UNSW AUSTRALIA

PHYS 3112 computational lab 2

Numerical simulations: the Ising model

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SKILLS GAINED

- Run existing Ising model code
- Connect bulk properties like magnetization and magntic susceptibility with the 2d distribution of spin in a lattice

ASSUMED KNOWLEDGE

- Editing and running python code
- Spin and magnetism

1 Experimental aim

To calculate the spin alignment behaviour and calculate the temperature of phase transition between magnetic and chaotic in a regular lattice material.

2 Introduction

There is a lab on magnetism in rare earth elements, which you may have done. This section on magnetism is from the introduction section of that lab.

Electrons 'orbiting' around a nucleus possess magnetic dipole moments both due to their orbital 'motion' around the nucleus and due to their intrinsic spin. In the case of Russel-Saunders (or L-S) coupling, the individual electronic spins couple to give a resultant spin $\mathbf{S}$ for the ion (atom), while the individual orbital angular momenta couple to give a resultant orbital momentum $\mathbf{L}$. These two magnetic components couple magnetically to give the ion a total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$. If the number of electrons orbiting the nucleus is such that some of the atomic subshells are only partially filled, $\mathbf{L}$ and/or $\mathbf{S}$ are non-zero and the ion as a whole will have a net magnetic dipole moment.

Consider now a crystalline solid made up of ions, some of which possess permanent magnetic moments. Each magnetic ion interacts with its surroundings. Some important interactions that may occur are:

(a) The exchange interactions between the spin part of the total electronic angular momentum on the magnetic ions. These interactions (electrostatic in origin) are due to overlap of the electronic wave functions on neighbouring ions and the interaction strength depends on the relative directions of the interacting spins. Indirect (or RKKY) exchange via intermediary electrons (e.g. conduction electrons in metals) may also occur and is in fact the dominant exchange mechanism between the 4f electrons in rare earth metals and alloys (Elliott 1972, Taylor 1972).

(b) The interaction of the orbital part of the electronic angular momentum with the surrounding charge distribution in the crystal. The charge distribution is considered to set up an effective electric field at the ionic known as the crystal (or anisotropy) field. The field has the same

symmetry as the crystal and tends to align the orbital electronic moments in a preferred direction relative to the crystal axes (i.e. the interaction is anisotropic).

(c) The long-range ($\propto 1/r^3$) dipole-dipole interaction between magnetic moments. This interaction is the same as that between two magnets on a macroscopic scale. This interaction tends to align magnetic dipoles antiparallel to one another, however it is much weaker than the exchange interactions of (a) on an atomic scale.

The energies of the above interactions depend on the individual ionic magnetic moments relative to one another and relative to the crystal lattice. Since the free energy of a solid in thermal equilibrium tends to a minimum, the final arrangement of the ionic magnetic moments at a given temperature will then depend on the size of each of the energy terms due to (a), (b) and (c) (the magnetostrictive energy associated with (c) is neglected here). In the Ising model, only the exchange interaction matters, and only with the nearest neighbours in the lattice.

2.1 The Ising model

The Ising model is an idealized study of magnetic behaviour in a solid. In the model, there is a regular n-dimensional grid of electrons with spin S that can have a value of +1 or -1, which can only interact with their nearest neighbours. The spins as a group will align into the lowest energy state, as determined by the Hamiltonian. If the grid is isolated, the total energy is $E = -\sum J_{ij} S_i \cdot S_j$ where J_{ij} is the interaction energy between neighbouring spins. If there is also a magnetic field applied, the energy has an additional $-\mu \sum S \cdot B$ term, where μ is the magnetic moment of each electron.

If the interaction energy J_{ij} is positive, then the lattice is ferromagnetic, and the spins prefer to align. If J_{ij} is negative, then the lattice is antiferromagnetic, and neighbouring spins prefer to be opposed. With an external magnetic field, the spins prefer to align with the field.

However, thermal energy in the lattice will tend to interfere with the spin alignment by spontaneously flipping spins. This limits the degree to which the whole lattice can be organised. At a critical temperature T_c, the lattice can no longer maintain its ordered behaviour, and it undergoes a phase transition and becomes paramagnetic (so that it has no fixed magnetization but can have one induced by an external magnetic field). As the temperature rises past Tc, the magnetization falls rapidly, and the magnetic susceptibility has a sharp maximum.

The magnetization M of the lattice is the average spin, calculated as $\frac{\sum S}{N}$ where N is the number of spins in the lattice. The magnetic susceptibility χ of the lattice is calculated as $\frac{(\langle M^2 \rangle - \langle M \rangle^2)}{k_B T}$, and it measures both how much the magnetization changes with increasing temperature and the ratio of induced to external magnetic field. Both of these quantities, and the total energy of the system, are calculated by the code we will be using in this lab.

From a study of susceptibility and magnetization as a function of temperature, we can determine the magnetic transition temperature of a magnetic solid.

3 Ising model code

The course Moodle page has code from https://github.com/red-starter/Ising-Model, which is well organized with functions and classes to do the calculations and make the plots we need for this lab. It also has a jupyter notebook for you to use during this lab.

