# Magnetic Waves, their Dispersion Relation and Phase Transitions

Computer Simulation Course Spring Semester 2023

February 14, 2023

**Abstract**

In this task, we will learn the concept of finding a dispersion relation and a critical curve numerically by the example of magnetic waves, or magnons, in magnetic insulators. In order to do so, the technique of atomistic spin simulations will be used. In the first part, we will focus on spin dynamics. In the second part, we will explore the dispersion relation of magnetic waves. Finally, we will have a look at magnetic phase transitions.

*In section 1 you will find a short general introduction to magnons and atomistic spin simulations after [Rez20, Blu01, EC14], a short overview of dispersion relations, and the system parameters. The most important information is highlighted. In section 2 you will find your task.*

## 1 Information

### 1.1 Atomistic spin simulations: The Heisenberg model and the equation of motion (LLG)

In order to simulate magnetic properties in an insulator, let's be aware of the two ingredients. First, insulating means, that electrons don't move. This we describe by a lattice with fixed lattice sites. Second, using the word 'spin' is actually inexact, since most often we talk about the overall magnetic moment $\vec{\mu}$ of the atom that sits on the lattice site. Where exactly this magnetic moment comes from and how strong it is, might be of general interest, but not relevant within this context. We will just use normalized magnetic moments and call them $\vec{S} = \vec{\mu}/|\vec{\mu}|$.

Spin waves in insulating magnets can be described on a lattice based on the Heisenberg model. This is very similar to the Ising model, where spins on fixed lattice positions can point in two directions, for example up and down (see lower panel of fig. 1 on the right-hand side). In the Heisenberg model, the spins are also fixed on space positions, but can point to arbitrary points on the unit sphere (see upper panel of fig. 1 on the right-hand side). Because of an interaction (Heisenberg coupling $J$) between the spins, a wave can travel through the system. Different additional effects might be included, for example different kinds of magnetic anisotropy or magnetic fields that can couple to the spins. In the ground state, the spins are aligned parallel if ferromagnetic ($J > 0$) or antiparallel if antiferromagnetic ($J < 0$) interaction is assumed, see fig. 1 on

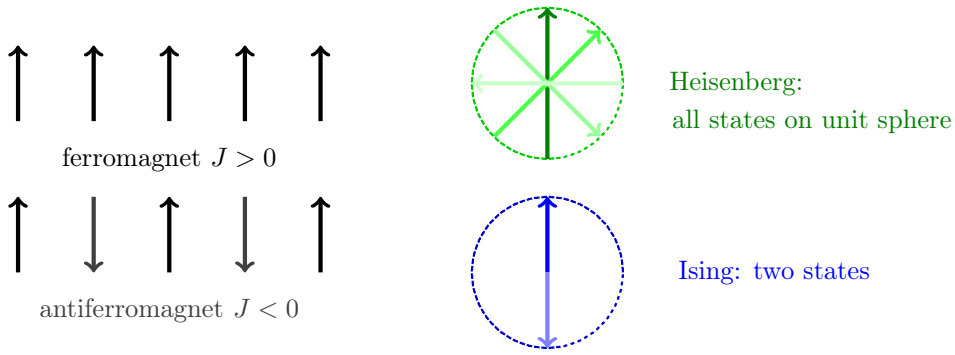


Figure 1: Models for a spin chain: On the left you can see a ferromagnet ($J > 0$, top) and an antiferromaget ($J < 0$, bottom) in the ground state. There are different ways to describe the spins in this chain, on the right you can see two of them: The Ising model allows only for two states, commonly called 'up' and 'down' (bottom, blue). The Heisenberg model allows all states on the unit sphere (green, top).

