PHYS379: Group Project – Spin System Modelling Topic

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Introduction

In PHYS379, you should undertake an open-ended group project and submit a group report describing the project. The group project is worth twenty credits. Please see the document "PHYS379-group-project-notes.pdf" for details about organisation and assessment.

Open-ended project

Your task in the project is to model the properties of spins on a lattice. Precisely what you do is your choice - the project is open-ended. You will need to formulate a research question (or questions) that is more specific than simply "model the properties of spins on a lattice". What are you trying to discover? You should do some research in the library or on the internet to find out what the interesting questions are. It may be that you will not finalise the research question until the latter stages of the project, once you have found what is (or is not) interesting. Remember that this is group work - it will make sense to plan for parallel tasks in order to use your personnel effectively. For example, you might want parallel numerical and analytic investigations, investigations looking at different aspects of the same problem, or you might deliberately duplicate effort in order to check important results (in the "real" world, results should always be checked before publication, getting different people to work independently is the best way to do this). There are some ideas below, you can follow some or all of them, or you can follow your own ideas.

Getting started

Ising model

The Ising model [1,2,3] consists of a lattice of N sites (e.g. a 1-d chain, a 2-d square lattice). The ith site ($i = 1,2,\cdots,N$) has a number s_i associated with it, where $s_i = 1$ or $s_i = -1$. This can be thought of as a spin (spin "up" or spin "down"). The energy E and magnetisation M of the Ising model are given by

$$E = -J\sum_{\langle i,j\rangle}^{N} s_i s_j - h\sum_{i=1}^{N} s_i\,; \qquad M = \sum_{i=1}^{N} s_i \qquad (1)$$

The first term in E describes the energy due to interactions between spins. Notation $\langle i,j\rangle$ indicates that only the interactions between nearest neighbours are taken into account, and the strength of this interaction is characterised by the exchange constant J. For $J > 0$, the lowest energy of a pair of spins occurs when they are parallel, this is called a ferromagnetic interaction, whereas for $J < 0$, the lowest energy of a pair of spins occurs when they are antiparallel, this is called an antiferromagnetic interaction.

The second term in the energy, Eq.1, describes the interaction of the spins with an external magnetic field of strength proportional to parameter h. As an example, three possible

configurations of a one-dimensional chain with $N = 4$ is shown in Fig.1. There are $2^N = 16$ possible configurations (microstates), and there are different possible energies and magnetistations. Usually we are interested in determining thermodynamic averages $\langle E \rangle$, $\langle M \rangle$ and fluctuations, e.g. $\langle M^2 \rangle - \langle M \rangle^2$.

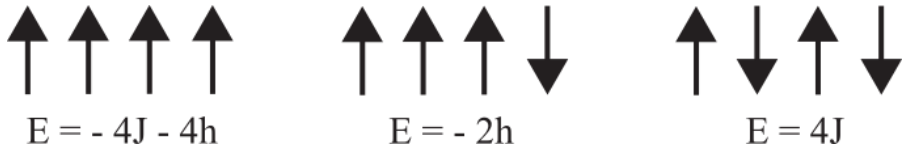

Figure 1 Three of the $2^N = 16$ possible configurations of a one-dimensional system of $N = 4$ Ising spins. The corresponding energy Eq.1 of each configuration is given, using periodic boundary conditions.

Metropolis algorithm

The canonical ensemble describes a system in thermal equilibrium with a heat bath of fixed temperature T, the system reaching equilibrium by exchanging energy with the heat bath. The system has fixed V, N, T.

The probability P_ℓ for the system to be in the ℓth microstate of energy E_ℓ is given by

$$P_\ell = \frac{1}{Z} e^{-E_\ell / k_B T}; \qquad Z = \sum_\ell e^{-E_\ell / k_B T} \qquad (2)$$

where the sum in the partition function Z is over all microstates with fixed V and N. Observable quantities of interest include

$$\langle E \rangle = \frac{1}{Z} \sum_\ell E_\ell e^{-E_\ell / k_B T}; \qquad \langle E^2 \rangle = \frac{1}{Z} \sum_\ell E_\ell^2 e^{-E_\ell / k_B T}$$

$$\langle M \rangle = \frac{1}{Z} \sum_\ell M_\ell e^{-E_\ell / k_B T}; \qquad \langle M^2 \rangle = \frac{1}{Z} \sum_\ell M_\ell^2 e^{-E_\ell / k_B T}$$

$$C = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2); \qquad \chi = \frac{1}{k_B T} (\langle M^2 \rangle - \langle M \rangle^2)$$

where, for the susceptibility χ, the magnetisation is evaluated for zero external field, $h = 0$.

