NTNU

Kunnskap for en bedre verden

Department of Physics

TFy4235 - Numerical Physics

Exercise 2 2023 - 10039

1 Tasks

1.1 Preparations

1.1.1 Single spin

Setting a single spin leads to a spinning trajectory around the z-axis. With a damping, the spin will slow down and the velocity will go to zero. With temperature the spin will as expected "shake", as this term moves the spin in random directions.

1.1.2 One dimensional chain

The expected ground state for positive J is all magnets pointing up in the z-direction. My simulation shows the same ground state. For negative J the ground state would be anti-ferromagnetic, that every second magnet points in positive z-direction, and the others point in negative z-direction. Examples can be seen in Figure 1.

1.1.3 Magnetic waves

The middle chain couples together with the magnets beside it, forcing them to move in the same motion it does. Then those magnets couple with the ones beside them, and so on. The motion of going back and forth is transferred from the middle and out in the chain, making a wave motion.

1.2 Dispersion relations

1.2.1 Preparations

Since $\hbar$ is in the order of 10^{-34} and both d_z and J is in the order of 0.1 - 1 meV, the frequency range would be in the order of magnitude $10^{11} - 10^{12}$.
Since d_z is only a constant, changing this value would only lead to a constant difference. So the shape of the dispersion relation would not be changed. It could be worth noting that, since cos(x) is equal to 1 at x = 0, the frequency w is equal to d_z at k = 0.J, however, does change the slope of the dispersion relation. A larger J leads to a steeper slope.

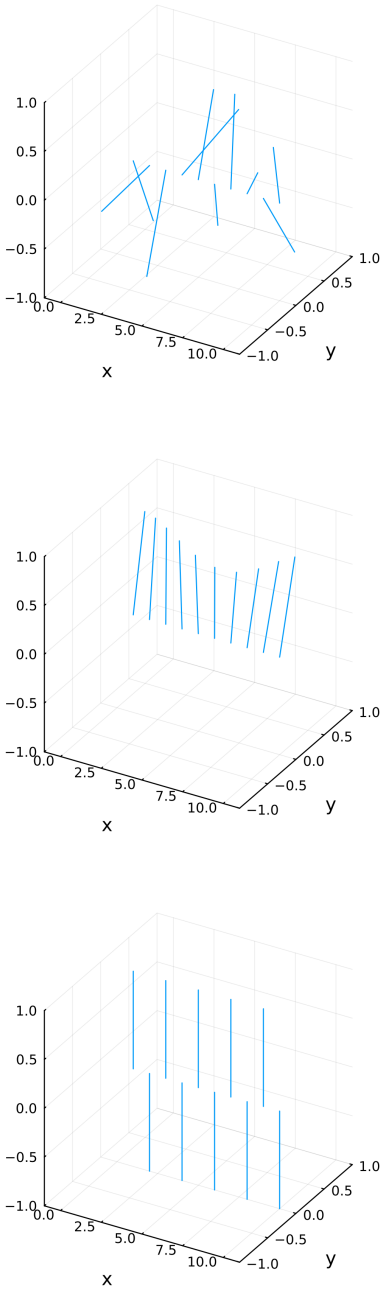

Figure 1: Top: Chain at start of simulation
Middle: Ground state found for positive J
Bottom: Ground state found for negative J

1.2.2 Finding the dispersion relation numerically

I initialized a chain of 100 magnets for a better resolution result. For all simulations in this section, $\alpha = 0.1meV$ was used. The step size used was $0.5fs$, and $kbt = 0.2meV$. The result of the Fourier transform can be seen in Figure 2. To fit the analytical plot, d_z had to be multiplied by 10, and I am uncertain of the reason for this, but I believe it lies in the way the Fourier matrix was found.

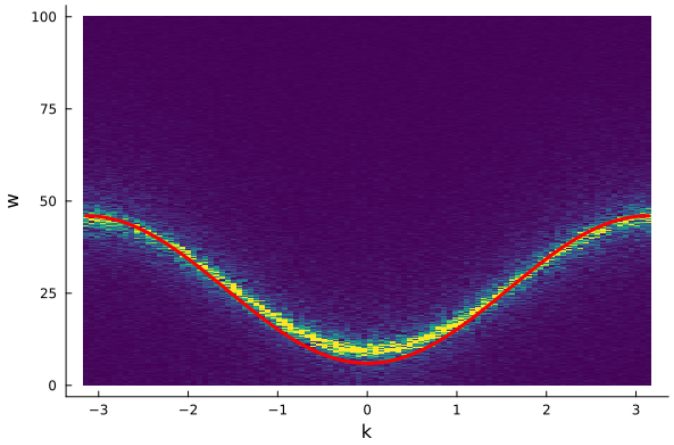

Figure 2: Heat map and plot of a two dimensional DFT.

