Low-lying spin excitations due to next-nearest neighbour interactions in a ferromagnetic lattice with a body-centred cubic (bcc) crystal structure

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Abstract. Spin excitations due to the next-nearest-neighbour interactions are investigated for a ferromagnetic lattice with a body-centred cubic (bcc) crystal structure. Using the three-dimensional Heisenberg spin model in a uniform external magnetic field, both the nearest-neighbour (NN) and next-nearest-neighbour (NNN) exchange interactions are considered. The spin wave energies at low temperatures are calculated for which the system is close to its ground state. From the dispersion plots, the additional exchange interactions by the NNN cause an increase in the spin excitation energies. Furthermore, there is a critical NNN/NN exchange ratio for which the effect of the NNN interactions becomes evident as characterized by the presence of two maximum energy peaks in the energy spectra.

1. Introduction
Spin waves (SWs) are collective excitations of spins in a magnetic lattice. Many factors that cause the occurrence of SWs include the short exchange and long range dipolar interactions, magnetic anisotropies, distortions due to magnetic impurities and application of an external field. These spin excitations can be derived using the Heisenberg spin Hamiltonian. For the case where both the nearest- and next-nearest-neighbour exchange interactions are considered, the Hamiltonian has the form

\[ \hat{H} = -\sum_{NN} J_{uv} \vec{S}_u \cdot \vec{S}_v - \sum_{NNN} J_{uv'} \vec{S}_u \cdot \vec{S}_{v'} \]  

(1)

Here the first and the second terms are summed over all pairs of nearest-neighbour (NN) and next-nearest-neighbour (NNN) spins, respectively. The exchange constants \( J_{uv} \) and \( J_{uv'} \) denote the strength of the interaction between a spin \( \vec{S}_u \) at site \( u \) with its NN spin \( \vec{S}_v \) at site \( v \) and its NNN spin \( \vec{S}_{v'} \) at site \( v' \). By convention, the exchange constant is positive (negative) to indicate ferromagnetic (anti-ferromagnetic) alignment.

Although NN interactions are dominant, the coupling between NNN spins are also important particularly at low temperatures. The inclusion of such interactions can bring about the following effects - magnetic frustration [1], competing exchange interactions [2] and spatial anisotropy - which can alter the properties of most magnetic systems. Xue et al., on one hand, attributed
the increase of the absolute spin wave energy of both isotropic and anisotropic two-sublattice ferrimagnets to the NNN exchange interaction [3].

The coupling between NN and NNN spins in a lattice generally depend on their spatial arrangement. Nguyen et al., for example, have shown that SW frequencies vary for ultra-thin ferromagnetic films of different lattice structures having different NN and NNN spin distribution [4]. Here they analytically obtained an expression for the SW mode frequencies and performed numerical evaluation to derive the dispersion plots. The spin excitations were taken perpendicular to the film with spin waves propagating along the film surface oriented either parallel or transverse to the saturation magnetization.

In most materials, these excitations may have components in three dimensions (3D). The Hamiltonian in (1) must be expressed accordingly in three dimensions. However such spin Hamiltonian problem in 3D has no exact solution and can only be solved numerically by various means - Monte Carlo (MC) simulations, effective-field theory [2], among others. For the case of a ferromagnet at its ground state, this 3D problem becomes analytically solvable - with all spins aligned along the saturation magnetization. From this, the spin waves energies near the ground state can be calculated. This was shown in our previous work wherein using a semi-classical approach [5] we obtained the dispersion relation for an isotropic ferromagnetic lattice with simple cubic (sc) crystal structure [6]. In the semi-classical approach, the spins are treated as classical 3D vectors that obey commutation relations as quantum mechanical operators. The relative effects of the NN and NNN interactions on the spin excitations were shown by varying the exchange interaction ratio $J_2/J_1$, where $J_{uv} ≈ J_2$ and $J_{uv} ≈ J_1$ (isotropic case). The results that we obtained agrees with that found by Xue et al. [3].

In this paper, we present an extension of our formulation for the case of ferromagnetic body-centred crystal (bcc) structure and compare the dispersion plot with that obtained for the sc case. Thus the results may be used to characterize elements, such as Cr and Fe, that exist in cubic phase with body-centred crystal structure.