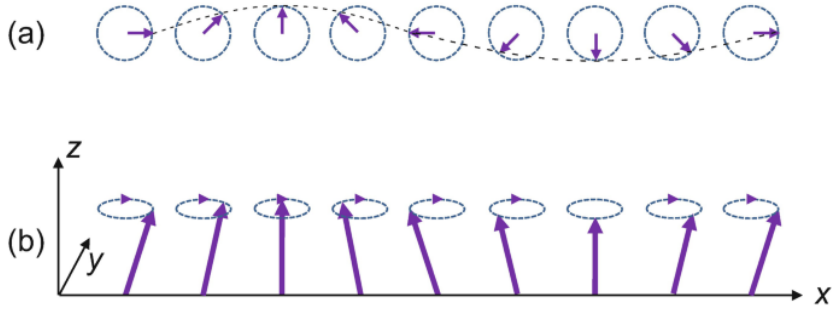


Figure 2: Illustration of a spin wave, from [Rez20]. In (b) one can see a linear chain of spins that oscillate around their ground state, the $z$-direction. In (a), the top view is shown, which illustrates the magnetic wave.

the left hand side. The excitation of the system can be visualized by the tilting of the spin away from its ground state.

Be aware that this picture is semi-classical. It does not capture all quantum properties.

The Heisenberg Hamilton function describing the energy of our system is given by

$$\mathrm{H} = -\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N}\frac{J_{j,k}}{2}\vec{S}_j\cdot\vec{S}_k - d_z\sum_{j=1}^{N}\left(\vec{S}_j\cdot\hat{e}_z\right)^2 - \mu B_0\sum_{j=1}^{N}\vec{S}_j\cdot\vec{B}_j \qquad (1)$$

with the coupling $J$[1], the normalized spins $\vec{S}_j$, the easy axis anisotropy constant

[1]Different authors use different conventions for the prefactor J. The factor of $\frac{1}{2}$ mainly depends on how you count the sum: you can either count every pair double by running over all indices $j, k$ and use a prefactor $J/2$, or you count every pair only once by counting only pairs with $j < k$ and use $J$.

$d_z > 0$ and the unit vector along the $z$ direction $\hat{e}_z$ and the absolute value of the magnetic moment $\mu$. $\vec{B}$ is a normalized vector which carries the direction of the magnetic field, and $B_0$ is the strength of the magnetic field, which may vary in space and time, $\vec{B}(t, j)$.

The first term describes the Heisenberg interaction (direct interaction, coming from an overlap of atomic orbitals). The sums run over all the spins and in general the coupling constant can be different for every pair of spins, but we will consider homogeneous coupling, this is $J_{jk} = J \quad \forall j, k$. For further simplification, only nearest neighbor interaction will be considered. This means, that the second sum runs only over $k$ if $j$ and $k$ are nearest neighbors: in a linear chain for example, spin two is *only* coupled to spin one and three, all the other spins do not have direct influence on spin two. There are different ways to treat the first and last spin: either they just couple to the inside, which is called 'closed boundary condition', or they couple also to each other, called 'periodic boundary conditions'. We will use the latter. Note that this first term minimizes for $J > 0$ if the spins are parallel, but is invariant under rotation (which means, it is energetically favorable for all spins to be aligned, but they don't care about the space direction).

The second term describes an easy uniaxial anisotropy (crystalline on-site anisotropy), which gives a preferred direction (in this case the $z$-direction). Thus, we break the rotational symmetry.

The third term is called the Zeeman term and makes it possible for an external magnetic field to couple to each spin individually. For simplicity, we will assume a magnetic field that is homogenous in space and time, $B_j(t) = B \quad \forall j$.

The equation of motion is called the Landau-Lifshitz-Gilbert equation and the time derivative $\partial_t$ of every spin $\vec{S}_j(t)$ is given by

$$\partial_t \vec{S}_j = -\frac{\gamma}{1+\alpha^2}\left[\vec{S}_j \times \vec{H}_j^{\text{eff}} + \alpha \vec{S}_j \times (\vec{S}_j \times \vec{H}_j^{\text{eff}})\right] \tag{2}$$

$$\vec{H}_j^{\text{eff}} = \frac{-1}{\mu}\frac{\partial \mathrm{H}}{\partial \vec{S}_j} + \vec{\xi}_j, \tag{3}$$

with the absolute value of the gyromagnetic ratio $\gamma > 0$ and the Gilbert damping constant $\alpha > 0$ [2]. The LLG eq. (2) consists of two parts. The first term describes the precession of the spin $\vec{S}_j$ around its effective field $\vec{H}_j^{\text{eff}}$ and the second is a damping term that causes the spin to align back with its effective field.