The case for $J = 20meV$ can be seen in Figure 3. As expected, the slope is much steeper for these parameters.

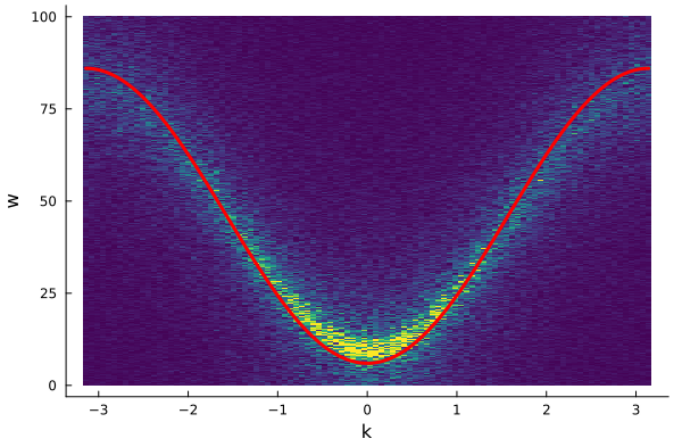

Figure 3: Heat map and plot of a two dimensional DFT, here with $d_z = 0.3meV$ and $J = 20meV$.

The final case, for $dz = 0.6eV$ and $J = -10meV$, can be seen in Figure 4. As expected, the slope is identical to Figure 2. It is worth noting: for this simulation there was no need to scale d_z with a factor of 10, even though no changes were made to the code. Thus it is in the way the Fourier matrix was found. It is probably in the fftshift() function used.

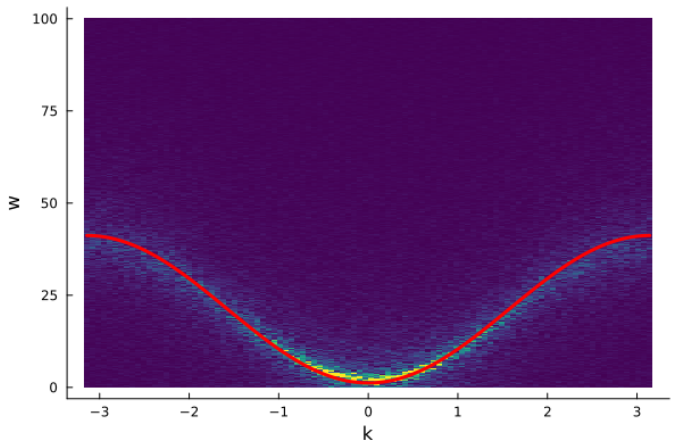

Figure 4: Heat map and plots of two dimensional DFT, here with $d_z = 0.6meV$ and $J = 10meV$

The AFM dispersions were first simulated using $d_z = 0.3meV$ and $kbt = 0.2meV$. The results are shown in Figure 5.

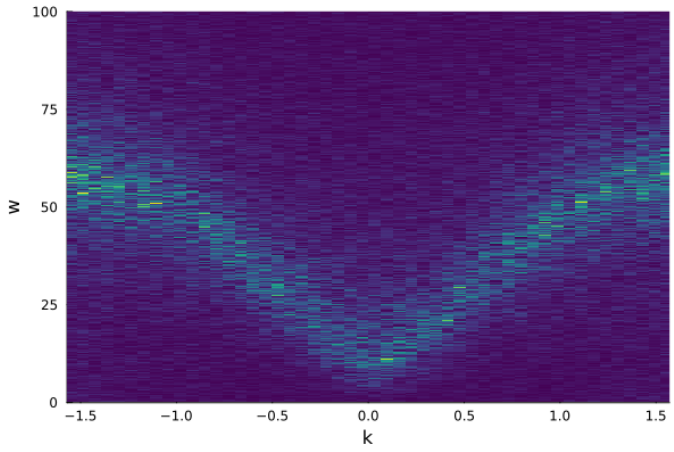

Figure 5: Heat map and plots of two dimensional DFT for antiferromagnetic dispersions.

