Simulated lifetime of magnons and short wavelength distortion of magnons in bcc iron and fcc cobalt

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Abstract

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distortion of magnons in bcc iron and fcc cobalt

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The topic of this report is in electron spin dynamics where simulations where made using the UppASD simulations software based on the Landau-Lifshits-Gilbert equation. When many spins act together they form a wavelike movement called a magnon. It is believed that the magnon can be used as information carrier in next generation of technology.

We found that the lifetime of magnons in zero Kelvin in bcc iron and fcc cobalt decreases with higher damping and with smaller simulated structures for magnons with the same wavelength as the structure. Magnons with shorter wavelength than the structure are unstable and restructures itself to form a magnon of the same size as the structure.

In a structure with a temperature, magnons with short wavelengths can exist at many energy levels. The short wavelength distortion was measured to increase linearly with higher temperature and linearly with higher damping for bcc iron and fcc cobalt.

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1 Introduction
If a magnetic crystalline material, such as iron, receives energy from an external source then that energy will create magnetic excitations in the form of magnons, a.k.a. spin waves. These magnons can be seen as a wave when the magnetic moments are displaced over several atoms to form a characteristic wavelength. A magnon is defined by its wave vector, $\mathbf{q}$. In time these waves will transfer their energy to the underlying crystal. In that way you can say that the magnetic system is dampened.

Figure 1: 9 electron spins that together form one wavelength of a magnon

It is possible to model a single magnon in a crystalline magnetic material with computational experiments and observe the characteristics of a single magnon existing in systems with a certain crystalline structure, damping and size of the structure within the periodic boundaries.

2 Theory
The UppASD\textsuperscript{[1]} magnetization dynamics simulation software uses the commonly used theoretical description of magnons and other magnetization dynamics based on Landau-Lifshits-Gilbert equation\textsuperscript{[1]} (LLG) that describes magnetic moment as a function of time.

$$\frac{\partial \mathbf{m}_i}{\partial t} = -\gamma \mathbf{m}_i \times \mathbf{B}_i - \gamma \frac{\alpha}{m} \mathbf{m}_i \times \{ \mathbf{m}_i \times \mathbf{B}_i \}$$

\textit{eq. 1}

The first term in the LLG equation describes a conservative precision motion around the effective magnetic field $\mathbf{B}_i$ that work on the magnetic moment $\mathbf{m}_i$. The second term describes a damping motion that in time makes $\mathbf{m}_i$ align with the field $\mathbf{B}_i$. The magnitude of the damping is determined by the damping parameter $\alpha$. $\gamma$ is the gyromagnetic ratio.

Some contributions to the damping parameter can be calculated but determining the complete $\alpha$ is still difficult and produces varying results for experiments and simulations. The damping parameter is generally set to suit the needs of the experiment. We have used an experimental value for bcc iron and fcc cobalt as a reference when choosing $\alpha$.

In order to study the presence of magnons it is convenient to use Fourier transformation on the system so that the magnons become visible in the Fourier space. The result is that we can find the magnon intensity for a certain wavelength in the system. \textit{Equation 2} describes the magnon intensity $S^h(\mathbf{q}, \omega)$ as a Fourier transform of the magnetic moments in discrete space and continuous time. $N$ is the number of atoms and $\mathbf{r}$ is the directions of the magnetic moments.
Equation 3 is called the correlation function and it calculates the average difference of magnetic moments from zero to any given time between one atom and all the other atoms in the system while treating directions separately.

\[ C^k(r - r', t) = \langle m^k_{i}(t) m^k_{i}(0) \rangle - \langle m^k_{i}(t) \rangle \langle m^k_{i}(0) \rangle \]  

\[ S^k(q, \omega) = \frac{1}{\sqrt{2\piN}} \sum_{r,r'} e^{i q (r-r')} \int_{-\infty}^{\infty} e^{i \omega t} C^k(r - r', t) dt \]  

\[ eq. 2 \]

\[ eq. 3 \]

3 Problem statement

3.1 Magnon lifetime

By modeling a single axial magnon in a zero Kelvin magnetic crystalline structure we can analyze the life time of that magnon by measuring the decay to the ferromagnetic ground state. The lifetime of that magnon is dependent on the damping parameter and possibly the underlying structure as well as the wavelength.