The effective field consists of two parts: first, the derivation of the Hamilton function eq. (1) with respect to the according spin. Formally, this is a functional derivative, but treating it as a partial derivative will give you the same result in this context. This means, that you see the spin $\vec{S}_i$ as a variable and do the derivative of eq. (1) with respect to that. For example, the Hamilton function for *two spins with only anisotropy and Heisenberg interaction and non-periodic boundary conditions*, the Hamilton function would be

$$\mathrm{H} = -\frac{J}{2}\vec{S}_1 \cdot \vec{S}_2 - \frac{J}{2}\vec{S}_2 \cdot \vec{S}_1 - d_z \left(S_1 \cdot \hat{e}_z\right)^2 - d_z \left(S_2 \cdot \hat{e}_z\right)^2 .$$

[2] Some authors call this damping parameter $\lambda$.

This means, that the effective field of spin 1 at zero temperature would be

$$\vec{H}_1^{\text{eff}} = \frac{-1}{\mu}\frac{\partial \mathrm{H}}{\partial \vec{S}_1} = \frac{-1}{\mu}\frac{\partial\left[-J/2\vec{S}_1\cdot\vec{S}_2 - J/2\vec{S}_2\cdot\vec{S}_1 - d_z\left(\vec{S}_1\cdot\hat{e}_z\right)^2 - d_z\left(\vec{S}_2\cdot\hat{e}_z\right)^2\right]}{\partial\vec{S}_1}$$
$$= \frac{-1}{\mu}\left[-J/2\vec{S}_2 - J/2\vec{S}_2 - 2d_z(\vec{S}_1\cdot\hat{e}_z)\hat{e}_z\right]$$

or

$$\vec{H}_1^{\text{eff}} = \frac{J\vec{S}_2 + 2d_z\vec{S}_1^z\hat{e}_z}{\mu}$$

Note how the anisotropy only acts on the according lattice site (this is also called 'on-site anisotropy') and how the exchange term gives coupling to the other lattice site.

The second part of the effective field is a noise term $\vec{\xi}$. This allows to include temperature. We will use Gaussian thermal noise which is white, this means there is neither temporal- nor spatial correlation. For each time step and every single spin, a different random distribution

$$\vec{\xi}(t) = \vec{\Gamma}(t)\sqrt{\frac{2\alpha k_B T}{\gamma\mu\Delta t}} \tag{4}$$

is drawn, where $\vec{\Gamma}$ is a 3D vector that contains a random number taken from a Gauss distribution with Zero mean and variance one in each component, $\mathcal{N}(0,1)$. Furthermore, $\Delta t$ is the step size of your simulation, $k_B$ the Boltzmann constant and $T$ the temperature. [3]

Note that the damping constant $\alpha$ appears in this noise; here we can see the dissipation-fluctuation-theorem, that links the dissipation (given in this case by the Gilbert damping) to the fluctuation (random forces acting on the system through the noise term). Through this type of noise, all magnon modes in the system are occupied.

We will use the Heun method to solve the problem numerically. It is a predictor-corrector procedure for ordinary differential equations $\partial_t y(t) = f(t, y(t))$ – which in our case is the LLG eq. (2) – with

$$y_{n+1}^p = y_n + \Delta t_n f(t_n, y_n) \tag{5}$$
$$y_{n+1} = y_n + \frac{\Delta t_n}{2}\left[f\left(t_n, y_n\right) + f\left(t_{n+1}, y_{n+1}^p\right)\right] \tag{6}$$

where $\Delta t$ is the step size. The index $n$ in this case runs over discrete time steps. The Heun method can be solved iteratively when the initial conditions $(t_0, y_0)$ are known. The time step we will set to 1 fs. [4]

[3] For each time step, you can alternatively initialize one big random number matrix for all $N$ spins directly, so the shape of $\vec{\Gamma}$ will be $(N, 3)$. This might be more time-efficient compared to calling the function separately for each spin, since calling a random number generator might take some time.

[4] The spins are normalized, which means that the spins are in the unit sphere, their absolute value is 1. This normalization has to be conserved! Make sure throughout your simulation that your spins remain normalized, which means you have to project the solution back into the unit sphere after each time step.

