Finite temperature magnon spectra in yttrium iron garnet from a mean field approach in a tight-binding model

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Abstract
We study magnon spectra at finite temperature in yttrium iron garnet using a tight-binding model with nearest-neighbor exchange interaction. The spin reduction due to thermal magnon excitation is taken into account via the mean field approximation to the local spin and is found to be different at two sets of iron atoms. The resulting temperature dependence of the spin wave gap shows good agreement with experiment. We find that only two magnon modes are relevant to the ferromagnetic resonance.

1. Introduction

Since its discovery decades ago [1], yttrium iron garnet (YIG) has been regarded as one of the most important magnetic materials due to its extremely low magnetic damping and other intriguing properties [2]. As an insulator, YIG is free from Joule heating, revealing its promising applications in future low energy consumption devices, which makes it a popular material in recent studies on magnonics [3, 4] and spin caloritronics [5]. While the applications in magnonics mainly rely on the coherent transport properties of the spin waves with relatively long wavelengths (\(\sim \mu m\)) and low frequencies (\(\sim GHz\)), in spin caloritronic devices, the short-wavelength spin waves dominate because of their significant population due to thermal excitation. In the latter case, recent experiments show that the diffusion length of the thermal magnons can reach up to tens of microns [6, 7] and presents very interesting behaviors with respect to the variation of the external magnetic field and temperature [8–10], which have not been well understood so far. Moreover, the magnon diffusion length appears to be sensitive to the measurement technique used [6, 7]. The full understanding of these observations requires a comprehensive study of the dissipation processes in a wide range of magnon frequency up to several THz.

In the literature, great efforts [11–13] have been devoted to explain the origin of the magnetic damping in YIG measured by ferromagnetic resonance [14–19] or parametric pumping [20, 21]. Several mechanisms were proposed to be relevant, such as the magnon-impurity scattering, the magnon–phonon scattering, and the magnon–magnon scattering. Since the frequencies in both ferromagnetic resonant experiment and parametric pumping mainly lie in the GHz regime, the applicability of the conclusion there to the THz thermal magnons is questionable. In some recent works, the lifetime of the thermal magnons in YIG was estimated using a single parabolic dispersion [8], which however is valid only for GHz magnons and deviates far from the real spectra for GHz magnons. Moreover, at room temperature, several magnon bands in YIG are thermally excited [22, 23], which also reveals the limitation of the single band model.

The full magnon band structure of YIG was modeled by Harris [24] with nearest-neighbor exchange interaction and measured from neutron scattering by Plant [22], from which the values of the exchange interaction coefficients were obtained [2]. The next nearest-neighbor exchange interactions were recently also taken into account with the exchange integrals obtained from the first principle calculation [25] or fitting to the neutron scattering data [26, 27]. An atomistic dynamic simulation shows that the nearest-neighbor exchange model with stochastic thermal fluctuation is sufficient to quantitatively reproduce the decrease of the spin wave gap, i.e., the minimal frequency of the antiferromagnetic-like mode, with increasing temperature [23].
reason for such a redshift is that the effective magnetic field acting on a local spin is suppressed by the reduction of the expectation value of neighboring spins due to the magnon excitation. A similar redshift was recently also observed in the acoustic magnon branch by An et al [28]. At low temperature, the reduction of the spin magnitude is too small to be relevant, resulting in a saturate spin wave gap and magnetization as observed in experiment. The gap and magnetization obtained from the atomistic dynamic simulation of classical spins however keep linearly increasing and fail to saturate at very low temperature [23], in contrast to the results from the experiment and Harris’s quantum model with the same parameters.