2. Dispersion relation

Our ferromagnetic system consists of magnetic ions arranged on a body-centred crystal structure as shown in figure 1 with an applied magnetic field along the z-axis. The Heisenberg Hamiltonian in (1) has the form

$$
\hat{H} = -J_1 \sum_{u} \sum_{v=1}^{8} \vec{S}_u \cdot \vec{S}_v - J_2 \sum_{u} \sum_{v'=9}^{14} \vec{S}_u \cdot \vec{S}_{v'} - g\mu_B \sum_u \vec{B} \cdot \vec{S}_u .
$$

(2)

Figure 1. Schematic representation of magnetic ions on a ferromagnetic bcc lattice with unit cell size $a$. A spin $\vec{S}_u$ on site $u$ has eight NNs (white spheres) and six NNNs (black spheres) at a distance $\sqrt{3}a/2$ and $a$, respectively.

where $g$ and $\mu_B$ are the Landé factor and the Bohr magneton constant, respectively. Here the corresponding exchange constants are taken to be equal between NN and NNN spins, i.e.
$J_{xy} \approx J_1$ and $J_{uv} \approx J_2$. Also, the spins are assumed dimensionless; with units of energy assigned to the NN and NNN exchange constants. The last term is the Zeeman effect which causes an upward or downward shift to the excitation energy depending on the applied field $B_{\text{ext}}$. The ground state of the system is characterized by magnetic moments oriented parallel to the external magnetic field. For bulk materials, the dispersion relations are obtained for spins which are far from the boundaries or edges and are, thus, free of surface-related effects.

Spin waves in ferromagnetic lattices are brought about by the precession of the spins about the external field. Spin excitations are calculated from the equations of motion using semi-classical which are far from the boundaries or edges and are, thus, free of surface-related effects.

Spin excitations are small enough such that the magnitude of the spin z-component (parallel to $B_{\text{ext}}$) causes an upward or downward shift to the excitation energy depending on the applied field $J_1$. Here the spins are treated as classical vectors given by superscripts $x$, $y$ and $z$. How they propagate in time can be derived from the commutation relation given by

$$\frac{d\vec{S}_u}{dt} = \frac{1}{\hbar} [\vec{S}_u, \hat{H}],$$  \hspace{1cm} (3)

where $\hbar$ is the Planck’s constant divided by $2\pi$. These spin vectors satisfy the following identities: $[S_1^\alpha, S_2^\beta] = [S_2^\alpha, S_1^\beta] = [S_1^\alpha, S_2^\beta] = 0$ and $[\vec{S}_u, \vec{S}_v] = [\vec{S}_u, \vec{S}_v] = 0$, where indices $\alpha$ and $\beta$ denote the spin component. Labels $A$ and $B$ represent two different lattice sites.

The average value of the spin fluctuations at site $u$ can be expressed as

$$\frac{d\langle \vec{S}_u \rangle}{dt} = \frac{dS_{ux}^u}{dt} \hat{x} + \frac{dS_{uy}^u}{dt} \hat{y} + \frac{dS_{uz}^u}{dt} \hat{z},$$  \hspace{1cm} (4)

where each term represents the spin excitations in three coordinate axes. We then evaluate (4) near the ground state for which all spins align to the external field $B_{\text{ext}}$. Using the random phase approximation [7], we have considered that $S_{ux}^u$ is approximately equal to the mean value of the z-component of all the spins, $S$. For a spin 1/2 particle, $S = 1/2$. In addition to this, the spin excitations are small enough such that the magnitude of the spin z-component (parallel to $B_{\text{ext}}$) is considered to be larger than the x- and y-components, i.e. $S_{ux}^u >> S_{uy}^u, S_{uz}^u$. The mean spin fluctuations are then reduced to

$$\frac{dS_{ux}^u}{dt} \approx \frac{8J_1}{\hbar} S_{uy}^u - \frac{J_1}{\hbar} \sum_v S_{vy}^v + \frac{6J_2}{\hbar} S_{uy}^u - \frac{J_2}{\hbar} \sum_{v'} S_{vy}^{v'} - g\mu_B B_{\text{ext}} S_{uy}^u,$$  \hspace{1cm} (5)

$$\frac{dS_{uy}^u}{dt} \approx -\frac{8J_1}{\hbar} S_{ux}^u + \frac{J_1}{\hbar} \sum_v S_{vx}^v - \frac{6J_2}{\hbar} S_{ux}^u + \frac{J_2}{\hbar} \sum_{v'} S_{vx}^{v'} + g\mu_B B_{\text{ext}} S_{ux}^u,$$  \hspace{1cm} (6)

and

$$\frac{dS_{uz}^u}{dt} \approx 0$$  \hspace{1cm} (7)

since the fluctuations along the z-axis is approximately zero for the case near the ground state.