This dispersion relation seems to be sharper at k = 0, instead of a smooth curve like one would expect from a harmonic function. It looks similar to a phonon dispersion relation from solid state physics. Since phonons are just the quanta of lattice vibrations, one could compare them to the magnons in this situation. The magnons are results of magnetic spins coupled together where they all move chaotically as a result from the temperature. The vibrations in a solid is much the same, and it would be reasonable to assume their dispersion relations have similarities.

Adding a homogeneous magnetic field did not seem to alter the results from the simulations. The results are seen in Figure 6.

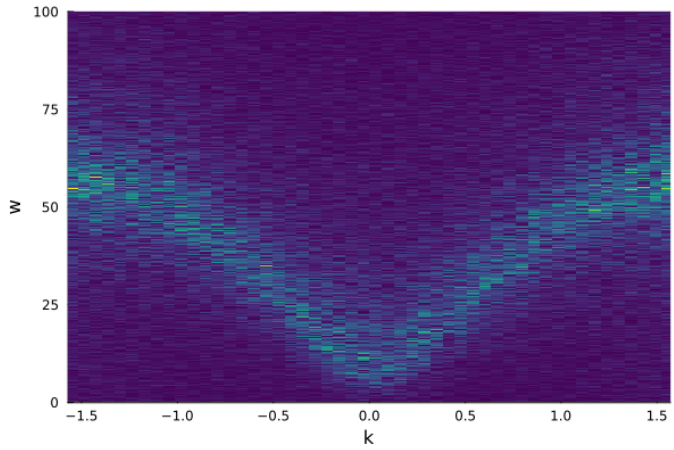

Figure 6: Heat map and plots of two dimensional DFT for antiferromagnetic dispersions with a homogeneous magnetic field $\mu B_0 = 0.05J$.

1.2.3 Ferromagnetic phase diagrams

For this section, $J = 10meV$, $d_z = 0.3meV$, and $\alpha = 0.1$ was used. The time steps were $1fs$.

I first set up a toy system with 10x10x10 magnets and set $kbt = 0$. A collinear ground state, where all magnets pointed in positive or negative z-direction, was found, see Figure 7

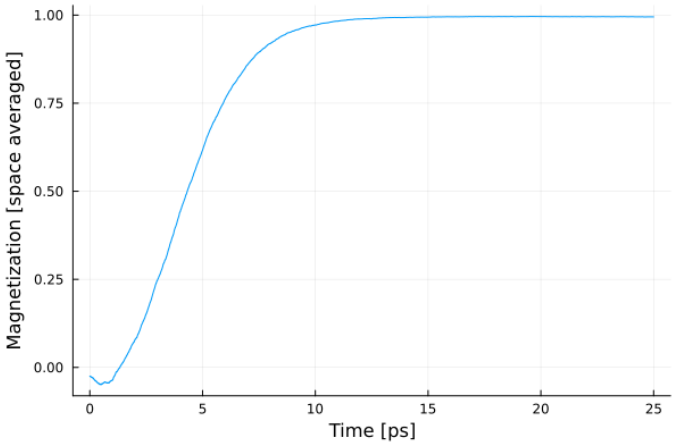

Figure 7: Simulation of the magnetization of 10x10x10 magnets starting from random spinstates.

The difference is that in the first plot, the magnetization goes to 1. Since we have an unaxial constant all the magnets are driven to have [0,0,1] or [0,0,-1] spin. But when you have a temperature term, the spins will receive random velocities at each time steps (although small changes) and thus will fluctuate around the desired spin. So instead of the z-component being 1 in the spin, it is almost 1. See Figure 8.

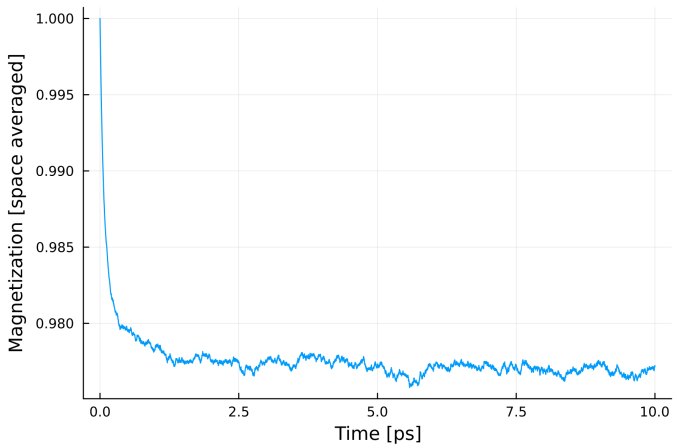

Figure 8: Simulation of the magnetization of 20x20x20 magnets starting from the ferromagnetic ground state, at T = 0.1J.

