NTNU **Institutt for fysikk**

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Exam in TFY4235/FY8904 Computational Physics

Apr 28, 2022
09:00

Allowed help: Alternativ **A**

This problem set consists of 9 pages.

This exam is published on Thursday Apr 28 at 09:00 hours. You can work on your solution till **Sun May 01, 2022 at 23:00** ("the deadline"). Before the deadline you should submit your final report in the pdf-format and a zip-file containing the documented source code. For the names of the files that you will submit, please use `<lastname>_TFY4235_report.pdf` and `<lastname>_TFY4235_code.zip`; for those of you taking the course using the FY8904 code, replace TFY4235 with by this code. The submission of your work you will do via the system "Inspera" that you can find at `https://ntnu.inspera.no/`. You will receive an email at the start of the exam, detailing how to log in to this system and how to submit your report via it.

Prior to the deadline you are *also* expected[1], to send the final report to me at email `Ingve.Simonsen@ntnu.no` with subject TFY4235 or FY8904.[2]

There are no constraints on the kind of aid you may want to use in connection with this exam, including discussing it with anybody. However, *the report and the computer code you*

[1] Useful in the unlikely event that something should go wrong with the digital submission via "Inspera" (or you cannot get it to work properly).

[2] Warning: If your email is too large, the gmail system, to which I also forward my email, may notify you that the message was too large to be delivered to my gmail account. This means that your message was received successfully by the ntnu email system, if you were not informed otherwise.

will have to write yourself. Please attach your computer codes as appendices to the report. Give as a footnote the names of your collaborators during the exam. The report may be written in either Norwegian (either variants) or in English.

Should you run out of time, you are advised to spend the time on properly explaining what you did and the results you obtained instead of following a strategy of doing a little bit here-and-there without much explanation.

Information posted during the exam, like potential misprints, links to papers, extended deadline etc. will be posted on the web-page of the course at `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Exam/`. It is your responsibility to *check this information regularly!*

There are no formal requirements for the format of the report in addition to what was said above. The report should explain what you have been doing, your results, and how you interpret these results. Details should be included to the extent that we as graders can follow your way of reasoning. General background theory that, for instance, can be found in textbooks, is not needed in the report. It is documentation of your work we are interested in! Remember that if you have written an original and/or clever code for solving the problem, but are not able to explain it well in the report, it is hard to give you full credit.

The first point of contact for questions to this exam are the TAs

- Verena Johanna Brehm (verena.j.brehm@ntnu.no)
- Guillermo Garrido Hernandez (guillermo.g.hernandez@ntnu.no)

Good luck to everyone of you!

Problem 1

Your suggested solution for *Assignment no 2* [1] should be handed in as part of the report. It will count 15% towards the final grade of the course. Recall that the assignment text says that the report should be maximum 6 pages and take the form of a scientific report. You do NOT have comply with this.

Problem 2

Spin is a property carried by most elementary particles that we know; you may think about it is an intrinsic form of angular momentum. In magnetic materials, the collection of all the elementary particles (electrons, nucleus,...) that compose an atom of that material, gives an overall atomic magnetic moment. These overall atomic magnetic moments can interact if sufficiently close to each other. This exam problem is related to the study of *magnetic waves* and phase transitions that can exist in insulating magnets (where the position of the magnetic atom is fixed). A magnet can be modeled as a set of non-overlapping atomic magnetic moments and the sum of all the moments represents the magnetization of the system. Since "atomic magnetic moment" is a mouth-full, we commonly call these atomic magnetic moments "spin" and thus call this type of modeling *atomistic spin simulation* [3]. The magnetic waves that can exist in these models are a collective excitation of the spin structure and are referred to as *spin waves*. The quantized version of it is called a *magnon* [2] (which is a quasiparticle). There are different models to describe magnetism and spin waves, and here we take the *semi-classical* approach. There is also a quantum mechanical description which we will not cover here. In Sec. 3.2 of the supporting material you can find some comments on this topic if you are interested.

In the first part of this exam, we will focus on spin dynamics. In the second part, we will see phase diagrams that describe the transition from an ordered phase to an unordered magnetic phase.

2.1 Heisenberg model

Spin waves in insulating magnets can be described on a linear spin chain based on the semi-classical *Heisenberg model*. This model is very similar to the celebrated Ising model, where spins at fixed spatial positions can point in two opposite directions, for example, up or down. In the Heisenberg model on the other hand, the spins are also fixed at spatial positions, but they can point in arbitrary directions, or equivalently, point to arbitrary points on the unit sphere (see the top of Fig. 1). Because of an interaction between the spins, controlled by the Heisenberg coupling J, a wave can travel through the system. Different additional effects might be included, for example, anisotropies or external magnetic fields that can couple to the spins. In the ground state, the spins are aligned parallel if ferromagnetic interaction ($J > 0$) is assumed or antiparallel if antiferromagnetic interaction ($J < 0$) is assumed, see left-side of Fig. 1 for details.

