Another quantity of interest is the mean magnetization $\langle M \rangle$ (see (16.7)) and the corresponding thermodynamic derivative χ:

$$\chi = \lim_{H \to 0} \frac{\partial \langle M \rangle}{\partial H}, \tag{17.13}$$

where H is proportional to the external magnetic field. In the following, we will refer to H as the magnetic field. The zero field magnetic susceptibility χ is an example of a linear response function, because it measures the ability of a spin to "respond" due to a change in the external magnetic field. In analogy to the heat capacity, χ is related to the fluctuations of the magnetization (see Appendix 17.31):

$$\chi = \frac{1}{kT}\big(\langle M^2 \rangle - \langle M \rangle^2\big), \tag{17.14}$$

where $\langle M \rangle$ and $\langle M^2 \rangle$ are evaluated in zero magnetic fields. Relations (17.12) and (17.14) are examples of the general relation between linear response functions and equilibrium fluctuations.

Now that we have specified several equilibrium quantities of interest, we implement the Metropolis algorithm for the Ising model. The possible trial change is the flip of a spin, $s_i \to -s_i$. The Metropolis algorithm was stated in Section 17.2 as a method for generating states with the desired Boltzmann probability, but the flipping of single spins also can be interpreted as a reasonable approximation to the real dynamics of an anisotropic magnet whose spins are coupled to the vibrations of the lattice. The coupling leads to random spin flips, and we expect that one Monte Carlo step per spin is proportional to the average time between single spin flips observed in the laboratory. We can regard single spin flip dynamics as a time dependent process and observe the relaxation to equilibrium after a sufficiently long time. In the following, we will frequently refer to the application of the Metropolis algorithm to the Ising model as "single spin flip dynamics."

In Problem 17.4 we use the Metropolis algorithm to simulate the one-dimensional Ising model. Note that the parameters J and kT do not appear separately, but appear together in the dimensionless ratio J/kT. Unless otherwise stated, we measure temperature in units of J/k, and set $H = 0$.

Problem 17.4. One-dimensional Ising model

from Gould-Tobochnick

a. Write a Monte Carlo program to simulate the one-dimensional Ising model in equilibrium with a heat bath. (Modify `SUB changes` in `Program demon` (see Chapter 16) or see `Program ising`, listed in the following, for an example of the implementation of the Metropolis algorithm to the two-dimensional Ising model.) Use periodic boundary conditions. As a test of your program, compute the mean energy and magnetization of the lattice for $N = 20$ and $T = 1$. Draw the microscopic state (configuration) of the system after each Monte Carlo step per spin.

b. Choose $N = 20$, $T = 1$, `mcs` $= 100$, and all spins up, that is, $s_i = +1$ initially. What is the initial "temperature" of the system? Visually inspect the configuration of the system after each Monte Carlo step and estimate the time it takes for the system to reach equilibrium. Then change the initial condition so that the orientation of the spins is chosen at random. What is the initial "temperature" of the system in this case? Estimate the time it takes for the system to reach equilibrium in the same way as before.

And in case the spins are alternatively up and down?

c. Choose $N = 20$ and equilibrate the system for `mcs` ≥ 100. Let `mcs` ≥ 1000 and determine $\langle E\rangle$, $\langle E^2\rangle$, $\langle M\rangle$, 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 $\langle E(T)\rangle$ to the exact result (for $H = 0$)

$$\langle E\rangle = -N \tanh \beta J. \tag{17.15}$$

Use the relation (17.12) to determine the T dependence of C.

d. What is the qualitative dependence of $\langle M\rangle$ on T? Use the relation (17.14) to estimate the T dependence of χ. One of the best laboratory realizations of a one-dimensional Ising ferromagnet is a chain of bichloride-bridged Fe^{2+} ions known as FeTAC (Greeney et al.). Measurements of χ yield a value of the exchange interaction J given by $J/k = 17.4\,\mathrm{K}$. (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?

e. 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?

f. Compute the probability density $P(E)$ for a system of 50 spins at $T = 1$. Choose `mcs` ≥ 1000. Plot $\ln P(E)$ versus $(E - \langle E\rangle)^2$ and discuss its qualitative features.

We next apply the Metropolis algorithm to the two-dimensional Ising model on the square lattice. The main program is listed in the following.

```
PROGRAM ising
! Monte Carlo simulation of the Ising model on the square lattice
! using the Metropolis algorithm
DIM spin(32,32),w(-8 to 8),accum(10)
LIBRARY "csgraphics"
CALL initial(N,L,T,spin(,),mcs,nequil,w(),E,M)
FOR i = 1 to nequil          ! equilibrate system
    CALL Metropolis(N,L,spin(,),E,M,w(),accept)
NEXT i
CALL initialize(accum(),accept)
FOR pass = 1 to mcs          ! accumulate data while updating spins
    CALL Metropolis(N,L,spin(,),E,M,w(),accept)
    CALL data(E,M,accum())
NEXT pass
CALL output(T,N,mcs,accum(),accept)
END
```

In `SUB initial` we choose the initial directions of the spins, and compute the initial values of the energy and magnetization. To compute the total energy, we consider the interaction of a spin with its nearest neighbor spins to the north and the east. In this way we compute the energy of each interaction only once and avoid double counting. One of the most time consuming parts of the Metropolis algorithm is the calculation of the exponential function $e^{-\beta\Delta E}$. Because there are only a small number of possible values of $\beta\Delta E$ for the Ising model (see Fig. 16.3), we store the