Computational Laboratory in Statistical Mechanics
PHYS 31453 Spring 2021

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STUDYING MAGNETISM WITH THE ISING MODEL

A ferromagnet can be approximately described by the Ising model. If s_i is the state of the i-th spin ($s_i = \pm 1$), B is the external magnetization, μ is the magnetic moment of a spin, and J is the interaction between neighboring spins, the Hamiltonian for the 1-dimensional Ising model is

$$H_{\text{Ising}} = \mu B \sum_{i=1}^{N} s_i - J \sum_{i=1}^{N} s_i s_{i+1} \tag{1}$$

Let $\mathbf{S}$ be the state of the system, given by the state of each spin in the system, $\mathbf{S} = \{s_1, \ldots, s_N\}$. At thermal equilibrium, the probability of finding the system in a given state $\mathbf{S}$ is

$$P_{eq}(\mathbf{S}) = \frac{1}{Z} \exp\left\{-\frac{H(\mathbf{S})}{k_B T}\right\}, \quad \text{where } Z = \sum_{\text{all } S} \exp\left\{-\frac{H(\mathbf{S})}{k_B T}\right\}. \tag{2}$$

The magnetization per spin, $\mathbf{M}$ of a state $\mathbf{S}$ is defined as $\mathbf{M}(\mathbf{S}) = (1/N)\sum_{i=1}^{N} s_i$. The magnetic susceptibility, $\chi = (\partial \mathbf{M}/\partial B)|_{B=0}$. Do you know how the specific heat is defined?
We will use the Metropolis Monte Carlo algorithm to simulate the behavior of the Ising model. The procedure is as follows:

1. Select one lattice site i at which the spin s_i is considered for flipping ($s_i \to -s_i$).
2. Compute the energy change δH associated with that flip.
3. Calculate the transition probability p for that flip.
4. Draw a random number Z uniformly distributed between zero and unity.
5. If $Z < p$ flip the spin, otherwise do not flip it. In any case, the configuration of the spins obtained in this way at the end of step (5) is counted as a "new configuration".
6. Analyze the resulting configuration as desired.

For example, you may plot the following:

1. $\mathbf{M}$ vs. time, to make sure that your system has reached equilibrium
2. $\langle M \rangle$ vs. T for fixed B, and different values of J.
3. $\langle M \rangle$ and χ (it actually denotes $\langle \chi \rangle = (\partial \langle \mathbf{M} \rangle / \partial B)|_{B=0}$) versus temperature, for a fixed magnetic field (a) $B = 0$ and (b) $B = 1$ (in units of $k_B T = 1,\ \mu = 1$) and fixed $J \neq 0$.
4. Energy and specific heat versus temperature.

Write the Hamiltonian for the 2D and 3D Ising model similar to the 1D model above and extend your program accordingly. Try plotting the above quantities in 2D (and 3D, if time permits). Your chain should have at least 100 spins and your 2D lattice should be at least 50×50.

We have also discussed the following details of the simulation in class:

1. Considerable freedom exists in the order in which subsequent lattice sites (i) are selected when one repeats this process. One may go through the lattice in a regular fashion or one may select the lattice sites at random; for equilibrium properties this does not matter.
2. Since subsequent states differ only by a single spin flip, they are almost identical. It may be better not to perform step (6) after every (attempted) flip, but only after much larger "time" intervals. We define one Monte Carlo step (MCS) per site by carrying out the above (5 or 6) steps once for every lattice site, if the spins are selected consecutively. If we select them at random, the MCS/site is defined by requiring that on the average each spin is selected once. It is then advisable to perform step (6) only once every MCS/site.
3. Although the distribution of generated states $P(\mathbf{S})$ asymptotically (that is, for $t \to \infty$) tends to the equilibrium distribution $P_{eq}(\mathbf{S})$ there is no reason to assume that the states immediately following the (arbitrary) initial configuration already have a distribution close to $P_{eq}(\mathbf{S})$. On the contrary, it will be necessary to generate a large number of configurations until the "memory" of the initial state is lost. ***Note:*** *The number of steps needed to reach equilibrium may depend on parameters such as temperature, magnetic field and the coupling.*
4. **Initial spin configuration:** A random spin configuration corresponds to the infinitely high temperature state $T = \infty$ with zero magnetization. We now let the system evolve in time. If there is a spontaneous magnetization at the temperature we are interested in, we need to essentially cool the system from a disordered phase to an ordered phase. It will take a long time to reach equilibrium, since all the excess energy needs to be removed from the system. It is better to choose your intial state according to the given parameters.
5. **Boundary conditions:** In 1D, the spins at the ends of the chain have only one neighbor as opposed to two for all the other spins. A similar situation arises at the faces, edges and corners of a 2D or 3D lattice. Using periodic boundary conditions helps reduce the disturbances from the boundaries of the system.
6. **Tip:** You can save computer time by storing at the beginning the small number of different values that the transition probability p can have, rather than evaluating the exponential function again and again. This method works for all problems with discrete degrees of freedom.

For more information, you can refere to: Kurt Binder and Dieter W. Heermann, *Monte Carlo Simulation in Statistical Physics*, Sixth Ed., Springer (2019). You have access to the electronic version of this book through the library (link).