Problem 15.9 Planar spin in an external magnetic field

(a) Consider a classical planar magnet with magnetic moment μ_0. The magnet can be oriented in any direction in the xy-plane, and the energy of interaction of the magnet with an external magnetic field $\mathbf{B}$ is $-\mu_0 B \cos\phi$, where ϕ is the angle between the moment and $\mathbf{B}$. Write a Monte Carlo program to sample the microstates of this system in thermal equilibrium with a heat bath at temperature T. Compute the mean energy as a function of the ratio $\beta\mu_0 B$.

(b) Compute the probability density $P(\phi)$ and analyze its dependence on the energy. ■

In Problem 15.10 we consider the Monte Carlo simulation of a classical ideal gas of N particles in equilibrium with a heat bath. It is convenient to say that one time unit or one Monte Carlo step per particle (mcs) has elapsed after N particles have had a chance to change their coordinates. If the particles are chosen at random, then during one Monte Carlo step per particle, some particles might not be chosen, but all particles will be chosen equally on the average. The advantage of this definition is that the time is independent of the number of particles. However, this definition of time has no obvious relation to a physical time.

Problem 15.10 Simulation of an ideal gas in one dimension

(a) Modify class `BoltzmannApp` to simulate an ideal gas of N particles in one dimension. For simplicity, assume that all particles have the same initial velocity of 10. Let $N = 20$ and $T = 10$ and consider at least 2000 Monte Carlo steps per particle. Choose the value of δ so that the acceptance probability is approximately 40%. What are the mean kinetic energy and mean velocity of the particles?

(b) We might expect the total energy of an ideal gas to remain constant because the particles do not interact with one another and, hence, cannot exchange energy directly. What is the value of the initial total energy of the system in part (a)? Does the total energy remain constant? If not, explain how the energy changes.

(c) What is the nature of the time dependence of the total energy starting from the initial condition in (a)? Estimate the number of Monte Carlo steps per particle necessary for the system to reach thermal equilibrium by computing a moving average of the total energy over a fixed time interval. Does this average change with time after a sufficient time has elapsed? What choice of the initial velocities allows the system to reach thermal equilibrium at temperature T as quickly as possible?

(d) Compute the probability $P(E)\Delta E$ for the system of N particles to have a total energy between E and $E + \Delta E$. Plot $P(E)$ as a function of E and describe the qualitative behavior of $P(E)$. Does $P(E)$ have the form of the Boltzmann distribution? If not, describe the qualitative features of $P(E)$ and determine its functional form.

(e) Compute the mean energy for $T = 10$, 20, 40, 80, and 120 and estimate the heat capacity from its definition $C = \partial E/\partial T$.

(f) Compute the mean square energy fluctuations $\langle(\Delta E)^2\rangle = \langle E^2\rangle - \langle E\rangle^2$ for $T = 10$ and $T = 40$. Compare the magnitude of the ratio $\langle(\Delta E)^2\rangle/T^2$ with the heat capacity determined in part (e). ■

You might have been surprised to find in Problem 15.10d that the form of $P(E)$ is a Gaussian centered about the mean energy of the system. What is the relation of this form of $P(E)$ to the central limit theorem (see Problem 7.15)? If the microstates are distributed according to the Boltzmann probability, why is the total energy distributed according to the Gaussian distribution?

15.7 ■ SIMULATION OF THE ISING MODEL

You are probably familiar with ferromagnetic materials, such as iron and nickel, which exhibit a spontaneous magnetization in the absence of an applied magnetic field. This nonzero magnetization occurs only if the temperature is less than a well-defined temperature known as the Curie or critical temperature T_c. For temperatures $T > T_c$, the magnetization vanishes. Hence, T_c separates the disordered phase for $T > T_c$ from the ferromagnetic phase for $T < T_c$.

The origin of magnetism is quantum mechanical in nature and its study is of much experimental and theoretical interest. The study of simple classical models of magnetism has provided much insight. The two- and three-dimensional Ising model is the most commonly studied classical model and is particularly useful in the neighborhood of the magnetic phase transition.

The thermal quantities of interest for the Ising model include the mean energy $\langle E\rangle$ and the heat capacity C. One way to determine C at constant external magnetic field is from its definition $C = \partial\langle E\rangle/\partial T$. An alternative way is to relate C to the statistical fluctuations of the total energy in the canonical ensemble (see Appendix 15B):

$$C = \frac{1}{kT^2}(\langle E^2\rangle - \langle E\rangle^2) \quad \text{(canonical ensemble).} \tag{15.19}$$

Another quantity of interest is the mean magnetization $\langle M\rangle$ and the corresponding zero field magnetic susceptibility:

$$\chi = \left.\frac{\partial\langle M\rangle}{\partial B}\right|_{B=0}. \tag{15.20}$$

The zero field magnetic susceptibility χ is an example of a linear response function, because it measures the ability of a spin to respond 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 15C):

$$\chi = \frac{1}{kT}(\langle M^2\rangle - \langle M\rangle^2), \tag{15.21}$$

where $\langle M\rangle$ and $\langle M^2\rangle$ are evaluated in zero external magnetic field. The relations (15.19) and (15.21) are examples of the general relation between linear response functions and equilibrium fluctuations.

The Metropolis algorithm was stated in Section 15.6 as a method for generating states with the desired Boltzmann probability, but the flipping of single spins can also 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