## 1.2 Dispersion relations

A dispersion relation $\omega(k)$ is a general expression that links the frequency of a wave $\omega$ to its momentum, or k-vector $k$. It carries information about the particle or wave you are looking at, for example its phase velocity $\omega/k$ and group velocity $d\omega/dk$. One dispersion relation you might have encountered in your life is the one of light (electromagnetic waves), which is in vacuum $\omega = ck$. It is linear: the frequency (and thus energy) is proportional to the $k$-vector via the proportionality constant $c$. Two examples for non-linear dispersion relations are particles that carry $\omega \propto k^2$ according to the De Broglie dispersion (from $E = \frac{p^2}{2m}$ with $p = \hbar k$ and $E = h\omega$), and phonons (lattice vibration in crystals) where you might for example have found $\omega \propto \sin(k)$ in some solid state physics course.

We will focus on magnon dispersion relations, which at zero temperature can be found analytically as

$$\hbar\omega = 2d_z + 2J(1 - \cos(ka)) \tag{7}$$

for a one-dimensional ferromagnetic square lattice when just including $J \neq 0, d_z \neq 0$. This you might have or will find in some other physics course using linear spin wave theory (for example in a Holstein-Primakoff transformation). Keep in mind that this expression changes for other lattice structures (for example hexagonal) and for ferri-/antiferromagnets (which will not be part of this assignment).

## 1.3 Model parameters

We set up a toy system that does not necessarily represent a real material, but reproduces typical behavior qualitatively. The Heisenberg coupling constant $J$ in units of milli electronvolt (meV) scales the system and will dominate the dynamics. All other parameters are set relatively to $J$. We will vary them a bit, but this is a starting point:

- Heisenberg coupling constant $J = 10\,\mathrm{meV}$
- Uniaxial anisotropy constant $d_z = 0.3J = 3\,\mathrm{meV}$
- Temperature $k_B T = 0.1J = 1\,\mathrm{meV}$.
- Homogenous magnetic field $\mu B_0(x,t) = \mu B_0 = const.$ along the $z$-direction, $\vec{B} \parallel \hat{e}_z$ with $\mu B_0 = 0.3J = 3\,\mathrm{meV}$

Furthermore, we will use the absolute value of the electron gyromagnetic ratio $\gamma = |\gamma_e| \approx 1.6 \times 10^{11}\,\mathrm{Hz\,T^{-1}}$ and the Bohr magneton $\mu = \mu_B \approx 5.8 \times 10^{-5}\,\mathrm{eV\,T^{-1}}$. As you can see, the parameters $J, d_z, k_B T$ and $\mu B_0$ carry the unit of an energy. Through $\mu$, the effective field has the units of T and through $\gamma$, one ends up with dynamics with the units of Hz.

# 2 Task

Our first aim is to find the one-dimensional magnon dispersion relation numerically. In order to achieve this, we suggest that you take the following steps. Along the way, find a plotting technique that helps you to observe the dynamics. Since we work with three-dimensional objects (Heisenberg spins) that are distributed over space (the lattice/chain) and each one will evolve differently in time, it is worth looking into (3D) animations (see section 2.4).

## 2.1 Preparations: Atomistic Spin Simulations

1. Show how one single spin behaves when you initialize it along a direction which is slightly tilted away from the $z$-direction (less than 45 degrees). Formally, that means that in your Heun procedure, you start with the initial condition $\vec{y}(0) = \left(S_0^x, S_0^y, \sqrt{1-(S_0^x)^2-(S_0^y)^2}\right)$ where $S_0^x$ and $S_0^y$ are the initial amplitude along the $x$ and $y$ direction at $t = 0$. Compare the undamped $\alpha = 0$ to two damped cases $\alpha_1 = 0.1, \alpha_2 = 0.5$. Inform yourself about how the trajectory should look like and what impact the damping should have. First, set $k_BT = 0, J = 0, B_0 = 0$, but use $d_z = 1\,\text{meV}$. When you have understood the dynamics, turn on low temperature $k_BT \approx 0.1 d_z$ together with $\alpha = 0.1$ and see how the trajectory changes.

