Introduction

Based on their response to external magnetic fields, materials are classified as diamagnetic, paramagnetic or ferromagnetic. A diamagnetic material produces a weak magnetization that opposes the applied magnetic field. A paramagnetic material produces a magnetization, stronger than that of a diamagnetic material, along the applied field. On the contrary, ferromagnetic effects are strong and yield a magnetization much stronger than the applied field. When an external magnetic field is applied to a ferromagnetic material, the individual atomic spins align themselves along one direction, yielding a macroscopic magnetic moment.

In this exercise we will use a Monte Carlo simulation to study the effect of temperature on ferromagnetism. We will use the 2D Ising model to treat our system as an array of N particles with non-zero spin $\{\mathbf{s}_j\}$, in an external magnetic field $\mathbf{B}$ perpendicular to the plane of the particles. Interaction amongst particles is assumed to be restricted to first neighbours. The Hamiltonian of this system reads:

$$H(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N) = -\frac{1}{2} J \sum_i \sum_{j \in \mathcal{N}_i} \mathbf{s}_i . \mathbf{s}_j - \mu \mathbf{B} \sum_{i=1}^{N} \mathbf{s}_i,$$

where $\mathcal{N}_i$ represents the neighbour list of particle i. The magnetization of system at a given state $\{\mathbf{s}_j\}$ is:

$$M(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N) = \mu \sum_{i=1}^{N} \mathbf{s}_i.$$

Let us consider a canonical ensemble of N particles at an inverse temperature β. The average energy and magnetization of the system can be calculated by the ensemble averages:

$$\langle E \rangle = \int d\mathbf{s_1} d\mathbf{s_2} \ldots d\mathbf{s_N} H(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N) e^{-\beta H(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N)}, \tag{1}$$

$$\langle M \rangle = \int d\mathbf{s_1} d\mathbf{s_2} \ldots d\mathbf{s_N} M(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N) e^{-\beta H(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N)}. \tag{2}$$

Invoking the ergodic hypothesis, the ensemble averages can be replaced by the following averages over the time:

$$\langle E \rangle = \int d\mathbf{s_1} d\mathbf{s_2} \ldots d\mathbf{s_N} H(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N) e^{-\beta H(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N)} \approx \langle H(\mathbf{s}(\tau)_1, \mathbf{s}(\tau)_2, \ldots, \mathbf{s}(\tau)_N) \rangle_t ,$$

$$\langle M \rangle = \int d\mathbf{s_1} d\mathbf{s_2} \ldots d\mathbf{s_N} M(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N) e^{-\beta H(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N)} \approx \langle M(\mathbf{s}(\tau)_1, \mathbf{s}(\tau)_2, \ldots, \mathbf{s}(\tau)_N) \rangle_t ,$$

$$\langle C \rangle \approx \frac{1}{k_B T^2} \mathrm{Var}(H(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N))_t,$$

$$\langle \chi \rangle \approx \frac{1}{k_B T} \mathrm{Var}(M(\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N))_t.$$

where, C and χ are heat capacity and magnetic susceptibility respectively.

To generate a time series $\{\mathbf{s}(\tau)_1, \mathbf{s}(\tau)_2, \ldots, \mathbf{s}(\tau)_N\}$ over which the averages of E and M will be performed, we will use the Markov Chain Monte Carlo (MCMC) algorithm.

Exercise 1 An Ising Model for a toy system [15 minutes]

The Markov Chain Monte Carlo algorithm with a Metropolis rule is implemented in the "**lab3_stepper.cdf**" file for a system of 64 particles on an 8x8 grid. The button "**reset**" allows you to start from either a random or a predefined configuration of $\{\mathbf{s}_j\}$. The button "**step**" performs one step of the algorithm *i.e.* one accepted or rejected "flip" of spin state of a random particle. The temperature of the simulation can be changed by moving the slider. Play around with it for a while!

(a) Begin with a randomly configured starting point. Try to observe the effect of temperature on the probability of accepting a "flip" with positive ΔE. Do you see a pattern ? Can you explain it?

(b) Begin with a configuration using the initialization style "disk". Run Monte Carlo steps at a high temperature . Do you see a relationship between the probability of accepting a "flip" and the location of the "flipped" particle?

Exercise 2

Open the file called "**lab3_ising.cdf**". It is an interface for simulating the Ising model and computing averages. The size of the system, temperature, magnitude of magnetic field and initial configuration can be varied using labeled sliders or buttons. The plots on the right give the average and variance of the energy and the magnetization.

Before beginning a simulation you must choose a starting configuration. Various "initialization styles" can be chosen by clicking the appropriate buttons. By clicking the buttons "run" and "stop" you can begin and end the simulation. The frequency at which the plots and the system grids are updated can be manipulated by the buttons labeled "Number of MC steps".

The expectation values of energy and magnetization are computed by averaging over time. The averages and the variance are printed at the upper right corner of the plots. The buffer of data over which the average is computed can be reset by pressing the button "reset".

To compute the average only over the equilibrium configurations it is suggested that you follow a two step procedure:

- **Equilibration:** Let the simulation run until the system reaches a state of equilibrium. This will be indicated by the convergence of magnetization and energy to an average value with finite fluctuations around it.
- **Production:** To discard the non equilibrium configurations, "reset" the average after the system has "equilibrated" and record the average value over a few million simulation steps.

(a) Begin from various initial configurations with the magnetic field set to zero and temperature $\approx 1.$. Do they end up in the same or different equilibrium states ? Can you explain the results you have found?

