from Gould-Tobochnick

Problem 17.15. Antiferromagnetic Ising model

a. Modify `Program ising` to simulate the antiferromagnetic Ising model on the square lattice in zero magnetic field. Because J does not appear explicitly in `Program ising`, change the sign of the energy calculations in the appropriate places in the program. To compute the staggered magnetization on a square lattice, define one sublattice to be the sites (x, y) for which the product $\texttt{mod}(x, 2) \times \texttt{mod}(y, 2) = 1$; the other sublattice corresponds to the remaining sites.

b. Choose $L = 16$ and the initial condition to be all spins up. What configuration of spins corresponds to the state of lowest energy? Compute the temperature dependence of the mean energy, specific heat, magnetization, and the susceptibility χ. Does the temperature dependence of any of these quantities show evidence of a phase transition?

c. Compute the temperature dependence of M_s and the staggered susceptibility χ_s defined as (see (17.14))

$$\chi_s = \frac{1}{kT}\left[\langle {M_s}^2\rangle - \langle M_s\rangle^2\right]. \tag{17.35}$$

Verify that the temperature dependence of M_s for the antiferromagnetic Ising model is the same as the temperature dependence of M for the Ising ferromagnet. Could you have predicted this similarity without doing the simulation?

d. In part (b) you might have noticed that χ shows a cusp. Compute χ for different values of L at $T = T_N \approx 2.269$. Do a finite size scaling analysis and verify that χ does not diverge at $T = T_N$.

e. Consider the behavior of the antiferromagnetic Ising model on a triangular lattice. Choose $L \geq 16$ and compute the same quantities as before. Do you see any evidence of a phase transition? Draw several configurations of the system at different temperatures. Do you see evidence of many small domains at low temperatures? Is there a unique ground state? If you cannot find a unique ground state, you share the same frustration as do the individual spins in the antiferromagnetic Ising model on the triangular lattice. We say that this model exhibits *frustration* because there is no spin configuration on the triangular lattice such that all spins are able to minimize their energy (see Fig. 17.3).

The Ising model is one of many models of magnetism. The Heisenberg, Potts, and x-y models are other examples of models of magnetic materials familiar to condensed matter scientists as well as to workers in other areas. Monte Carlo simulations of these models and others have been important in the development of our understanding of phase transitions in both magnetic and nonmagnetic materials. Some of these models are discussed in Section 17.11.

17.7 Simulation of Classical Fluids

The existence of matter as a solid, liquid and gas is well known (see Fig. 17.4). Our goal in this section is to use Monte Carlo methods to gain additional insight into the qualitative differences between these three phases.

Monte Carlo simulations of classical systems are simplified considerably by the fact that the velocity (momentum) variables are decoupled from the position variables. The total energy can be written as $E = K(\{\mathbf{v}_i\}) + U(\{\mathbf{r}_i\})$, where the kinetic energy K is a function of only the particle