2. Set up a one-dimensional chain with $N = 10$ and periodic boundary conditions and anisotropy along the $z$ direction $d_z = 0.3J$ where the spins are coupled via $J = 10\,\text{meV}$. Initialize all spins in (different) random directions, including up and down. Turn off temperature $k_BT = 0$ and use relatively high damping $0.1 < \alpha < 0.5$ and find the ground state by letting the system evolve in time until all movement is damped out. What ground state do you expect, and how does yours look? What changes if you change the sign of the coupling constant, so using the new coupling constant $\tilde{J}$ with $\tilde{J} = -J$?

3. Now, increase the length of the chain to $N = 100$ spins and initialize in the ground state. Keep the anisotropy. Then, tilt the spin in the center a little bit, less than 45 degrees away from the $z$-axis. Watch and compare what happens when $J = 0$ vs $J \neq 0$. Set the temperature to zero, $T = 0$. For the coupled case, you should see the excitation travelling along the chain. Can you see why we call this object a 'spin wave' or magnetic wave? Try different values for $\alpha$ and see how the dynamics changes.

## 2.2 Dispersion relations

### 2.2.1 Preparations

First some analytic considerations:

1. Estimate the frequency range (order of magnitude) you expect from eq. (7) and the given parameters.

2. First sketch (by hand) $\omega(ka)$ for $ka \in (0, \pi)$ for the case $J, d_z$ as given. Then, compare to the first other case $\tilde{J} = 2J, \tilde{d_z} = d_z$ and the second other

case $\hat{d}_z = 2d_z, \hat{J} = J$ in the same graph. How does each parameter impact the dispersion relation qualitatively? Now, if you want, plot the exact solution, you will need it later. *Hint: by sketching we mean schematically drawing the main qualitative features like the shape of the function and possible intersections with the axes. That you should be able to see from the analytic expression without actually computing the function values. By plotting we mean drawing the exact (quantitative) solution.*

Finally, you will need to use a Fourier transform (FT) in order to find the dispersion relation from your numerical data. A FT can be used to decompose a signal into its frequency components. In general, one can do FTs from any domain to its reciproce domain - for example, from time to frequency, or from space to k-space (where k is the wave vector or number) - and back, since the FT is symmetrical. One common application would be to record an instrument (or voice) over time, and find its frequency (so to say, the pitch) through a FT that goes from the time domain into the frequency domain. In space, an example from solid state physics is that if you transform the position of the lattice sites in a crystal, you can find the lattice constant. The general (analytical) expression for a FT from a function $y(t)$ to its Fourier-transformed $\hat{y}(\omega)$ in one dimension is

$$\mathcal{FT}[y(t)] = \hat{y}(\omega) = \int_{-\infty}^{\infty} y(t) \exp\left(-2\pi i \omega t\right) dt$$

and the back transform would be

$$\mathcal{FT}[\hat{y}(\omega)] = y(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{y}(\omega) \exp\left(2\pi i \omega t\right) d\omega$$

but there are different conventions concerning the prefactor $\frac{1}{2\pi}$ (for example, some authors use a factor $\frac{1}{\sqrt{2\pi}}$ in the there- and back-transform).

Numerically, we work in discrete time and space, which means we have to use a discrete FT, or DFT. It is comparable, but the integral is replaced with a discrete sum. Furthermore, the DFT uses some assumptions in order to make the calculation highly efficient, and the DFT is a very common tool in data analysis.

Now, get familiar with an implementation of a DFT in your language of your choice and read the documentation properly (for example numpys fft: `https://numpy.org/doc/stable/reference/routines.fft.html`). Pay special attention to how the frequencies are defined (sometimes, the found frequencies go like $[0, ..., f_{\max}, -f_{\max}, ..., 0]$ which requires a shift) and the prefactor (there are different standards where to include the $\frac{1}{2\pi}$). We do not expect you to implement the FT yourself!

### 2.2.2 Finding the dispersion relation numerically

Now we are good to go: We have checked that the spins couple to each other and magnons can propagate, magnon modes at all frequencies will be occupied by thermal noise, and the dispersion relation will be found using a DFT.

