Final projects
Computational Physics course

Part 1: Ising model

Please note that the deadline for the final projects is midnight of 28th March, 2025.

Consider the following text for Projects 1 and 2.

and estimate the uncertainty in your answer. Study how your results depend upon where the random walker is started and on how many thermalization steps you take before beginning the sampling. Compare the efficiency of the Metropolis algorithm with that of a calculation that uses one of the methods discussed in Section 8.2 to generate the normal distribution directly.

8.4 The Ising model in two dimensions

Models in which the degrees of freedom reside on a lattice and interact locally arise in several areas of condensed matter physics and field theory. The simplest of these is the Ising model [Hu63], which can be taken as a crude description of a magnetic material or a binary alloy. In this example, we will use Monte Carlo methods to calculate the thermodynamic properties of this model.

If we speak in the magnetic language, the Ising model consists of a set of spin degrees of freedom interacting with each other and with an external magnetic field. These might represent the magnetic moments of the atoms in a solid. We will consider in particular a model in two spatial dimensions, where the spin variables are located on the sites of an $N_x \times N_y$ square lattice. The spins can therefore be labeled as S_{ij}, where i, j are the indices for the two spatial directions, or as S_α, where α is a generic site label. Each of these spin variables can be either "up" ($S_\alpha = +1$) or "down" ($S_\alpha = -1$). This mimics the spin-1/2 situation, although note that we take the spins to be classical degrees of freedom and do not impose the angular momentum commutation rules characteristic of a quantum description. (Doing so would correspond to the Heisenberg model.)

The Hamiltonian for the system is conventionally written as

$$H = -J \sum_{(\alpha\beta)} S_\alpha S_\beta - B \sum_\alpha S_\alpha. \tag{8.18}$$

Here, the notation $(\alpha\beta)$ means that the sum is over nearest-neighbor *pairs* of spins; these interact with a strength J (see Figure 8.2). Thus, the spin at site ij interacts with the spins at $i \pm 1j$ and $ij \pm 1$. (We assume periodic boundary conditions on the lattice, so that, for example, the lower neighbors of the spins with $i = N_x$ are those with $i = 1$ and the left-hand neighbors of those with $j = 1$ are those with $j = N_y$; the lattice therefore has the topology of a torus.) When J is positive, the energy is lower if a spin is in the same direction as its neighbors (ferromagnetism), while when J is negative, a spin will tend to be anti-aligned with its

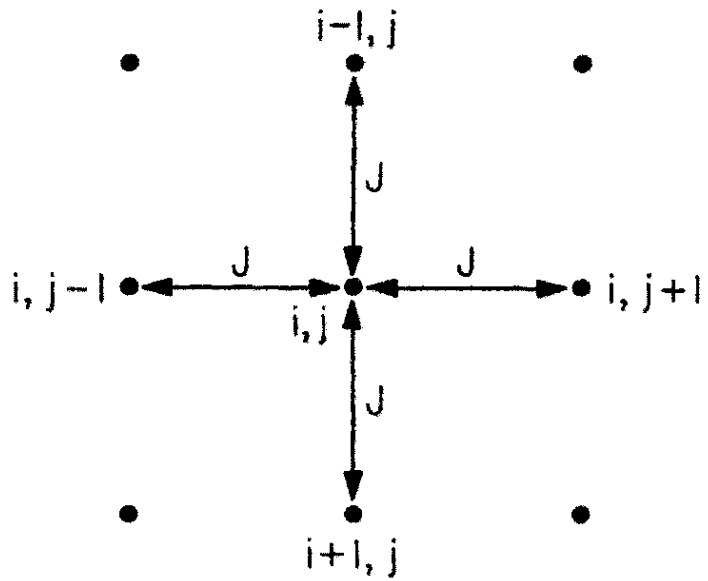

Figure 8.2 Schematic illustration of the two-dimensional Ising model.

neighbors (anti-ferromagnetism). The term involving B represents the interaction of the spins with an external magnetic field, which tends to align all spins in the same direction.

We will be interested in the thermodynamics of this system. In this case, it is convenient to measure the coupling energies J and B in units of the temperature, so that heating the system corresponds to decreasing these couplings. Configurations of the system are specified by giving the values of all $N_x \times N_y \equiv N_s$ spin variables and the weighting of any one of the 2^{N_s} spin configurations, $\mathbf{S}$, in the canonical ensemble is

$$w(\mathbf{S}) = \frac{e^{-H(\mathbf{S})}}{Z}\,, \tag{8.19}$$

where the partition function is

$$Z(J,B) = \sum_{\mathbf{S}} e^{-H(\mathbf{S})}\,. \tag{8.20}$$

The thermodynamic quantities we will be interested are the magnetization

$$M = \frac{\partial \log Z}{\partial B} = \sum_{\mathbf{S}} w(\mathbf{S}) \Big(\sum_{\alpha} S_\alpha \Big) , \tag{8.21a}$$

