Problem 15.11 One-dimensional Ising model

(a) Write a program to simulate the one-dimensional Ising model in equilibrium with a heat bath. Modify method `doOneMCStep` in `IsingDemon` (see class `IsingDemon` on page 600 or class `Ising` on page 611). Use periodic boundary conditions. Assume that the external magnetic field is zero. Draw the microscopic state (configuration) of the system after each Monte Carlo step per spin.

(b) Choose $N = 20$ and $T = 1$ and start with all spins up. What is the initial effective temperature of the system? Run for at least 1000 mcs, where mcs is the number of Monte Carlo steps per spin. Visually inspect the configuration of the system after each Monte Carlo step per spin and estimate the time it takes for the system to reach equilibrium. Does the sign of the magnetization change during the simulation? Increase N and estimate the time for the system to reach equilibrium and for the magnetization to change sign.

(c) Change the initial condition so that the orientation of each spin is chosen at random. What is the initial effective temperature of the system in this case? Estimate the time it takes for the system to reach equilibrium.

(d) Choose $N = 50$ and determine $\langle E \rangle$, $\langle E^2 \rangle$, and $\langle M^2 \rangle$ as a function of T in the range $0.1 \leq T \leq 5$. Plot $\langle E \rangle$ as a function of T and discuss its qualitative features. Compare your computed results for $\langle E \rangle$ to the exact result (for $B = 0$):

$$E(T) = -N \tanh \beta J. \tag{15.22}$$

Use the relation (15.19) to determine the T-dependence of C.

(e) As you probably noticed in part (b), the system can overturn completely during a long run and thus the value of $\langle M \rangle$ can vary widely from run to run. Because $\langle M \rangle = 0$ for $T > 0$ for the one-dimensional Ising model, it is better to assume $\langle M \rangle = 0$ and compute χ from the relation $\chi = \langle M^2 \rangle / kT$. Use this relation (15.21) to estimate the T-dependence of χ.

(f) One of the best laboratory realizations of a one-dimensional Ising ferromagnet is a chain of bichloride-bridged Fe^{2+} ions known as FeTAC (see Greeney et al.). Measurements of χ yield a value of the exchange interaction J given by $J/k = 17.4\,\mathrm{K}$. Note that experimental values of J are typically given in temperature units. Use this value of J to plot your Monte Carlo results for χ versus T with T given in Kelvin. At what temperature is χ a maximum for FeTAC?

(g) Is the acceptance probability an increasing or decreasing function of T? Does the Metropolis algorithm become more or less efficient as the temperature is lowered?

(h) Compute the probability $P(E)$ for a system of $N = 50$ spins at $T = 1$. Run for at least 1000 mcs. Plot $\ln P(E)$ versus $(E - \langle E \rangle)^2$ and discuss its qualitative features. ∎

You may select some items among these suggestions and you may also go beyond these. For example, the formula (15.22) can be generalized to finite N. However, please keep the following points in mind:

- Show that your results are correct. In particular, address the issue of proper thermalization.
- Compute error bars and include these into your plots. One way to get this is to repeat the simulation a number of times (for example 10 times) with different sequences of pseudorandom numbers and then compute the mean and variance of these repetitions.