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Computational Physics

In section 1 you will find information about the problem [1,3]. *The most important information is highlighted. In section 2 you will find your task.*

1 Information

Spin waves can be described on a linear spin chain based on the Heisenberg model. This is very similar to the Ising model, where spins on fixed positions can point in two directions, for example up and down. In the Heisenberg model, the spins are also fixed on space positions, but can point to arbitrary points on the unit sphere (see 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 anisotropies 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 the left hand side. The excitation of the system can be visualized by the tilting of the spin away from its ground state.

In this task we will find the numerical solution of a magnon on a linear spin chain and visualize the magnon. The Hamilton function describing the system is given by

$$\mathrm{H} = -\frac{1}{2}\sum_{j,k}^{N} J_{j,k}\vec{S}_j \cdot \vec{S}_k - d_z \sum_{j=1}^{N} (S_{j,z})^2 - \mu \sum_{j=1}^{N} \vec{B}_j \cdot \vec{S}_j \tag{1}$$

with the coupling J, the spins $\vec{S}_j$, the anisotropy constant $d_z > 0$ and the absolute value of the magnetic moment μ. The magnetic field $\vec{B}$ will not be of interest for the moment. The sum runs over the spins and in general the coupling constant can be different for every pair of spins, but we will consider homogenous coupling, this is $J_{jk} = J \quad \forall j, k$. For further simplification, only nearest neighbour interaction will be considered. This means, that the sum of the first term (Heisenberg interaction) runs only over j, k if j and k are nearest neighbours: for example, spin two is *only* coupled to spin one and three, all the other spins do not have direct influence on spin two.

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

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

$$\vec{H}_j = \frac{-\partial \,\mathrm{H}}{\partial \vec{S}_j} + \vec{\xi}_j, \tag{3}$$

with the gyromagnetic ratio $\gamma > 0$ and the Gilbert damping constant $\alpha \geq 0$. The LLG (eq. (2)) consists of two parts. The first term describes the precession of the spin $\vec{S}_j$ around its effective field $\vec{H}_j$ 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 derivative of the Hamilton function (eq. (1)) with respect to the spin and second, a noise term $\vec{\xi}$. This allows one to include temperature. Gaussian thermal noise is white, this means it there is neither temporal- nor spatial correlation, with $\langle \vec{\xi_l} \rangle = 0$ and

$$\langle \xi_l^\beta(t) \xi_k^\zeta(t') \rangle = \frac{2\mu^s \alpha k_B T}{\gamma} \delta_{lk} \delta_{\beta\zeta} \delta(t-t'), \quad \beta, \zeta \in \{x, y, z\}.$$

Unfortunately it is not within the scope of this task to include the temperature. All our simulations will be conducted at zero temperature and thus the second term in the effective field will be Zero.

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

$$y_{j+1}^p = y_j + h_j f(t_j, y_j) \tag{4}$$

$$y_{j+1} = y_j + \frac{h_j}{2} \left[f(t_j, y_j) + f\left(t_{j+1}, y_{j+1}^p\right) \right] \tag{5}$$

where h is the step size. It can be solved iteratively when the initial conditions (t_0, y_0) are known.

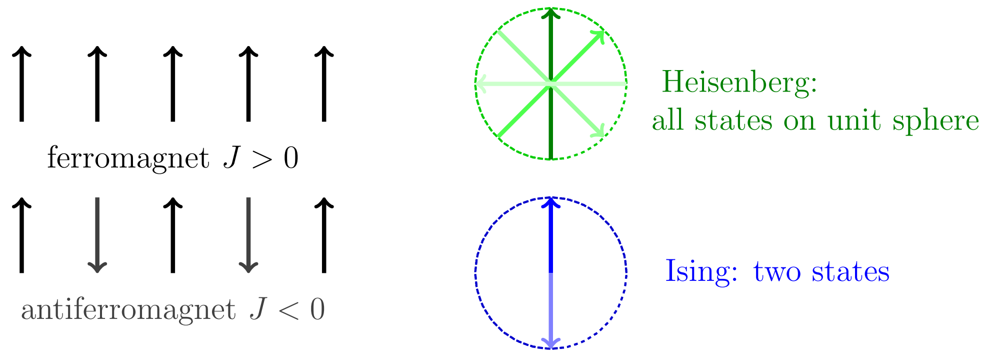

Figure 1: Models for a spin chain: On the left you can see a ferromagnet ($J > 0$, top) and an antiferromaget ($J < 0$, bottom) in the ground state. There are different ways to describe the spins in this chain, on the right you can see two of them: The Ising model allows only for two states, commonly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

2 Task

Our aim is to understand a magnon (a spin wave) on a spin chain. We will go there step by step building it up from scratch and validating our little simulation program as we go along.

You can either think about realistic values for the parameters (this includes some research and you should give the references) or calculate in natural units, this means giving the results in units of J, γ, μ and B_0.

2.1 One spin

We start with one spin that precesses around its effective field. Implement a Heun algorithm that can solve the LLG (eq. (2)). For the moment, disregard damping ($\alpha = 0$) and all the terms in the Hamilton function (eq. (1)) besides a homogenous magnetic field along the z-direction $\vec{B} = (0, 0, B_0)$. Start with a small step size ($h = 0.01$). Try to structure your program in a general way, so that you will be able to extend it easily to more spins, different solution procedures and a general Hamilton function.