For the purpose of this exam, we will limit ourselves to two simple cases: first, a one-dimensional line with equal distances (commonly called *linear spin chain*). Second, we will consider a flat layer modeled by a two-dimensional quadratic (or *square*) lattice where the sites are arranged on equally-distanced points in a plane. Furthermore, it will be assumed that the system consists of N spins in total. The Hamilton function describing the energy of

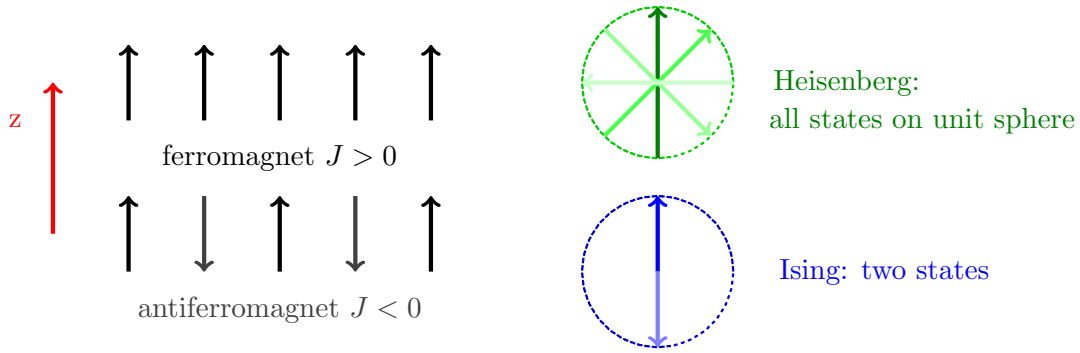

Figure 1: Models for a spin chain: On the left you can see the *semi-classical* ground states of a ferromagnet ($J > 0$, top) and an antiferromaget ($J < 0$, bottom) aligned along the z-direction. There are different ways to describe the spins in this chain, on the right you can see two of them: The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

the system is given by

$$\mathrm{H} = -\sum_{j\neq k}^{N} J_{jk}\,\mathbf{S}_j \cdot \mathbf{S}_k - d_z \sum_{j=1}^{N} (\mathbf{S}_j \cdot \hat{\mathbf{e}}_z)^2 - \mu_s \sum_{j=1}^{N} \mathbf{S}_j \cdot \mathbf{B}_j \tag{1}$$

with the coupling J, the normalized spins $\mathbf{S}_j$ at site j, the anisotropy constant[3] $d_z > 0$, the unit vector along the z direction $\hat{\mathbf{e}}_z$ and the absolute value of the magnetic moment μ_s. The vector $\mathbf{B}_j$ that appears in Eq. (1) represents the possible external magnetic induction field at site j.

The sums in Eq. (1) run over all the spins in the system. In the first term, in general the coupling constant J_{jk} can be different for every pair of spins j, k. However, for some materials, it is a good approximation to only assume nearest neighbor interaction[4]. In other words, in the first term we will just include pairs of j, k if j and k are nearest neighbors: for example, spin two is *only* coupled to spin one and three, all the other spins do not have direct influence on spin two. For further simplification, we will assume a constant, homogeneous coupling, this is $J_{jk} = J = const.$ for all j and k. In Sec. 3.1 you can find more information about these parameters.

2.2 Landau-Lifshitz-Gilbert equation

The equation of motion for each of the spins is called the Landau-Lifshitz-Gilbert (LLG) equation and the time derivation $\partial_t = \partial/\partial t$ of every spin $\mathbf{S}_j$ is given by

$$\partial_t \mathbf{S}_j = \frac{-\gamma}{1+\alpha^2}\left[\mathbf{S}_j \times \mathbf{F}_j + \alpha \mathbf{S}_j \times (\mathbf{S}_j \times \mathbf{F}_j)\right], \qquad j = 1, \ldots, N, \tag{2}$$

with the gyromagnetic ratio $\gamma > 0$ and the Gilbert damping constant $0 < \alpha < 1$ [5]. In writing Eq. (2), we have introduced an effective field $\mathbf{F}_j$ at site j that will be defined in detail below.

[3] Different authors use different conventions for the constants, for example you can find an additional factor of $\frac{1}{2}$ in front of J and d_z.

