Problem 15.27. Characterization of a phase transition

a. Use your modified version of class `Ising` from Problem 15.26 to determine $H(E, M)$. Read the $H(E, M)$ data from a file, and compute and plot $F(E)$ for the range of temperatures of interest. First generate data at $T = 2.27$ and use the Lee-Kosterlitz method to verify that the Ising model in two dimensions has a continuous phase transition in zero magnetic field. Consider lattices of sizes $L = 4$, 8, and 16.

b. Do a Lee-Kosterlitz analysis of the Ising model at $T = 2$ and zero magnetic field by plotting $F(M)$. Determine if the transition from $M > 0$ to $M < 0$ is first-order or continuous. This transition is called field-driven because the transition occurs if we change the magnetic field. Make sure your simulations sample configurations with both positive and negative magnetization by using small values of L such as $L = 4$, 6, and 8.

c. Repeat part (b) at $T = 2.5$ and determine if there is a field-driven transition at $T = 2.5$.

***Problem 15.28.** The Potts Model
In the q-state Potts model, the total energy or Hamiltonian of the lattice is given by

$$E = -J \sum_{i,j=\mathrm{nn}(i)} \delta_{s_i,s_j}, \tag{15.59}$$

where s_i at site i can have the values $1, 2, \ldots, q$; the Kronecker delta function $\delta_{a,b}$ equals unity if $a = b$ and is zero otherwise. As before, we will measure the temperature in energy units. Convince yourself that the $q = 2$ Potts model is equivalent to the Ising model (except for a trivial difference in the energy minimum). One of the many applications of the Potts model is to helium absorbed on the surface of graphite. The graphite-helium interaction gives rise to preferred adsorption sites directly above the centers of the honeycomb graphite surface. As discussed by Plischke and Bergersen, the helium atoms can be described by a three-state Potts model.

a. The transition in the Potts model is continuous for small q and first-order for larger q. Write a Monte Carlo program to simulate the Potts model for a given value of q and store the histogram $H(E)$. Test your program by comparing the output for $q = 2$ with your Ising model program.

b. Use the Lee-Kosterlitz method to analyze the nature of the phase transition in the Potts model for $q = 3$, 4, 5, 6, and 10. First find the location of the specific heat maximum, and then collect data for $H(E)$ at the specific heat maximum. Lattice sizes of order $L \geq 50$ are required to obtain convincing results for some values of q.

Another way to determine the nature of a phase transition is to use the Binder cumulant method. The cumulant is defined by

$$U_L \equiv 1 - \frac{\langle E^4 \rangle}{3\langle E^2 \rangle^2}. \tag{15.60}$$

It can be shown that the minimum value of U_L is

$$U_{L,\min} = \frac{2}{3} - \frac{1}{3}\Big(\frac{E_+^2 - E_-^2}{2E_+E_-}\Big)^2 + O(L^{-d}), \tag{15.61}$$

where E_+ and E_- are the energies of the two phases in a first-order transition. These results are derived by considering the distribution of energy values to be a sum of Gaussians about each phase at the transition, which become sharper and sharper as $L \to \infty$. If $U_{L,\mathrm{min}} = 2/3$ in the infinite size limit, then the transition is continuous.

Problem 15.29. The Binder cumulant and the nature of the transition

a. Suppose that the energy in a system is given by a Gaussian distribution with a zero mean. What is the corresponding value of U_L?

b. Consider the two-dimensional Ising model in the absence of a magnetic field and consider the cumulant

$$V_L \equiv 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}. \tag{15.62}$$

Compute V_L for a temperature much higher than T_c. What is the value of V_L? What is the value of V_L at $T = 0$?

c. Compute V_L for values of T in the range $2.20 \leq T \leq 2.35$ for $L = 10$, 20, and 40. Plot V_L as a function of T for these three values of L. Note that the three curves for V_L cross at a value of T that is approximately T_c. What is the approximate value of V_L at this crossing? Can you conclude that the transition is continuous?

d. Repeat Problem 15.28 using the Binder cumulant method and determine the nature of the transition.

15.12 *Other Ensembles

So far, we have considered the microcanonical ensemble (fixed N, V, and E) and the canonical ensemble (fixed N, V, and T). Monte Carlo methods are very flexible and can be adapted to the calculation of averages in any ensemble. Two other ensembles of particular importance are the constant pressure and the grand canonical ensembles. The main difference in the Monte Carlo method is that there are additional moves corresponding to changing the volume or changing the number of particles. The constant pressure ensemble is particularly important for studying first-order phase transitions because the phase transition occurs at a fixed pressure, unlike a constant volume simulation where the system passes through a two phase coexistence region before changing phase completely as the volume is changed.

In the NPT ensemble, the probability of a microstate is proportional to $e^{-\beta(E+PV)}$. For a classical system, the mean value of a physical quantity A that depends on the positions of the particles can be expressed as

$$\langle A \rangle_{\mathrm{NPT}} = \frac{\int_0^\infty dV e^{-\beta PV} \int d\mathbf{r}_1 d\mathbf{r}_2 \ldots d\mathbf{r}_N A(\{\mathbf{r}\})\, e^{-\beta U(\{\mathbf{r}\})}}{\int_0^\infty dV e^{-\beta PV} \int d\mathbf{r}_1 d\mathbf{r}_2 \ldots d\mathbf{r}_N\, e^{-\beta U(\{\mathbf{r}\})}}. \tag{15.63}$$

The potential energy $U(\{\mathbf{r}\})$ depends on the set of particle coordinates ($\{\mathbf{r}\}$). To simulate the NPT ensemble, we need to sample the coordinates $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N$ of the particles and the volume