For N sites, there are 2^N possible microstates, so calculating thermodynamic averages directly is very difficult for large N. One possible approach is to use a Monte Carlo numerical method. Monte Carlo is a generic term describing algorithms which use repeated random sampling. Here we describe the Metropolis algorithm [2,3,4] which is used for the Boltzmann distribution Eq.2. To begin the numerical approach, consider the zero field case, $h = 0$, and introduce dimensionless parameters describing energy $\epsilon = E/J$ and temperature $\tau = k_B T/J$:

$$\epsilon_\ell = -\sum_{\langle i,j \rangle}^{N} s_i s_j; \qquad \langle \epsilon \rangle = \frac{1}{Z} \sum_\ell \epsilon_\ell e^{-\epsilon_\ell / \tau}$$

Then, for fixed values of N and τ, take the following steps [2]:

1. Choose an initial microstate, calculate its energy.

2. Create a "trial" state by choosing one of the spins at random and flipping its spin.
3. Calculate $\Delta\epsilon = \epsilon_{\text{trial}} - \epsilon_{\text{old}}$, the change in energy due to the flip.
4. If $\Delta\epsilon \leq 0$, accept the trial microstate, go to step 8.
5. If $\Delta\epsilon > 0$, calculate the quantity $w = \exp(-\Delta\epsilon/\tau)$.
6. Generate a random number r in the unit interval $[0,1]$.
7. If $r \leq w$, accept the trial microstate. If $r > w$, keep the old microstate.
8. Determine the value of the required physical observables.
9. Repeat steps 2. to 8. to obtain a large enough number of microstates.
10. Compute averages over the microstates.

It is conventional to say that one "time" unit or one "Monte Carlo step per particle" (mcs) has elapsed after N spins have had a chance to flip. You should ensure that your results converge (i.e. you reach equilibrium), this will probably require at least several thousand mcs. Plot the dependence on temperature, τ. Compare with analytic results, e.g. in 1d, $\langle\epsilon\rangle = -N\tanh(1/\tau)$.

Open-ended part

Please note:

1. **The aim is for your group to do its own, original calculations.** A literature review and, perhaps, reproduction of other people's results may be important steps along the way, but these are not the final aim.
2. This topic has been offered for many years, but only done a couple of times. One main difficulty is to be able to numerically model a large enough system. Model a series of ever larger systems and extrapolate. For critical exponents, this is the topic of "finite-size scaling".

Ideas include:

- Ising model for the two-dimensional square lattice. Is it possible to check your numerical program? What are its properties? Phase transition? See Sections 15.7, 15.8 of Ref.[2].
- Ising model in an external magnetic field. See Section 15.9 of Ref.[2].
- Antiferromagnetic Ising model. Triangular lattice and frustration. See Section 15.9 of Ref.[2].
- Other types of thermodynamic ensemble. See Section 15.12 of Ref.[2].
- Different models, e.g. xy model, Heisenberg model, Kitaev model. See Projects 15.37, 15.38 of Ref.[2].
- What is the role of next-nearest neighbour interactions?
- What happens if there is a defect in the lattice? What models of defects can you imagine, e.g. a bond (or series of bonds) with different J? a missing site? What is the role of disorder - adding defects with a fixed density but at random positions or with random characteristics?
- What happens if there are regions of space with different properties, e.g. different J values or different lattices?
- Which analytic methods are useful? Transfer matrix method?

Bibliography

[1] “Ising model”, http://en.wikipedia.org/wiki/Ising_model

[2] “An Introduction to Computer Simulation Methods” by H. Gould, J. Tobochnik, and W. Christian (Pearson, San Francisco, 2007)

[3] “Physics Simulations in Java” by D. V. Schroeder, http://physics.weber.edu/schroeder/javacourse/javamanual.pdf

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