(b) Compute the following plots for the option size=100 in the absence of external magnetic field.
   - energy vs temperature.
   - magnetization vs temperature.
   - heat capacity vs temperature.
   - magnetic susceptibility vs temperature.

Cont.

Start from a random configuration. Each member of your group should run a separate simulation so that you can plot all your results together. If you see any abnormal behaviour, take note. What kind of phase transition do you see? Can you estimate the critical temperature? *HINT:*

- *Start with about 8 equally-spaced temperatures within the given range, and then refine in the region where you observe interesting effects.*
- *Note that near the critical temperature the growing fluctuations in energy and magnetization will affect your average. In order to get a statistically significant average you will have to run longer simulations.*

(c) How does the heat capacity, as estimated from the derivative of the internal energy, compare with the heat capacity computed from the fluctuations of the energy? *HINT:*

- *The average energy and variance of energy are given in scaled form, so the units are* $\frac{unit\ of\ observable}{number\ of\ particles}$ *and* $\frac{(unit\ of\ observable)^2}{(number\ of\ particles)^2}$ *respectively.*
- *Pay attention while using the expression for the heat capacity in terms of energy fluctuations, that this is written for the* extensive *quantity. So make sure the unit of heat capacity and magnetic susceptibility is not scaled by (number of particles)*^{2}*.*

Exercise 3

Computer simulations are often affected by “finite size effects"; that is, results depend on the number of sites included in the simulation, and differ from the results predicted in the limit of a system of infinite size.

(a) Try to estimate the critical temperature for size $L = 20$ and $L = 10$, by looking at the maximum in heat capacity. How are the plots different form the ones you obtained in exercise 2 (b)? Also plot the critical temperature as a function of $1/L$. What kind of a trend do you observe? Do you think you can extrapolate the result to the large size limit ? You will need longer simulations to converge averages at the smaller sizes (but correlation time will be shorter, so you can print more often). Use a stride of 100k steps, and a buffer size of 2k or 4k samples.

(b) Using the data of average energy vs temperature obtained in the previous section and exercise 2 part (a) compute the heat capacity curves by finite differences. How do these compare with the ones you computed using the variance of energy? Do you see a size effect and can you explain it?

Exercise 4 Magnetic hysteresis in an Ising model

Use the notebook **lab3_ising.cdf** to perform this exercise.

(a) For Size$= 100$ compute the hysteresis curve by following the instructions:

- Start at $T = 1.0$ and $B = 0.60$. Record the magnetization $M(T = 1.0, B = 0.6)$.
- Record the magnetization as the B is decreased to about $B = -0.6$, proceeding in steps of about 0.1 and letting the system equilibrate before collecting the average magnetization. *Hint: you can use the Reset avg. button!*
- Record the magnetization as the the magnetic field is increased to $B = 0.60$

Plot M vs B for the process.What is the integral $\oint đQ$ over the cycle ?

(b) Can you repeat (a) at $T = 2.0$? How is the hysteresis plot different from the one obtained in (a) ?

Exercise 5 Linear response in an ising model

Cont.

Use the notebook **lab3_ising.cdf** to perform this exercise.

(a) For Size= 100 compute the magnetic susceptibility curve for $T \in (1.0, 3.0)$ by computing finite differences, i.e. by computing

$$[\langle M\rangle\,(B = 0.05) - \langle M\rangle\,(B = -0.05]/0.1 \tag{3}$$

Compare the curves with the one one obtained by averaging χ over the trajectory in the Exercise 2.

(b) Try different $\Delta B \in \{0.1, 0.01, 0.001\}$ and explain which order of magnitude is optimum for approximating a derivative with a finite difference? Do you think a very small ΔB give the best result? What happens if you use a value of ΔB that is too large (think also about the previous exercise)?

Exercise 6 Spin correlation functions

Use the notebook **lab3_rng.cdf** to perform this exercise.

(a) Compute the pair wise spin correlation functions $c_j = \langle s_i s_{i+j}\rangle$ for Size $= 256$ at $T \in \{2.1, 2.2, 2.24, 2.26, 2.3, 2.5, 3.0\}$. By pressing the "analyze" button a number of times you can get an estimate of the pair wise spin correlation. You'll have to wait a long time (at least one minute) between evaluations, so as to obtain uncorrelated samples. It might help to use the largest MC step delay. Comment qualitatively on the shape of the curve at the different temperatures, and explain how this relates to what you know about the critical point of the Ising model. *Hint: Particularly below the critical temperature it might be better to initialize your simulations in an "all up" or "all down" configurations, to avoid the formation of long-lived magnetic domains (which are a non-equilibrium feature)*

The "RNG ANALYSIS" box makes it possible to perform a renormalization group analysis of a snapshot by decimating the spins. The simulation box is too small and the simulation time too short to allow for a quantitative analysis, but this is good enough to give you an idea of how RNG theory works, and what is the effect of applying a RNG transformation onto a 2D lattice. *Hint: stop the main simulation before you perform a RNG analysis, or you might hang your computer!*

(b) Perform a RNG analysis for a few temperatures below, at and above T_c. What do you observe as the grid is coarsened? Comment both on the qualitative patterns you observe on the grid, and on the decay of the spin correlation function. *Hint: you may not observe exactly what you expect for* $T = T_c$. *This is both because of the approximate nature of RNG theory for the 2D lattice, and because of finite size effects.*

The End.