In the present work, we develop a mean field approach based on the nearest-neighbor exchange model, where the magnon excitation at finite temperature is taken into account. In our approach, the temperature dependence of the entire magnon spectra can be easily obtained with the magnon thermal excitation and its influence on the dispersion treated in a self-consistent manner. With a set of temperature independent exchange constants, the resulting spin wave gap and magnetization show good agreement with the experiment from zero up to room temperature. In addition to a better description of the entire spectra compared to the widely used long wavelength approximation, another apparent advantage of our approach is that the output tight-binding wave functions contain only twenty components and are convenient for quantitative computation of various spin wave properties, such as the spin wave dissipation rate due to different mechanisms and the responses to different driving sources, e.g., light or microwave. Moreover, the information of the magnon polarization, which is responsible to the sign of the spin Seebeck coefficient [23], is also naturally included in the wave functions and is easy to read out. Therefore our approach should be useful for the study of various physics in YIG at finite temperature. As an application, we discuss the ferromagnetic resonance and its quantum model with the same parameters.

2. Exchange model

In one unit cell in YIG, the collinearly aligning iron atoms at ground state are separated into two sets, eight a atoms and twelve d atoms, according to the spin polarization direction or the configuration of the neighboring oxygen atoms [2]. The closest distances are $r_{aa} = (\sqrt{3}/4)a_0$ between two a atoms, $r_{dd} = (\sqrt{6}/8)a_0$ between two d atoms, and $r_{ad} = (\sqrt{5}/8)a_0$ between one a and one d atom with $a_0$ being the lattice constant of the face-centered cubic lattice. Following Harris [24], we start from the nearest-neighbor exchange Hamiltonian

$$H = -\sum_{n=1}^{N} \left[ J_{aa} \sum_{i \in \{r_{aa}\}} S_a(R_{in}) \cdot S_a(R_{in} + r_i) + J_{dd} \sum_{i \in \{r_{dd}\}} S_d(R_{in}) \cdot S_d(R_{in} + r_i) + J_{ad} \sum_{i \in \{r_{ad}\}} S_a(R_{in}) \cdot S_d(R_{in} + r_i) + \sum_{i=1}^{8} g\mu_B B \cdot S_a(R_{in}) + \sum_{i=9}^{20} g\mu_B B \cdot S_d(R_{in}) \right],$$

(1)

where $J_{aa}, J_{dd}$ and $J_{ad}$ represent the corresponding exchange coupling constants. In YIG, all these coupling constants are negative [2]. $N$ is the number of unit cells. The last two terms are Zeeman energies. The coordinates of atoms can be found in [24].

Without loss of generality, we assume that the equilibrium magnetization follows the small external magnetic field along z axis. By defining transverse components $S^\pm = S^x \pm iS^y$, the Holstein-Primakoff transformation of the two sublattices can be written as [29, 30]

$$S^+_a = S_a - a^\dagger a, \quad S^-_a = \sqrt{2}S_a - a^\dagger a a, \quad S^+_d = -S_d + d^\dagger d, \quad S^-_d = d^\dagger \sqrt{2}S_d - d^\dagger d$$

(2)

and $S^\pm_{ad} = (S^\pm_a d^\dagger + S^\pm_d a^\dagger)$ where we have taken into account the antiferromagnetic alignment of the two sublattices. $a^\dagger$ and $d^\dagger$ are the creation operators of the clockwise spin rotation at a-site and the anticlockwise rotation at d-site, respectively. Applying equation (2) and Fourier transform $a_n = \frac{1}{\sqrt{N}} \sum_{k} a_{in}(k) e^{ikR_{in}}$ to equation (1), one obtains the tight-binding-type Bogoliubov–de Gennes Hamiltonian (the quadratic order) for an arbitrary wave vector $k$ [2, 24]
At very low temperature, fluctuations of local spins are then given by
\begin{align}
\langle a_i^+ a_i \rangle &= \frac{1}{N} \sum_k |C_{1,k}^i|^2 \langle \alpha_{1,k}^+ \alpha_{1,k} \rangle + |C_{2,k}^i|^2 (\beta_{2,k}^+ \beta_{2,k}^i) + 1, \\
\langle d_j^+ d_j \rangle &= \frac{1}{N} \sum_k |C_{1,k}^j|^2 (\alpha_{1,k}^+ \alpha_{1,k}^j + 1) + |C_{2,k}^j|^2 (\beta_{2,k}^+ \beta_{2,k}^j).
\end{align}