The goal is to find out how the life time relates to these factors.

Figure 2: Visualization of a 8^3 cell bcc iron system with a single magnon

3.2 Magnon short wavelength distortion

If a crystalline system is excited by heat then one can calculate the intensity of selected magnon wavelengths via the UppASD\textsuperscript{[1]} simulation software. The high energy waves i.e. short wavelength magnons in that system are distorted where a single magnon seem to exist within a wide energy range. From experience we know that the magnitude of this distortion is dependent on temperature and \( \alpha \).
Figure 3: A collective of normalized spin vectors for bcc iron where the distorted region is marked by the red line

The goal is to determine the relationship and magnitude of the distortion in relation to temperature and $\alpha$ for iron and cobalt.

4 Methods

For the lifetime experiment the magnons where created by altering the spins in an input file so that they represent a magnon moving in a single direction. The magnon was evaluated through time in a bcc iron structure with periodic boundaries at 0 K via UppASD\textsuperscript{[1]}. The average magnetization was then measured until the system reached equilibrium. The same experiment was then repeated for cobalt.

The q-vectors were created via UppASD\textsuperscript{[1]} from a $30^3$ cell bcc iron structure with periodic boundaries. Tests were made by varying temperature while keeping the damping fixed. The fixed damping was set to 0.0019, which is an experimental value for iron \textsuperscript{[2]}, and a higher damping of 0.01. Additional tests were made for various damping parameters while keeping the temperature fixed at 293 K. To compare the distortion we decided that the 29\textsuperscript{th} q-vector (out of 30) would be representative of the distorted area which is a short wavelength, high energy magnon. The norm of the perpendicular magnetic moments to our effective magnetic field of the 29\textsuperscript{th} q-vector was then calculated. The distortion was measured by taking the 95 % uncertainty distance of a Gaussian curve fit with an offset variable. The curve fit was calculated using the MATLAB \textit{lsqcurvefit} function. The same simulations where then repeated for fcc cobalt but with $\alpha$ as the experimental value of 0.011\textsuperscript{[2]} and 0.001.

\textit{Equation 4} is used for the Gaussian curve fit where $a(4)$ is an offset, $a(3)$ is the peak amplitude, $a(2)$ is the expected value and $a(1)$ is the $\sigma$ standard deviation.

$$F = a\,(4) + a\,(3) \times e^{-\frac{(x-a\,(2))^2}{2a\,(1)^2}} \quad \text{eq. 4}$$
5 Results

5.1 Magnon lifetime

Figure 4, 5 and 6 shows that a maximum wavelength magnon have the same path for 89° to equilibrium as for 45° to equilibrium. Figure 7 reveals a deviation between 89° and 45° for a system with half of the maximum wavelength. This deviation has been analyzed with animations of many systems and one can conclude that all wavelengths for $\alpha = 0.0019$ that are not the maximum wavelength are unstable. This means that the simulation will run well for a short time and then form a chaotic motion that subsequently seems to recreate a magnon with a maximum wavelength with added noise and later reach equilibrium. Animations also show that very high damping such as $\alpha = 0.1$ are stable. The system reaches equilibrium faster, within one or two circular motions, making it stable enough for a complete $10^3$ system with five cell long magnon simulations.

UppASD\(^[1]\) simulations were used to calculate the lifetime of the magnon.