1. Set up a chain with $N \approx 50$ and initialize in the FM ground state. The spins are coupled via $J = 10\,\mathrm{meV}$ and aligned along the $z$-direction due

to $d_z = 0.3J$. Turn on low temperature $k_B T < d_z$ [5]. Run over 30 ps with a step size $h < 1$ fs and record the $x$-component of all the spins over time. If $r$ is the position of the spin on the chain, this means you need to record $S_x(r,t)$. [6]

2. Do a two-dimensional DFT (for example in python numpy.fft.fft2) on these data $x(r,t)$; one is for the time-to-frequency, one for the space-to-k-space transformation. This will find both the frequencies $\omega$ and the k-vectors and correlate them. The output of this should be a 3D matrix with a FT intensity for each pair of $(\omega, k)$ values. You can plot the signal, which we define as the absolute value of the FT amplitudes, using a color map, so a graph with $k$ on the x-axis (ranging from $ka = -\pi$ to $ka = \pi$, with the lattice constant a), $\omega$ on the y-axis, and the value of the FT signal color coded. We expect a result that will show a strong signal along one curved line, and weak signals everywhere else.

3. Add your plot of the analytic solution (from the preparation) to your numerical plot. Compare. Note: if you find that your numeric solution is off by an overall scaling factor compared to the analytic solution, that is ok. We will focus on the qualitative observations. In that case, scale your relsults so that they overlap, and state the scaling factor you use (this could be something like 2, or $\pi$).

4. Next, vary the coupling constant and the anisotropy constant as before – first, $J, d_z$ as given, then the cases $\tilde{J} = 2J, \tilde{d_z} = d_z$ and finally $\hat{d_z} = 2d_z, \hat{J} = J$ – and observe what happens. Can you reproduce the behavior that you expected from the analytic expression? Take a while to reflect on what the qualitative changes in the dispersion mean.

5. Now, add a homogenous magnetic field (constant in time and space) with strength 0.1–0.5$J$. Show and describe the impact on the dispersion relation.

6. Next, we will have a look at antiferromangetic (AFM) dispersions. Set the coupling constant to $J = -30$ meV, the anisotropy low, $dz << J$, and start without a magnetic field ($\mu B_0 = 0$). Keep in mind to use small temperature, $k_B T < d_z$. Initialize the system in the AFM ground state. Then run your disperison calculation. Note: the Brillouin zone of AFM magnons [RARS19] is half the size of the FM, thus only plot from $ka = -\pi/2$ to $ka = \pi/2$ – you will find a dispersion that is minimum at $k = 0$ and maximum at the edges, but has a different shape compared to the FM one. Describe. If you have seen similar effects in other courses before, comment and make a connection.

7. Finally, add a homogenous magnetic field along the $z$-direction with $\mu B_0 \approx 0.05J$ and see the impact on the AFM dispersion. What happened? Describe in detail and try to explain using the knowledge you have from other

[5] It is important that the temperature is smaller than the anisotropy, so that there are only small fluctuations around a set ground state

[6] In this square lattice, easy axis FM configuration, the $x$ and $y$ component carry the same information (if you want validation, have a look at a plot of $S_x(r,t)$ and $S_y(r,t)$ and notice they show the same behaviour, only with a phase difference, or find the trajectory for a single spin analytically and come to the same conclusion).

courses or try to find out in the literature (give references). *Hint: AFM have two sublattices – think about degeneracy.*

## 2.3 Ferromagnetic phase diagrams

The second main task is to find a FM phase diagram in 3D. This means that now we scale the system up. Increase your system to a 3D cube with only nearest neighbor (which will be 6 now) interaction and periodic boundary conditions. Try to implement in an efficient way, so that you can have at least $N_x = N_y = N_z = 20$ spins in each direction.

Using this system, our last aim will be to a phase transition from the ordered (ferromagnetic) to the unordered (paramagnetic) phase. We will use the temperature $T$-dependent, space- and time $t$-averaged magnetization

$$M(T) =: \left\langle \frac{1}{N} \sum_{i=0}^{N} S_i^z(T,t) \right\rangle_{t>t_{\mathrm{eq}}} \tag{8}$$

as the order parameter, where the sum runs over all spins and averages their $z$-components. The final result we want to obtain is a graph that shows $M(T)$. In order to get there, we suggest these steps:

1. Check the ground state of your 3D system by initializing all spins in random directions (also up and down), set $k_BT = 0$ and let it evolve over time. Include $J > 0$ and $d_z > 0$. Verify that you find a collinear ground state. For that you need to save the whole spin configuration (where all spins point at all times), which is a lot of data, but this is the only time you need to do that for the 3D case. Along this simulation, also print out the space-averaged magnetization over time $M(0,t)$. Plot and describe.

