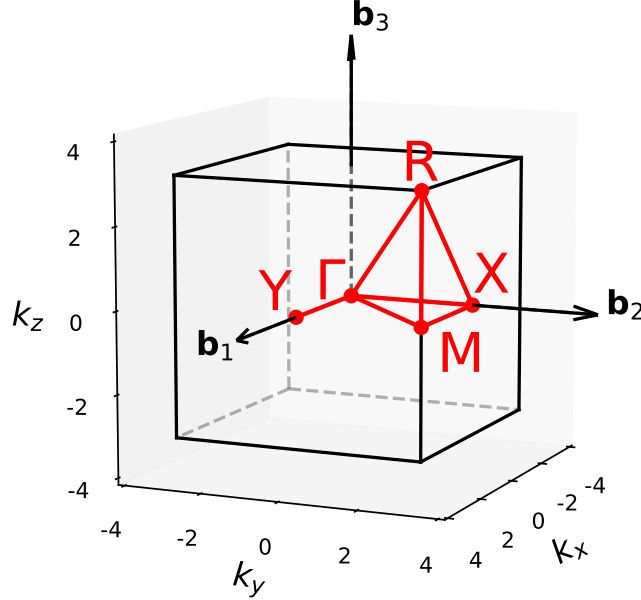Magnon dispersion plots will use the following path: Y-Γ-X-M-Γ-R-X|M-R (see Fig. 2).

Figure 2: Path in reciprocal space for the magnon dispersion plot: 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:

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

3 Main magnon dispersion

In Appendix I magnon dispersion is derived from the Hamiltonian in (1). The final result is present in equation 2.

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

In Fig. 3 is plotted 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.
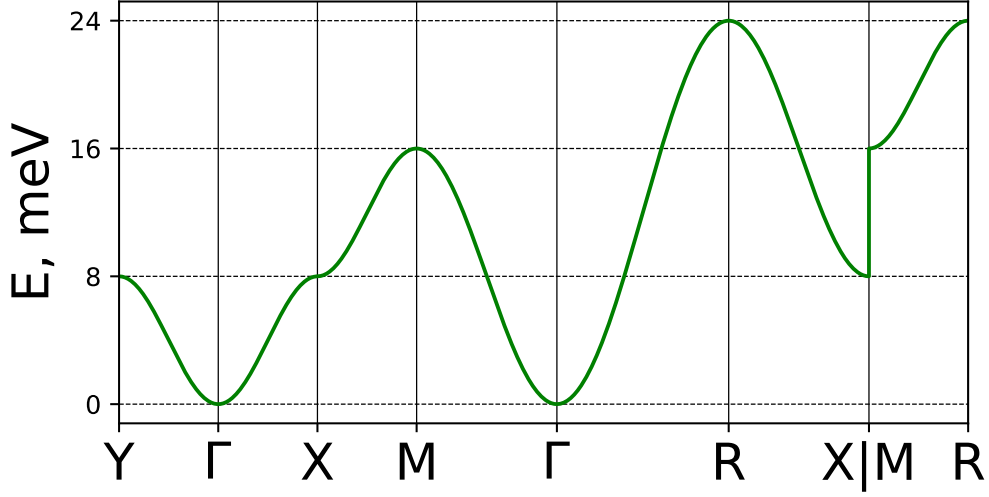
2

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

4 Literature check

In this section I will compare the result in equation (2) with the textbook results. For each source Hamiltonian definitions are compared with the equation (1) and make conversion if necessary. Detail consideration of each source is provided in Appendix II. In Table 1 the summary of textbooks review is provided.

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

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

3

5 Appendix I

In this section I will derive the magnon dispersion formula from the Hamiltonian in (1). First of all I rewrite the Hamiltonian using the raising and lowering spin operators:

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

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

since

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

and $i \neq j$ in the sum:

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

From this point the Hamiltonian is treated in the linearised Holstein–Primakoff formalism.

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

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

$$\hat{H} = E_0 + \hat{H}^{(2)} + \dots$$

$$E_0 = -JS^2Nn \tag{3}$$

$$\hat{H}^{(2)} = -JS\sum_{ij}\left(\hat{a}_j^\dagger\hat{a}_i + \hat{a}_i^\dagger\hat{a}_j - \hat{a}_i^\dagger\hat{a}_i - \hat{a}_j^\dagger\hat{a}_j\right) \tag{4}$$

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 I focus on the quadratic part of the Hamiltonian $\hat{H}^{(2)}$.

In the next step the Fourier transform is used 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 $\hat{a}_k$:

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

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

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

By substituting it into eq. (4) I get:

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

$$+ \left(\sum_k e^{-i\mathbf{k}\mathbf{r}_i} \hat{a}_k^\dagger \right) \left(\sum_{k'} e^{i\mathbf{k}'\mathbf{r}_j} \hat{a}_{k'} \right)$$

$$- \left(\sum_k e^{-i\mathbf{k}\mathbf{r}_i} \hat{a}_k^\dagger \right) \left(\sum_{k'} e^{i\mathbf{k}'\mathbf{r}_i} \hat{a}_{k'} \right)$$

$$\left. - \left(\sum_k e^{-i\mathbf{k}\mathbf{r}_j} \hat{a}_k^\dagger \right) \left(\sum_{k'} e^{i\mathbf{k}'\mathbf{r}_j} \hat{a}_{k'} \right) \right]$$