1. Tilt the spin a little bit (this is your initial condition) and watch what happens. Remember that the length of the spin has to be constant. Find an appropriate way to present the result, for example plots of the trajectory (you can plot the

time dependent in-plane components x and y separately). Or you can do 3D plots of the spins, for example represented by arrows.

2. We will do a short error analysis of the algorithm. For this, think about an analytical solution. What ansatz do you know for a precessional motion?
   - Compare the analytical and numerical solution (plot).
   - What happens if you decrease or increase the step size h? Quantify the error[1] as the difference between the numerical and analytical solution after a certain simulation time, in dependence of the step size. Do a simulation with five different step sizes between 0.1 and 1×10^{-5} and present the step size dependent error in a log-log plot. It is enough if you do this analysis for only the x or the y component.
   - Implement an Euler procedure (easy one-step procedure) and compare the results for the step size dependent error. What's the difference? How can you explain it? What do you learn from this comparison? If you want, you can include runtime in this discussion.
3. Finally, we include the damping term. Start small, for example $\alpha = 0.05$, and choose a simulation time for which both several oscillations and a clear decay of the amplitude can be seen.
   - Plot the solution (x-y-components or 3D arrow video).
   - Compare the decay of your simulation to the relation between the lifetime τ, the damping α and the frequency ω

     $$\tau = \frac{1}{\alpha\omega} \tag{6}$$

     that is known from linear spin wave theory for ferromagnets. Can you qualitatively reproduce this relation (try for three different damping constants)?
   - Extra point: fit the decay of the amplitude and show that your simulation reproduces eq. (6) for one $\alpha > 0$ of your choice.

[1] If you mess up the time when plotting the analytical solution, you can just compare the amplitudes. The amplitude has to be constant in time for one spin without damping.

2.2 The spin chain

We will now proceed to the spin chain. Turn of damping for the moment ($\alpha = 0$).

2.2.1 Ground states

1. Set up the easy problem $J > 0$, $B_0 = 0$, $\alpha = 0.05$ with a small uniaxial anisotropy $d_z \approx 0.1$ (see eq. (1)). Initialize ten spins in random directions[2] – that also includes 'up' and 'down'.
    - Plot the z-component of each spin over time. What can you observe?
    - Now set $J < 0$ and plot the time dependent z-component. What's the difference? How can this be explained?

2.2.2 Magnon

1. Initialize your system again with ten spins in a linear chain but do not couple them yet ($J = 0$) - only include uniaxial anisotropy $d_z > 0$.
    - Test if all spins precess if you tilt them (see task 2.1.1).
    - Next, tilt only the first spin and initialize all the other spins along the z-direction. If you have done it right, only the first spin should precess and the others should not move. Explain why.
2. Now turn on ferromagnetic coupling $J > 0$. Again, tilt only the first spin and initialize the other spins along the z-axis. Observe the behaviour of all the spins over time.
    - What happens? Why?
    - Think about boundary conditions (concerning the first and last spin in the chain): where is the difference? Present your solution. What can you observe? How could you simulate an infinite system?
3. Note that we have found a fundamental property in the last step: If the spins are coupled, the excitation at one spin (the tilting of the first) does not remain on this spin, but propagates along the chain; **a magnon is a collective motion, the excitation is distributed on all the spins!**
4. Again, include damping $\alpha > 0$.
    - What can you observe?
    - Think about a way to create a video. For example, you can generate many plots/pictures and render it to a video using FFMPEG, pythons

[2] Pick random initial amplitudes but keep in mind that the length of all spins is the same and constant.

ANIMATEGRAPHICS package or another software of your choice. In the video the following aspects should be visible: In the beginning only the first spin is tilted. Then the magnon propagates through the spin chain with time. Eventually, damping should cause the excitation to cease.

5. Now switch to antiferromagnetic coupling $J < 0$. What can you observe?
6. The z-component is commonly linked to the magnetization.
   - Referring to section 2.2.1: what is the magnetization in the ground state? (That means, after the system is equilibrated and not in the randomly initialized state any more).
   - Imagine the precession of the first spin models a local excitation[3]. Observe the magnetization by plotting the z-component of each spin in task item 2 (the ferromagnetic chain with $J > 0$, $\alpha > 0$ and the first spin tilted while all the other spins are initialized along the z-axis). How can you explain the curve?

2.3 Comment on magnetization

What we did not analyse is the temperature dependence. This you can include with the Gaussian thermal noise. The solution algorithm can be the Stochastic Heun procedure [2]. Basically what happens is that in each time step, random (uncorrelated) forces act on each spin. This will induce many magnons with different frequencies. The higher the temperature, the stronger the random the force, and the more magnons (but always with the same spectrum) will be excited. As you have seen, magnons decrease the magnetization. So if you think about the phase transition of a magnet, where the magnetization is fairly constant at low temperatures and eventually drops to zero at a certain critical temperatures, this can also be explained in the magnon picture: With increasing temperature, more magnons propagate in the system, reducing the overall magnetization.

References

[1] Stephen Blundell, *Magnetism in condensed matter*, Oxford University Press, 2001.

[2] David Garcia-Alvarez, *A comparison of a few numerical schemes for the integration of stochastic differential equations in the stratonovich interpretation*, arxiv (2011).

[3] Ulrich Nowak, *Classical spin models* (Helmut Kronmueller and Stuart Parkin, eds.), John Wiley and Sons, 2007.

[3] for example by an applied field or by a material that would be attached on the left side and induce magnons via the Spin Hall effect in your spin chain