2. Now increase the temperature to $k_BT = 0.1J$ and initialize the system in the ground state. Then let it evolve in time while only recording $M(T,t)$. Plot and compare to the previous plot. What is the difference?

3. Repeat for at least 10 values $k_BT \in (0, 2J)$. Make sure you simulate long enough so that $M(T,t)$ reaches a plateau after some time $t_{\mathrm{eq}}$ (fluctuating around a constant value) - there, the system is in steady state. From this point onward, you can calculate the time average $< \cdot >_t$ in order to find $M(T)$. Plot the time average you find along with your $M(T,t)$ plot and mark the time you started the average. The $M(T,t)$ curve should fluctuate around that constant line.

4. Finally, plot $M(T)$ over $T$. Describe and interpret. Can you find the theoretical critical temperature $k_BT_c \approx 1.7J$ [EC14]?

5. If your system remains ordered in the temperature range suggested above, try to increase the temperature until you find the phase transition. Make the same $M(T)$ diagram.

Note that a numerically found critical curve can never show the same critical exponent as an analytical one. The order parameter will not show a discontinutiy at the critical temperature. However, we can use our smooth curve to estimate the critical temperature.

**Final conclusions.** In this task, you have seen two different aspects of magnons: in the first part, we got to know them as magnetic waves. Be aware that the description of magnons as spin waves in this atomistic picture is the most accurate at low temperatures.

In the second part, we could see that by exciting these waves, or 'occupying magnonic states', the magnetization is reduced.

## 2.4 Hints

### 2.4.1 Setting up the system

- Make sure you understand what the LLG eq. (2) looks like. It helps to write it down for one spin in order to understand what the effective field looks like. Changing the step size in the simulation makes a huge difference. Remember what you learned about error scaling for Runge Kutta algorithms and use a time step that is small enough.

- Concerning the trajectory of a single spin: remember the top spin in a gravitational field and its precession. The dynamics observed here should be similar, you will find precession around the $z$-axis. What function do you think describes the trajectory, for example the time-dependent x-component $x(t)$? When you turn on damping, $x(t)$ will look different; you have seen this kind of function before and know how to describe that (think about the damped harmonic oscillator). If you compare the time-dependent $z$-component the following relation between the lifetime $\tau$, the damping $\alpha$ and the frequency $\omega$,

$$\tau = \frac{1}{\alpha\omega} \tag{9}$$

  that is known from linear spin wave theory for ferromagnets, can you qualitatively reproduce this relation (try for three different damping constants)? You can also fit and compare quantitatively.

- For testing the chain: initialize a chain along the $z$ axis and first turn off coupling ($J = 0$). Nothing should precess. Tilt single spins and observe that they will start precessing while the others remain still. Finally, just tilt one spin and turn on coupling $J > 0$. Observe how the other spins will follow the precession.

- There are different ways to show your result: videos, polar plots, trajectories,... Play around and see which one helps you understand what is going on. You can also try video rendering, for example with FFMPEG or pythons ANIMATEGRAPHICS package. Find a way that helps you understand the physics. If you can't make that work, choose one of the transverse components ($x$ or $y$) and the $z$- component and plot that over time, for selected spins.

- Concerning the DFT: Use what is implemented, but make sure you understand how to use it. You can for example do a quick test where you Fourier transform a signal $y(t) = \sin(\omega t)$ which gives two delta peaks at $\pm\omega$. Read out the achieved frequency and compare to the frequency you have put in. Follow examples from the documentation or on stack overflow.

### 2.5 If you are a bit lost...

...and the given references don't help, there are many lectures about this topic since it is a method actively used in research. For example you can watch Richard Evens from York (England) who is the author of the open-source atomistic spin simulation code VAMPIRE, `https://www.youtube.com/watch?v=648WAF4Czrk`, or meet Rembert Duine from Utrecht (the Netherlands): `https://www.youtube.com/watch?v=a-D5ja7Kmos`. Finally, if you like the topic, there is an institute at the NTNU called QuSpin `https://www.ntnu.edu/quspin`. Come and join us! :)

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