At very low temperature, \( \langle \alpha_{1,k}^+ \alpha_{1,k} \rangle \approx \langle \beta_{2,k}^+ \beta_{2,k}^i \rangle \approx 0 \), there is a residual fluctuation due to the inter-sublattice coupling \( B_d \) in equation (3) [33, 34].
3.1. Zero temperature spectra

Figure 1 shows all twenty magnon branches in [110] and [100] directions carried out at zero temperature in the weak external field limit. The polarization characteristics of $\alpha_{ik}$ and $\beta_{ik}$ are represented by red and blue, respectively. Typically, the eight clockwise modes have higher frequencies than the twelve anticlockwise modes, since the former correspond to the rotation of the a-site spins under the exchange field of six nearby d-site spins ($\sim 12 |J_{ad}| S_d$), which is stronger than the one acting on the d-site spins from the four nearby a-site spins ($\sim 8 |J_{da}| S_a$). This is confirmed by figure 1(b) from the calculation with the same parameters but without angular momentum exchange between the two sublattices, i.e., $B_{ij} = 0$. From the comparison between the results with and without $B_{ij}$ terms, we can see that the inter-sublattice angular momentum exchange partially lifts the degeneracy at high symmetry points, and more importantly gives the correct dispersion of the acoustic mode and the antiferromagnetic-like mode, labeled as $\beta_1$ and $\alpha_1$, separately. The $\beta_1$ mode is almost isotropic up to 5 THz and becomes anisotropic when approaching the boundary of the Brillouin zone.

In figure 1(c) we plot the instantaneous spin configurations of all the modes around the center of the Brillouin zone ($k = 0$). Each arrow in the figure represents the spin projection of one iron atom in the $x$–$y$ plane and its length and direction correspond to the magnitude of the transverse component and the precessing phase, respectively. The instantaneous spin configuration of a particular mode is given by one column consisting of eight a-site spins and twelve d-site spins. The transverse spin components in both $\alpha_1$ and $\beta_1$ are parallel within each sublattice and antiparallel between the two sublattices. The magnitudes of the transverse spins in $\beta_1$ mode are all the same, corresponding to a global rotation of the whole system. In other words, this tilted configuration is still a stable ground state, explaining its vanishing frequency. The a spins in $\alpha_1$ contain larger transverse spin components than the d spins and therefore dominate the rotation direction of this mode. Without $B_{ij}$, the two sublattices are decoupled and the fully parallel configuration of each sublattice ($\alpha_1'$ and $\beta_1'$) is of highest frequency due to the negative intra-sublattice exchange constant (see figure 1(b)). Note that the magnetic dipole–dipole interaction, which is neglected in our calculation, may cause an anisotropy in the dispersion in the long wavelength range and may slightly modify the wave functions there [35], but it will not change the main

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.pdf}
\caption{Zero temperature spin wave spectra (a) with and (b) without inter-sublattice coupling $B_{ij}$. The blue and red colors separate spin waves into two groups according to their polarization. (c) Instantaneous spin configurations projected in the $x$–$y$ plane of all twenty modes in (a) near $k = (0, 0, 0)$.}
\end{figure}
information given by figure 1(c). Moreover, the temperature effect discussed below is dominated by the thermally excited short-wavelength magnons, where the influence of the dipole–dipole interaction is negligible.