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

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

$$+ e^{i\boldsymbol{\delta}_j \mathbf{k}} \left(\frac{1}{N} \sum_i e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}_i} \right) \hat{a}_k^\dagger \hat{a}_{k'}$$

$$- \left(\frac{1}{N} \sum_i e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}_i} \right) \hat{a}_k^\dagger \hat{a}_{k'}$$

$$\left. - e^{i(\mathbf{k}'-\mathbf{k})\boldsymbol{\delta}_j} \left(\frac{1}{N} \sum_i e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}_i} \right) \hat{a}_k^\dagger \hat{a}_{k'} \right]$$

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

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

since for each $\boldsymbol{\delta}_j$ there is $-\boldsymbol{\delta}_j$ present in the sum over j we can rewrite the Hamiltonian one more time:

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

j runs from 1 to n, therefore:

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

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

$$\frac{1}{n} \sum_j e^{i\boldsymbol{\delta}_j \mathbf{k}} = \frac{1}{6} \left((e^{ik_x l} + e^{-ik_x l}) + (e^{ik_y l} + e^{-ik_y l}) + (e^{ik_z l} + e^{-ik_z l}) \right)$$

$$= \frac{1}{3} \left(\cos(k_x l) + \cos(k_y l) + \cos(k_z l) \right)$$

and the final formula for the magnon dispersion looks like

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

6 Appendix II

6.1 «Fundamentals of Magnonics»[5]

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, equation (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 (1): $i + \delta \rightarrow j$ and $\sum_{i,\delta} \rightarrow \sum_{i,j}$, therefore, no conversion is needed for parameters for this textbook.

Magnon dispersion is provided on page 78 in equations (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

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

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 equation (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 [5] 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 equation (2).

6.2 «Magnetism in condensed matter»[1]

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 equations (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 equations (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 ith 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 equation (6.9) corresponds to the definition in equation (4.7) and the equation (6.10) corresponds to the definition in equation (4.8). The definition in equation (4.7) is the same as in equation (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)

$$\hbar\omega = 4JS(1 - \cos(qa)), \tag{6.20}$$

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

which matches with the equations (3) and (2) if $n = 2$ is used and 1D-chain instead of 3D cubic system is considered. Magnon dispersion from equation (6.20) is plotted in the book on page 123 in figure 6.12 (Fig. 4). Path from 0 to π/a corresponds to the Γ-X path in Fig. 3. If the parameters from this paper are substitute into the eq. (6.20) then those two graphs are be exactly the same.
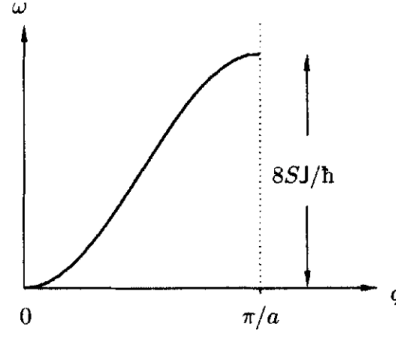
Fig. 6.12 The spin wave dispersion relation for a one-dimensional chain of spins.

Figure 4: Magnon dispersion plot from «Magnetism in condensed matter».

For the cubic system eq. 6.20 will look 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 will look like

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

6.3 «Magnetisation oscillations and waves»[3]

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 equations (7.82) and (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 equation (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

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

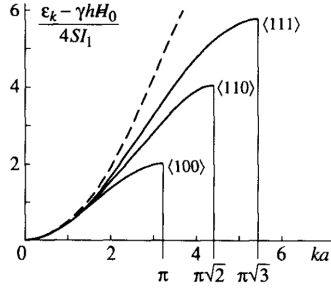For the cubic ferromagnet the textbook provides the figure 7.13 (Fig. 5)

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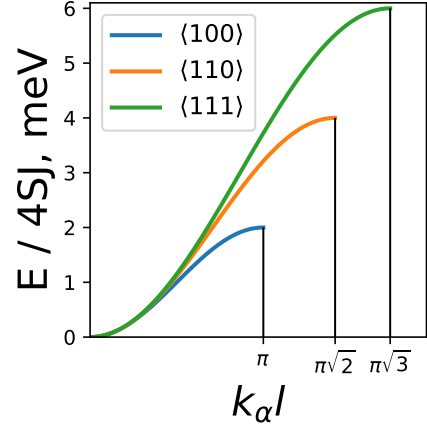
(b) Same plot with use of eq. (2)

Figure 5: 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. 5b the same graph is plotted by using the equation for magnon dispersion from this paper.

The dispersion law from eq. 7.99 for the cubic system will be

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

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

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

6.4   «The Oxford Solid State Basics»[6]

6.5   «Magnetism and magnetic materials»[2]

6.6   «Rare earth magnetism»[4]

References

[1] Stephen Blundell. Magnetism in condensed matter, 2003.

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[3] Alexander G Gurevich and Gennadii A Melkov. *Magnetization oscillations and waves*. CRC press, 1996.

[4] Jens Jensen and Allan R Mackintosh. *Rare earth magnetism*. Clarendon Press Oxford, 1991.

[5] Sergio M Rezende. *Fundamentals of magnonics*, volume 969. Springer, 2020.

[6] Steven H Simon. *The Oxford solid state basics*. OUP Oxford, 2013.