the susceptibility

$$\chi = \frac{\partial M}{\partial B} = \sum_{\mathbf{S}} w(\mathbf{S}) \Big(\sum_{\alpha} S_\alpha \Big)^2 - M^2 , \tag{8.21b}$$

the energy

$$E = \sum_{\mathbf{S}} w(\mathbf{S}) H(\mathbf{S}) , \tag{8.21c}$$

and the specific heat at constant field,

$$C_B = \sum_{\mathbf{S}} w(\mathbf{S}) H^2(\mathbf{S}) - E^2 . \tag{8.21d}$$

In the limit of an infinitely large lattice ($N_{x,y} \to \infty$), it is possible to solve the Ising model exactly; discussions of the solution, originally due to Onsager, can be found in [Hu63] and [Mc73]. The expressions are simplest at $B = 0$. In this limit, the energy is given by

$$E = -N_s J (\coth 2J) \Big[1 + \frac{2}{\pi} \kappa' K_1(\kappa) \Big] , \tag{8.22a}$$

and the specific heat is

$$C_B = N_s \frac{2}{\pi} (J \coth 2J)^2 \left(2K_1(\kappa) - 2E_1(\kappa) - (1 - \kappa') \Big[\frac{\pi}{2} + \kappa' K_1(\kappa) \Big] \right) , \tag{8.22b}$$

while the magnetization is given by

$$M = \pm N_s \frac{(1 + z^2)^{1/4} (1 - 6z^2 + z^4)^{1/8}}{(1 - z^2)^{1/2}} \tag{8.22c}$$

for $J > J_c$ and vanishes for $J < J_c$. In these expressions,

$$\kappa = 2 \frac{\sinh 2J}{\cosh^2 2J} \leq 1 , \quad \kappa' = 2 \tanh^2 2J - 1 ,$$

the complete elliptic integrals of the first and second kinds are

$$K_1(\kappa) \equiv \int_0^{\pi/2} \frac{d\phi}{(1 - \kappa^2 \sin^2 \phi)^{1/2}} , \quad E_1(\kappa) \equiv \int_0^{\pi/2} d\phi \, (1 - \kappa^2 \sin^2 \phi)^{1/2} ,$$

Project 1 (15 points)

Write a Monte Carlo code with Metropolis algorithm for a 2D Ising model using the Hamiltonian given in eqn. (8.18) in the above text. Consider ferromagnetic interactions (J>0) and zero magnetic field. Calculate and plot the order parameter (absolute value of the magnetization), susceptibility (fluctuations of magnetization) and specific heat (fluctuations of the internal energy) as a function of temperature and comment on the phase transition. Obtain the above quantities for 8x8, 16x16 and 32x32 lattices to observe the finite size effects. Obtain the phase transition temperature by calculating the 4th order cumulant defined as

$$U_L = 1 - \frac{\langle M^4 \rangle_L}{3\langle M^2 \rangle_L^2}$$

where M is the magnetization for a lattice size L. The crossing point of the cumulants for various lattice sizes plotted against temperauture gives an estimate of the phase transition temperature.

Project 2 (15 marks)

(a) Use your Monte Carlo code to study the thermodynamic properties for antiferromagnetic coupling (J<0) and for non-zero values of the external field B.

(b) An alternative method to calculate the thermodynamic quantities is to use a ’Heat bath’ algorithm. Here, for a zero external magnetic field, the chosen spin i may be set to +1 with probability p_i and -1 with probability 1-p_i, where

$$p_i = \frac{e^{2J\beta \sum_j S_j}}{1 + e^{2J\beta \sum_j S_j}} \qquad \beta = 1/k_B T$$

S_j’s are nearest neighbor spins of S_i.

Write a Monte Carlo code based on the *Heat bath* algorithm to compare the results and efficiency with *Metropolis* algorithm. Do the simulation in zero magnetic field.

Hints/tips

1. Strength of J: a clever thing is to use a dimensionless parameter $J/(k_B T)$ where k_B is the Boltzmann constant and T is the temperature. To study the phase transition, plot the observables as a function of an inverse of this parameter $k_B T/J$, which is proportional to T. The transition temperature happens for $k_B T/J \sim 2.3$, so a useful range is ca 0.5 to 5.0.

2. Don't forget that the Monte Carlo simulations (MCS) have two distinct phases: (i) the first phase is the thermalisation phase where no measurement is taken but only the system is allowed to evolve with Metropolis algorithm, (ii) second phase is the measurement/sampling phase where you take the measurements of essential quantities as energy and magnetization in regular intervals (not too small to avoid correlation) and store them. When you will be calculating the averages, the average is over all these measurements. Moreover, you can do several fresh starts of MCS with different seed values of the random number generator and finally take the grand average over all these configurations.

3. In plots compare the numerical results with the exact analytical expressions for magnetization [$z=\exp(-2J)$] and specific heat since especially the latter may converge slower with respect to the lattice size and without a reference it might look confusing.