### 3.2. Finite temperature spectra

At low temperature, the density of the thermally excited magnon is low enough so that the magnon dispersion calculated at zero temperature still works. However as more magnons are excited at high temperature, the enhanced magnon–magnon interaction can strongly affect the magnon dispersion. Physically, for example, the large magnon density reduces the magnitudes of the expectation values of all local spins and the resulting exchange field. The effect of the magnon–magnon interaction can be taken into account by including the higher order terms in form of \( \hat{a}_i^\dagger \hat{a}_j \hat{a}_j^\dagger \hat{a}_i \), \( \hat{d}_i^\dagger \hat{d}_j \hat{d}_j^\dagger \hat{d}_i \) and so on. The modification of the magnon spectra then can be carried out by a diagrammatic calculation of the real part of the magnon self-energy. Here, alternatively, we perform a mean field calculation with a self-consistent procedure, whose advantage has been discussed in the Introduction.

Specifically, we keep all magnon–magnon interactions with up to three magnon operators at the same site and apply

\[
a_i^\dagger a_i \rightarrow \langle a_i^\dagger a_i \rangle, \quad a_i^\dagger a_j^\dagger a_i \rightarrow 2 \langle a_i^\dagger a_i \rangle a_j^\dagger,
\]

\[
d_j^\dagger d_j \rightarrow \langle d_j^\dagger d_j \rangle, \quad d_j^\dagger d_j^\dagger d_j \rightarrow 2 \langle d_j^\dagger d_j \rangle d_j^\dagger,
\]

(17)

(18)

to reduce the interaction terms back to the quadratic order. The resulting effective Hamiltonian is exactly the same as equation (3) after a replacement of \( S_{a(d)} \) by effective spins

\[
S_{a(d)}^{\text{eff}} = S_{a(d)} - \Delta S_{a(d)}.
\]

Here \( \Delta S_{a(d)} \) stands for the average of the thermal excitation over all \( a(d) \)-site spins

\[
\Delta S_{a} = \frac{1}{N} \sum_k |C_{i,k}^{\dagger}t_i n_h(k\omega_{a,k}) + |C_{i,k}^{\dagger}t_i n_h(k\omega_{b,k})|, \\
\Delta S_{d} = \frac{1}{N} \sum_k |C_{i,k}^{\dagger}t_i n_h(k\omega_{a,k}) + |C_{i,k}^{\dagger}t_i n_h(k\omega_{b,k})|
\]

(20)

with \( n_h \) being the Plank distribution function. By diagonalizing equation (3) with \( S_{a(d)}^{\text{eff}} \), we obtain the modified spin wave spectra, from which we update \( S_{a(d)}^{\text{eff}} \) and repeat such a procedure until reaching a self-consistent solution.

In figures 2(a) and (b), we plot the convergent magnon spectra at 100 K and 300 K, respectively. As we can see, the shape of each band roughly remain the same at different temperatures. However, as the temperature increases, the clockwise rotating modes (in red) significantly move towards to lower frequency regime, which is consistent with the experimental observation [22] and the atomistic simulation [23]. The anticlockwise rotating modes are relatively insensitive to the temperature change.

In figure 2(c), the effective magnitudes of the two spin sets, i.e., equation (19), are plotted as a function of temperature, which show a weak dependence at low temperature, and approximately a linear decrease in the
high temperature regime. Interestingly, the reduction of the $d$-site is much larger than that of the $a$-site. The reason is that the $d$-site has larger components than the $a$-site in the lowest branch ($\beta_1$), which is most efficiently excited. At room temperature, the effective spins at the two sets reduce to 2.21 and 2.03 respectively. These distinct reductions are actually the origin of the relative shift between the anticlockwise and clockwise groups in figures 2(a) and (b), because the frequencies of the clockwise modes rely on the magnitude of $d$ spins. If the two effective magnon interaction strengths between nearest-neighboring $a$ sites are determined from the comparison of the calculated temperature dependence of the magnetization and the measured one [2], the determination of better exchange constants is beyond the scope of the present work.