The Ising model code uses a probabilistic approach and a series of steps to find the lowest energy state of the lattice, across a range of temperatures (measured in units of J_{ij}/k_B). For each temperature step, it begins with either a 'cold' start, in which all the spins are aligned, or a 'hot' start, in which the spins are randomly set. It then randomly chooses one of the electrons and uses a Metropolis algorithm to decide whether to flip it. The algorithm works like this:

1. If flipping the spin would reduce the total energy, flip it
2. If flipping the spin would increase the total energy by an amount dE, draw a random number between zero and 1 and flip it if the number is smaller than e^{-dE/k_BT}

This process is repeated until the system reaches equilibrium; that is, until the energy stops decreasing at each step. In the code we are using for this lab, it is run for a fixed number of steps, with a default of 50,000, which is sufficient. Then the code increases the temperature, resets the lattice to initial conditions, and runs the 50,000 steps again.

3.1 Using the code

To use this code, download it from the course Moodle page and put it into the same directory where you are running jupyter notebook. Import it with 'import Ising_model as model', and now there are a number of things you can do.

1. Set up your experiment with model.plots, which takes a number of inputs:
    - N - the size of the lattice (it will be an NxN grid)
    - B - the strength of the magnetic field (set to 0 by default)
    - start - whether use a cold start (start='Low') or a hot start (start='High') (set to 'Low' by default)
    - inc - the size of the temperature steps (set to 0.01 by default)
    - x0 - the lowest temperature to use (set to 1 by default)
    - x1 - the highest temperature to use (set to 5 by default)
    - steps - the number of steps to use when equilibrating the system (set to 50,000 by default)
    - T - the temperature to use when making a map of the spins (set to 1 by default)
- As an example: exp1=model.plots(N=15,start='High',inc=0.03)

2. Calculate energy and plot it versus temperature like this:
    - exp1.E()
    - exp1.show()
- For magnetization, use exp1.mag() and then exp1.show(); for magnetic susceptibility, use exp1.mag_sus and then exp1.show()

3. Make maps of the spin distribution using exp1.lattice() and then exp.show() - this creates a 2d plot with one pixel per spin, colour coded red/blue for up/down

4 Experimental Section

4.1 Experiments

Download the Ising model code for this lab from the course github page. Start a new jupyter notebook for this lab in the directory where the Ising model code is, and carry out the following experiments. Be sure to include enough comments that it is clear which experiment you are doing and which choices you are making for the model parameters.

4.1.1 Expt. 1: Magnetization versus temperature for a small lattice Generate an Ising model with 30x30 spins, and choose a 'cold' start (that is, with all spins aligned). Plot magnetization versus temperature. Now switch to a 'hot' start, with spins randomly distributed, and make the same plot. Make notes on any differences in your notebook.

4.1.2 Expt. 2: Magnetic susceptibility versus temperature for a larger lattice Using a 30x30 lattice with a 'cold' start, plot magnetic susceptibility as a function of temperature.

4.1.3 Expt. 3: Map out the spin distribution at fixed temperatures. Using a 100x100 lattice (or larger, if you want), make spin maps at T=1.5, 2, 3.5 and 4.

4.1.4 Expt. 4: Including an external magnetic field Turn on the external magnetic field in the model (with a strength between 0 and 2, so that the two terms in the Hamiltonian have comparable magnitudes), and remake the 'cold' start plots for magnetization, magnetic susceptibility and energy, and the spin maps for T=2.5.

If running these experiments seems overly simple, you are correct! What is important in this lab is your understanding of the Ising model and how it operates computationally, as well as what the results tell us about the behaviour of magnetisable substances in various conditions. In addition, you may wish to consider extended experiments (such as parameter changes not specified in the instructions) - these could also help you build your understanding of what is going on.

When composing your notebook, **please do your best to ensure readability!** You may wish to adopt a more formal structure to your notebook (eg Aim, Conduction of experiment, Discussion, Conclusion) to assist with this.

5 Discussion

You will be assessed via a “face-to-face” interview / video call, where you will need to screen-share your notebook. In your notebook, include in-depth responses to the following questions:

Question 1: Describe what is happening physically as you increase T in the 'cold' start lattice in experiment 1, and how your plot of magnetization versus temperature reflects that physical change. Describe the differences between the magnetization versus temperature plots for the 'cold' start and the 'hot' start. What in the program might be causing those differences?

Question 2: Based on your data from experiments 1 and 2, what is the value of Tc? How certain are you? Which measured quantity is most informative for answering this question? Describe two ways you could improve the accuracy of your measurement.

Question 3: Describe how the spin distribution maps in experiment 3 change with rising temperature. How does the behaviour you see in the maps correspond to physical properties like magnetization and susceptibility?

Question 4: What changes in your Ising model when you apply an external magnetic field? How can this be seen in your figures and your spin distribution maps?

6 References

6.1 Ising model code

https://github.com/red-starter/Ising-Model

6.2 Rare Earth Magnetism

Elliott R.J. (ed.), “Magnetic Properties of Rare Earth Metals” (1972).

Taylor K.N.R. and Darby M.I., “Physics of Rare Earth Solids” (1972).