I simulated for 20 different values of kbt varying from $0.1J$ to $2J$. The plots of 2 examples are shown in Figure 9. The start times for calculating the time average magnetizations were chosen by observing the plots for different temperatures. For example, for $kbt = 0.5J$, the start time was at $1ps$, while for $kbt = 1.4J$, the start time was at $3ps$.

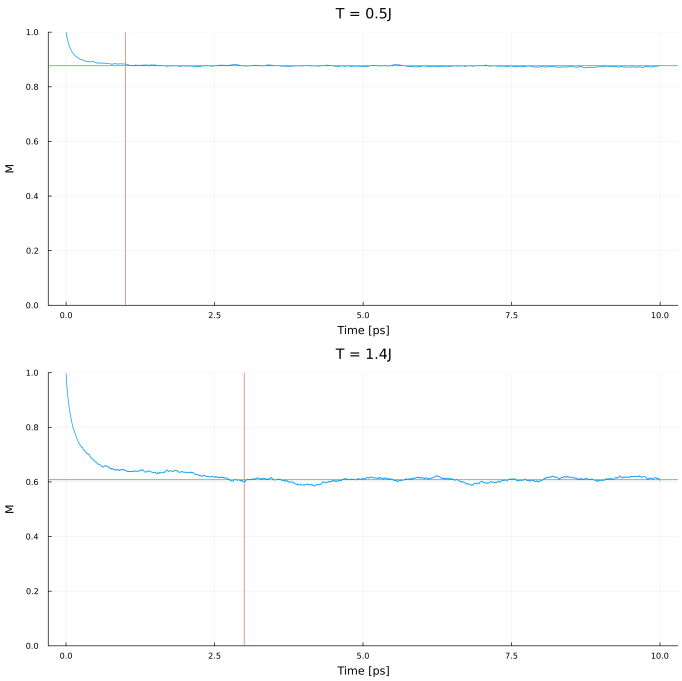

Figure 9: Simulations of the magnetization of 20x20x20 magnets starting from the ferromagnetic ground state, at $kbt = 0.5J$ and $kbt = 1.4J$. The orange line indicates the start point for the time averaged magnetization, and the green line is the calculated time averaged magnetization.

The space and time averaged magnetization is plotted in Figure 10. It is observed that the values seem to go in a zig-zag pattern. Since the simulations for this task took quite a long time, I had divided them into two simulations. The first simulated ten temperatures ranging from $0.2J$ to $2J$. The other simulated also ten temperatures, but ranging from $0.1J$ to $1.9J$. This is probably the cause for the zig-zag pattern, however I can not seem to find the specific reason as to why it happened. Nevertheless, the shape of the plot is still intact and it is possible to detect the theoretical critical temperature of around $1.7kbt$ as it is around that area the plot levels out. The overall shape is as expected. When the temperature gets large enough the magnetization will decrease, as the unaxial term contributes less and less compared to the temperature term. And since the temperature term contributes in random directions, it would be expected that more and more of the spins would point away from the z-axis as a matter of probability.

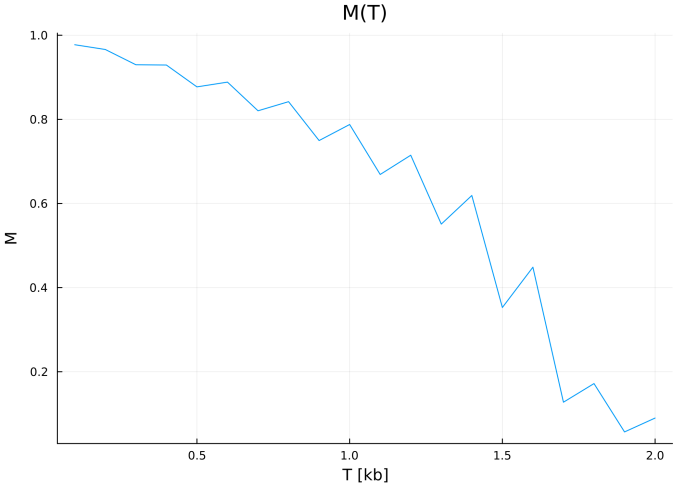

Figure 10: Time and space averaged magnetization as a function of temperature. NOTE: It should say [J], and not [kb] on the x-axis.

Appendix

I worked heavily with the candidates 10076 and 10069. They did not write their code in Julia, but we discussed the overall structure and methods to find the solutions.