Recently, two symmetry-distinct interaction strengths between nearest-neighboring $a$-site atoms and longer range interactions are proposed to be necessary to obtain a good fitting of the entire magnon dispersion to the neutron scattering data by Princep et al [27]. Since the change of the magnon dispersion at finite temperature is mainly caused by the thermal excitation of the well-defined and model-insensitive ferromagnetic branch, we expect that a more accurate set of interaction parameters may modify the spectra of the optical branches in detail, but it will not affect the temperature dependence. Actually, even in Princep’s model, each $a$-site atom interacts with the same number of neighboring $a$-site atoms via $J_{3a}$ and $J_{3b}$ bonds, therefore, the total effective magnetic field acting on the eight $a$ sites are all the same and equivalent to that in the simple model with $J_{a} = (J_{3a} + J_{3b})/2$. We expect that the spin configurations with different $J_{3a}$ and $J_{3b}$ should be very similar to those shown in figure 1(c), except a possible change in the order of their frequencies.

### 4. Ferromagnetic resonance

As discussed in the Introduction, with the knowledge of the wave functions, one can study various properties. Here, we take the ferromagnetic resonance as an example. In the presence of a spatially uniform ac magnetic field, we introduce a time-dependent perturbation Hamiltonian to describe its coupling with magnetic atoms

$$H'(t) = g \mu_B B(t) \cdot \left[ \sum_{i,n} S_i(R_{i,n}) + \sum_{j,n} S_d(R_{j,n}) \right].$$

For linear polarization magnetic field along $x$-direction,

$$H'(t) = \sqrt{N} g \mu_B B_x(t) \left( G^\alpha_2 \alpha_0 + G^\beta_2 \beta_0 \right) + \text{h.c.}$$

with $G^\alpha_2 = \sum_i C_{i,0} \chi^{\alpha}_{i,0}$, $G^\beta_2 = \sum_i C_{i,0} \chi^{\beta}_{i,0}$, and $B_x(t) = B_0 \cos(\omega t)$. Here, only $k = 0$ survives after the space integration. The absorption rates are then given by Fermi Golden rule

$$\Gamma_j(\omega) = \frac{\pi}{2\hbar} \left( g \mu_B B_0 \right)^2 N \left[ \left| G^\gamma_j \right|^2 \left| N_\gamma(\omega_{\gamma\alpha}) + 1 \right| \delta(\omega - \omega_{\gamma\alpha}) + \left| G^\gamma_j \right|^2 \left| N_\gamma(\omega_{\gamma\beta}) + 1 \right| \delta(\omega - \omega_{\gamma\beta}) \right],$$

which is proportional to the number of unit cells in the whole magnetic sample and the input power $(\propto B_0^2)$. By substituting the coefficients of the wave functions $C_{1,2,3,4}$, we find that only two of the prefactors $G^\gamma_2$ and $G^\gamma_2$ are non-zero. This actually can be easily understood from the spin configurations in figure 1(c), where only $\alpha$ and $\beta$ modes have net total transverse spins. The vanishing of the net transverse spin in other modes makes them transparent to the driving field.

### 5. Conclusion and discussion

In conclusion, we calculated the entire magnon spectra at finite temperature within a mean field approximation on the magnon–magnon interaction. The temperature dependence of magnon spectra shows good agreement with the experiment. We find that the reduction of the $d$-site spin is larger than that of the $a$-site spin. By using
the wave functions of the eigenstates, we analyze the ferromagnetic resonance and find that only two modes can be driven by a spatially uniform ac magnetic field. We suppose that our approach which provides proper magnon spectra and corresponding wave functions can be useful to the study of various properties in YIG at finite temperature.

One may notice that in figure 2 the residual magnetization (the effective local spins) near Curie temperature (560 K) is still finite, which reveals the limitation of the spin wave approximation in the high temperature regime [2]. In the literature, the mean field theory based on two sublattice-resolved magnetizations was found to perform well up to Curie temperature [37]. How to link this theory to our tight-binding-type mean field approach and how to extend the present spin wave-based model up to Curie temperature in ferrimagnetic systems are still under study. Moreover, the influence of the magnon–phonon interaction on the temperature dependence of the magnon dispersion is also an interesting and important issue, which is beyond the scope of our present work and left for future study.

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