![Figure 4](image1.png) A single 10 cell long magnon in a 10\(^3\) bcc iron system with starting angle of 89° vs. a starting angle of 45°, $\alpha = 0.0019$

![Figure 5](image2.png) A single 5 cell long magnon in a 5\(^3\) bcc iron system with starting angle of 89° vs. a starting angle of 45°, $\alpha = 0.0019$

![Figure 6](image3.png) A single 10 cell long magnon in a 10\(^3\) fcc cobalt system with starting angle of 89°, $\alpha = 0.0019$

![Figure 7](image4.png) A single 5 cell long magnon in a 10\(^3\) bcc iron system with starting angle of 89° vs. a starting angle of 45°, $\alpha = 0.0019$
Figure 8: Magnon lifetime of the maximum wavelength in three bcc iron structures, lifetime is calculated from 89° starting angle to 99% of the maximum magnetization.

5.2 Magnon short wavelength distortion

UppASD\(^1\) simulations were used calculating the short wavelength distortion of 30\(^3\) cell bcc iron and fcc cobalt. Figure 10, 11, 13, 14 shows distortion dependent on temperature. Figure 12, 15 shows distortion dependent on damping.

Figure 9: The 29\(^{th}\) q-vector with a Gaussian curve fit of the norm of the perpendicular magnetic moments to our magnetic field

Figure 10: The 95% error region for temperatures with \(\alpha = 0.0019\) for bcc iron, error = 2.60 meV
Figure 11: The 95% error region for temperatures with $\alpha = 0.01$ for fcc cobalt, error = 2.91 meV

Figure 12: The 95% error region for sample $\alpha$ at 293 K for bcc iron, error = 2.18 meV

Figure 13: The 95% error region for temperatures with $\alpha = 0.011$ for fcc cobalt, error = 2.91 meV

Figure 14: The 95% error region for temperatures with $\alpha = 0.001$ for fcc cobalt, error = 1.80 meV
6 Error sources
We chose not to include anisotropy in our calculations on the basis that we have high symmetry but from results we could conclude that anisotropy does affect the results but do not majorly effect the lifetime of a magnon.

Two points in figure 14 where removed (0.05 and 0.1) because of high distortion close to the simulation edge. This made it impossible for our curve fit to find a curve in the correct region.

7 Reflection
There is a clear correlation between magnon lifetime and damping where a higher $\alpha$ will always yield a shorter lifetime for maximum wavelength magnons shown in figure 8. This correlates well with the LLG equation. There is also a correlation between maximum wavelength magnons lifetime and the size of systems where larger systems have longer lifetimes.

It is unrealistic to define a lifetime for magnons that are not the maximum wavelength in the study of magnon lifetime wavelength because they change from their original wavelength. This is a big limitation factor when analyzing magnons. Also our simulations could not scale up in size with our limited computational power without sacrificing time.

We are currently considering that the instability of the system is caused by the 2nd order midpoint method. Increasing the order of accuracy might yield stable results. But we can also consider that the LLG equations is a semi classical first order non linear differential equation where as the system might better be described by a second order quantum mechanical differential equation.

Magnon lifetime simulations with cobalt show similarities to iron-based magnons, but with a shorter lifetime. This is most likely because of the stronger exchange coupling that cobalt has compared to iron.

If it is possible to measure short wavelength distortions in experiments for certain $q$-vectors then one can compare the short wavelength distortion to simulations and estimate $\alpha$. The accuracy of $\alpha$ can be sufficient for experiments since it is difficult to deal with material impurities that distorts the results. The
α-parameter can also serve as a cross reference to other experiments. Resolution in damping can also be increased to reduce inaccuracies.

8 Conclusions
There is a clear correlation between magnon lifetime and damping where higher α will yield a shorter lifetime for maximum wavelength magnons. For magnons that are not the maximum wavelength the study is unfortunately inconclusive where we have not implemented a solution to the instability problem.

The magnon short wavelength distortion simulations for bcc iron and fcc cobalt showed that there is a linear correlation between short wavelength distortion and temperature and a linear correlation between short wavelength distortion and damping.

9 References