[4] Because ferromagnetic coupling originates in overlapping orbitals and these decay rapidly in space.

[5] Some authors call this damping parameter λ.

The LLG equation (2) consists of two terms. The first term describes the precession of spin $\mathbf{S}_j$ around its effective field $\mathbf{F}_j$ (at site j) and the second term is a damping term that causes the spin to align back along its effective field.

We now turn to the definition of the effective field $\mathbf{F}_j$ that is needed to fully specify Eq. (2). This field we write as the sum of two separate contributions $\mathbf{F}_j = \mathbf{F}_j^{eff} + \mathbf{F}_j^{th}$. The first term is

$$\mathbf{F}_j^{eff} = -\frac{1}{\mu_s}\frac{\delta \mathrm{H}}{\delta \mathbf{S}_j} \tag{3}$$

and it is related to the functional derivative of the Hamiltonian function (1) of the system H with respect to the spin at site j. Here the notation $\delta/\delta\mathbf{S}_j$ means

$$\frac{\delta}{\delta \mathbf{S}_j} = \hat{\mathbf{e}}_x \frac{\delta}{\delta S_j^x} + \hat{\mathbf{e}}_y \frac{\delta}{\delta S_j^y} + \hat{\mathbf{e}}_z \frac{\delta}{\delta S_j^z}, \tag{4}$$

where $S_j^{x,y,z}(t)$ denote the time-dependent Cartesian components of the vector $\mathbf{S}_j$ on site j. If you don't know what a functional derivative is, you will formally get the correct answer if you replace all functional derivatives by partial derivative in Eqs. (3) and (4). The second term contributing to the effective field $\mathbf{F}_j$ is

$$\mathbf{F}_j^{th} = \boldsymbol{\xi}_j(T), \tag{5}$$

and it adds thermal noise to the problem. Here we will model the noise term as a Gaussian thermal noise that is both *temporally and spatially uncorrelated*. It is defined, similarly to what was done in Assignment 2, by

$$\boldsymbol{\xi} = \boldsymbol{\Gamma}(\mathbf{t})\sqrt{\frac{2\alpha k_B T}{\gamma \mu_s \Delta t}} \tag{6}$$

with the step size Δt of your simulation, the Bolzmann constant k_B, the absolute temperature T and a zero mean and unit variance Gaussian distribution $\boldsymbol{\Gamma}$. By including the noise term into the effective force, the temperature enters the problem. Watch out, it is not exactly the same as you used before, the constants are different!

2.3 Numerical method

To solve the LLG equation numerically we will apply the so-called Heun method. This is a predictor-corrector method, and when it is applied to the ordinary differential equations (ODE) $\partial_t y(t) = f(t, y(t))$ one gets[6]

$$y_{\tau+1}^p = y_\tau + \Delta t_\tau f(t_\tau, y_\tau) \tag{7a}$$

$$y_{\tau+1} = y_\tau + \frac{\Delta t_\tau}{2}\left[f\left(t_\tau, y_\tau\right) + f\left(t_{\tau+1}, y_{\tau+1}^p\right)\right], \tag{7b}$$

where the time-step is $\Delta t_\tau = t_{\tau+1} - t_\tau$ and $\tau = 0, 1, 2, \ldots$. Here y_τ^p is an approximation to the predictor function $y^p(t)$ at time $t = t_\tau$. The system in Eq. (7) can be solved iteratively when the initial conditions (t_0, y_0) are known.

[6]Note that the subscripts here refer to time while they for instance for $\mathbf{S}_j$ refer to site j. Make sure you do not confuse them.

When the Heun method is applied and a thermal noise term is included in the effective field it is stressed that the noise is not changed during a single Heun iteration described by Eqs. (7a) and (7a) [that is, for both the predictor step and the corrector step].

Note that the spins are normalized, which means that they are on the unit sphere. Hence, their absolute value is therefore unity so that $|\mathbf{S}_j(t)| = 1$ for all sites j and for all times. This normalization has to be conserved! Make sure throughout your simulation that your spins remain normalized. For example, you can project the solution back into the unit sphere after each time step.