The linearized equations in (5) and (6) have normal mode solutions of the general form

$$S_{ux}^{ul(mk)} = Ge^{iq_xkd_x}e^{iq_ymd_y}e^{iq_zkd_z}e^{-\omega t}, \quad S_{uy}^{ul(mk)} = iGe^{iq_xkd_x}e^{iq_ymd_y}e^{iq_zkd_z}e^{-\omega t}$$  \hspace{1cm} (8)

where $G$ and $\omega$ are the normalization constant and the SW angular frequency, respectively. We use subscript indices $l$, $m$ and $k$ to label the lattice site where the spin is located. The x-, y- and z-components of the distance between the spins are $d_x, d_y$ and $d_z$, respectively. Here we consider spin waves propagating in the solid uniformly along the x-, y- and z-axis with $q_x = q_y = q_z = q$.

Inserting equations (8) to (5) and (6), we obtain the spin wave energy given by

$$E_o = 2J_1[4 - \cos(3qa/2) - 3\cos(qa/2) + 3\lambda(1 - \cos qa)].$$  \hspace{1cm} (9)

Here $E_o$ represents only the energy due to the spin interactions and we have neglected the constant Zeeman energy. The coefficient $\lambda$ is the exchange interaction ratio equal to $J_2/J_1$. 

3
3. Spin wave spectra

Figure 2 shows the energy spectra for the ferromagnetic bcc lattice with unit cell size $a = 1\,\text{Å}$ and $J_1 = 1.602 \times 10^{-21}$ joule (spin fluctuations are of the order 10 meV) for exchange interaction ratios $\lambda = 0, 0.25, 0.50$ and 0.75. On the other hand, the figure on the right shows the recalculated spin wave energies for the sc case from our previous paper [6]. The dispersion curves for the sc case are periodic over the range $2\pi$, while the bcc spectra are periodic over the range $4\pi$. This difference in the period between the sc and bcc spectra can be traced from the chosen normal mode solutions in (8).

Clearly from figures 2 and 3, as the exchange ratio $\lambda$ is increased from 0 to 0.75 the spin wave energy increases in both ferromagnetic systems. This is a direct consequence of the additional exchange due to the NNN interactions. Taking the bcc case in figure 2, for example, the spin wave energy maximum increases from $E_o = 0.25632 \times 10^{-19}\,\text{J}$ to $E_o = 0.36846 \times 10^{-19}\,\text{J}$ as $\lambda$ is varied from 0 to 0.75. This agrees with the results of Majumdar [1] and of Almeida et al. [7], and is discussed thoroughly by Xue et al. [3]. Aside from this, increasing NNN interactions causes two peaks in both lattices which is more evident at $\lambda > 0.5$ for the sc and $\lambda = 0.75$ for the bcc case. These critical values of $\lambda$ can actually be determined analytically by minimizing the spin wave energies [6]. These two peaks feature in the energy can be related to the creation of two degenerate states with increasing NNN interactions.

The dispersion curves of the two systems behave differently if NNN interactions are ignored, i.e. $\lambda = 0$. As seen from figure 3 the sc dispersion only has a global maximum at $qa = \pi$ as compared to the bcc plot in figure 2 that has two relative maxima in addition to its maximum peak at $qa = 2\pi$. The presence of the two small peaks in the bcc spectra is caused by the diagonal arrangements of the NN spins. The central peak at $qa = 2\pi$ is attributed to the net lateral effects of the exchange interaction, similar to the sc case that has six lateral NN spins.

4. Conclusion

In this paper, we have shown that increasing next-nearest neighbour interactions yield spin waves with higher energies. Furthermore the NNNs leads to the creation of two degenerate states for both ferromagnetic bcc crystal structures.

References

[1] Majumdar K 2011 J. Phys.: Condens. Matter 23 116004-116009
[2] dos Anjos R, Viana R, de Sousa R and Plascak J A 2007 Phys. Rev. E 76 022103
[3] Xue D S, Gao M Z, Yang J B, Kong Y and Li F S 1996 Phys. Status Solidi (B) 193 161-166
[4] Nguyen H T and Cottam M G 2011 J. Phys.: Condens. Matter 23 126004-126012
[5] Keffer F, Kaplan H and Yafet Y 1953 Amer. J. Phys. 21 250-257
[6] Baldo C III and Villagonzalo C 2010 Proc. 28th SPP Phys. Congress (Antipolo City) p 11
[7] Almeida N S, Fulco P, Albuquerque E L and Tilley D R 1992 J. Phys.: Condens. Matter 4 8909-18