2.4 Exam questions

a) We start with the single-spin dynamics. To achieve this, initialize one spin in a direction that is almost aligned with the positive z-direction, but a little bit tilted (so $S_1^z(t=0) \gg S_1^{x/y}(t=0) > 0$). Then simulate its movement according to the introduced equations and plot the three components of the spin vector $\mathbf{S}_j$ as a function of time. To this end, assume $N = 1$, $T = 0$, $J = 0$, and no damping, that is, $\alpha = 0$. Furthermore, use only one symmetry-breaking term in the Hamiltonian that favors the z-direction. This means, including either an anisotropy term $d_z > 0$, or an external magnetic induction field $\mathbf{B} = (0, 0, B_0)$ where $B_0 > 0$ is a homogeneous in space and time (a constant).

b) Repeat problem 2.4(a) but now for the damped case with $0 < \alpha < 1$. You will find that the magnitude of the x and y components of the spin will decay over time. It is predicted by linear spin wave theory that, for ferromagnets, the decay constant of this exponential decay (also called lifetime) τ is related to the damping constant α and the frequency ω by

$$\tau = \frac{1}{\alpha\omega}. \tag{8}$$

Compare your results to this relation.

We will now consider a system consisting of several spins on a linear ferromagnetic chain so that we have $N > 1$ and $J > 0$. This system supports magnetic waves. For instance, they can be excited by first initializing all the spins along the positive z-direction and then tilting, say the first spin, slightly away from the z-direction, that is $S_1^z \gg S_1^x > 0$. This tilting we call an *excitation*. Because of the coupling J, this excitation is expected to travel through your chain. We will still assume $T = 0$ as before, and we will include either an anisotropy term $d_z > 0$, or an external magnetic induction field $\mathbf{B} = (0, 0, B_0)$.

c) Start with finite damping $0 < \alpha < 1$ and assuming non-periodic boundary conditions which means that spins at sites 1 and N are *not* interacting. Calculate the time-dependence of the spin vectors $\mathbf{S}_j(t)$ for all sites $j = 1, \ldots, N$. Make sure that the damping constant is small enough to allow the excitation to travel, but big enough that the last site will only be excited negligibly (that is, $S_N^z(t) \approx 1$ for all times). Graphically present and interpret your results. Focus on short times[7] and see how the first spin influences the second. Sooner or later, all spins will precess, but do they precess with the same frequency and are they in phase?

d) Repeat your calculation and interpretation for the undamped case $\alpha = 0$. What happens after the last spin $\mathbf{S}_N$ has started to move? What do you expect should happen in your closed system (non-periodic boundary conditions)?

[7] This means more or less a few period lengths, depending on your system size.

e) Now repeat problem 2.4(d) under the assumption of periodic boundary conditions. Compare for small times your results to what was obtained for the similar closed system.

We will now focus on the ground state of the magnetic system. A ground state is the state a system evolves to over time by minimizing its energy. You find it through initializing all spins in random directions and than letting the system evolve into a stable state (which means, it will not change any more with time). Once again it will be assumed that $T = 0$. Furthermore, an anisotropy term $d_z > 0$ is present but no magnetic induction field, that is, $\mathbf{B} = \mathbf{0}$. For this case you will need damping ($0 < \alpha < 1$). It is advisable to choose periodic boundary conditions and an even number of spins.

f) Find the ground states for $J > 0$ and $J < 0$ and interpret your results. Note that these are *semi-classical* ground states![8]

Finally, we will consider a single layer of ferromagnetic material. This we model with a two-dimensional[9] square spin lattice with periodic boundary conditions and only nearest neighbor interaction. This time, use a larger value for the damping ($0.1 < \alpha < 1$)[10] and the external magnetic induction field $\mathbf{B} = (0, 0, B_0)$. Before you proceed, find the ferromagnetic ground state again for your two-dimensional case, and make sure that it is qualitatively the same result as in 2.4(f) and Fig. 1.

Now we will assume finite temperature ($T > 0$). Our aim is to obtain the magnetic phase diagram of the system. In general a phase diagram shows the different phases a system can appear in depending on the values of the parameters defining it. For instance, in our case, the system can be in one of two possible phases, the ferromagnetic phase (ordered phase) or the paramagnetic phase (disordered phase) depending on the temperature T. Which of the two phases the system is in, is described by the temperature dependent average magnetization $M(T)$. It is defined by the following relation:

$$M(T) = \langle M(T,t) \rangle_t \tag{9a}$$

where

$$M(T,t) = \frac{1}{N} \sum_j^N \mathbf{S}_j \cdot \hat{\mathbf{e}}_z \tag{9b}$$

and $\langle \cdot \rangle_t$ denotes the temporal average of its argument *after* the system has reached thermal equilibrium.

g) Initialize all spins along the positive z-direction and start with a very low temperature $k_\mathrm{B}T < 0.1J$. Plot the time-dependent magnetization $M(T,t)$ and observe how it drops from the global maximum at $t = 0$ to a slightly lower value, from where on it fluctuates around a certain constant value. The latter is the equilibrium magnetization $M(T)$ that you want to find by the use of the temporal average[11]. Find $M(T)$ for your chosen temperature and plot it together with $M(T,t)$ as a function of time.

[8] See 3.2 for a comment on the compatibility with quantum models.

[9] For a short detour about the Mermin-Wagner theorem and the compatibility with quantum models, see 3.2.

[10] The larger the damping, the shorter the run time.

[11] In general, one would have to do a *ensemble average*, which means, doing this simulation many times and then average over the set these realizations. In some systems, however, one can replace an ensemble average by a temporal average. This is the case here and we advise you to use the temporal average *given that you start with that after the system has reached its equilibrium.* However, you can opt for the ensemble average. In this case, instead of the temporal average plot, you will have to show plots of your $M(T)$ curves for the realizations including the average value of all of them. Comment why you chose that method.

h) Repeat the calculations from 2.4(g) for gradually increasing temperatures till at least $M(T)$ vanishes and plot $M(T)$ as a function of T. Include a measure of the fluctuation, for example the standard deviation when calculating the mean value, as error bars in your plot. This is your phase diagram. Additionally, we will call the temperature at and above the magnetization drops to Zero the critical temperature T_c, so $M(T \geq T_c) \approx 0$ within the uncertainty. Write down this critical temperature along with your other simulation parameters (J, B_0, α and N). Describe and interpret your result.

i) Change the value of B_0. Show and discuss how it influences the critical temperature.

For your information it is mentioned that during grading, subproblems 2.4(a), (c), (g) and (h) will be given the highest and about equal weights; the remaining subproblems will be given approximately equal weight.

3 Supporting material

3.1 Concerning units and values for the constants

You can either find realistic values for the parameters (this includes some research and you should give the references) or use a toy system. In Ref. [3], Table 1, you can find an overview of the constants with units. A good place to start with is $J = 1\,\mathrm{meV}$, and giving all other constants in units of the coupling constant J: $d_z \approx 0.1J$, $\mu_s B_0 \approx 0.5J$, $\alpha \approx 0.01$, $\mu_s = \mu_B$, a time step of about 1 fs and a temperature range of $0 < k_\mathrm{B}T < 10J$ for the phase transition task. Since only the ratio of the energy scales matters, that is the relation between J, d_z, $mu_s B_0$ and $k_B T$, it is common to write down the constants in units of the coupling constant J. For example, $d_z \approx 0.1J$ means $d_z \approx 0.1\,\mathrm{meV}$.

3.2 Comment on the semi-classical nature of the used model

Atomistic spin simulations are of semi-classical nature. This means that they inherently can not capture quantum effects. One obvious difference is that, in the Heisenberg model, the assumed spin can move continuously on the unit sphere and is not restricted to quantized states. This is in contrast to quantum spin system where (assuming that you use the z-axis as the quantization axis) the z-component of the spin can only be multiples of $\hbar$. Furthermore, the formulation of Gaussian white noise we use here is an approximation for high temperatures and gives the classical distribution of the spin waves. But within the scope of this task, these assumptions are completely fine! Just remember that you expect different results here compared to what you learn in quantum physics courses. For example, the antiferromagnetic ground state (called the *Néel state*) that you find is not the quantum mechanical ground state!

Now let's shortly discuss the observed phase diagrams.

The Mermin-Wagner Theorem states that there cannot be long-range order at finite temperature for systems like the isotropic Heisenberg ferromagnet with nearest-neighbor interaction, that is, if you had only the first term with the $J\mathbf{S}_j\mathbf{S}_k$. However, we break the symmetry of the system by the use of the anisotropy or the magnetic field. That gives a preferred axis (the z-axis) and thus long-range order at elevated temperatures can be seen. And remember, we find a semi-classical phase diagram here, and this does not necessarily reproduce the results of a quantum mechanical approach. So don't be surprised that even if you try and set $B_0 = d_z = 0, J \neq 0$, which models a system that behaves semi-classically, you will still see finite magnetization at low temperatures — even though you would not expect that coming from a 2D quantum mechanical picture.

References

[1] Assignment 02 can be found at `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Assignments/TFY4235_Assignment_02.pdf`

[2] For instance, see `https://en.wikipedia.org/wiki/Magnon` and references therein.

[3] An article about atomistic spin simulations: `https://iopscience.iop.org/article/10.1088/0953-8984/26/10/103202/pdf` by Richard Evans.

[4] For instance, see `https://en.wikipedia.org/wiki/Square_lattice_Ising_model` and references therein.