# Exercises

8.1 **The Ising model.**[1] (Computation) ①

You will need a two-dimensional square-lattice Ising model simulation, one of which is available among the computational exercises section on the book web site [129]. The Ising Hamiltonian is (eqn 8.1):

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i, \qquad (1)$$

where $S_i = \pm 1$ are 'spins' on a square lattice, and the sum $\sum_{\langle ij \rangle}$ is over the four nearest-neighbor bonds (each pair summed once). It is conventional to set the coupling strength $J = 1$ and Boltzmann's constant $k_B = 1$, which amounts to measuring energies and temperatures in units of $J$. The constant $H$ is called the external field, and $\mathbf{M} = \sum_i S_i$ is called the magnetization. Our simulation does not conserve the number of spins up, so it is not a natural simulation for a binary alloy. You can think of it as a grand canonical ensemble, or as a model for extra atoms on a surface exchanging with the vapor above.

Play with the simulation. At high temperatures, the spins should not be strongly correlated. At low temperatures the spins should align all parallel, giving a large magnetization.

*Roughly locate $T_c$, the largest temperature where distant spins remain parallel on average at $T = 0$. Explore the behavior by gradually lowering the temperature from just above $T_c$ to just below $T_c$; does the behavior gradually change, or jump abruptly (like water freezing to ice)? Explore the behavior at $T = 2$ (below $T_c$) as you vary the external field $H = \pm 0.1$ up and down through the 'phase boundary' at $H = 0$ (Fig. 8.5). Does the behavior vary smoothly in that case?*

[1]From *Statistical Mechanics: Entropy, Order Parameters, and Complexity* by James P. Sethna, copyright Oxford University Press, 2007, page 174. A pdf of the text is available at pages.physics.cornell.edu/sethna/StatMech/ (select the picture of the text). Hyperlinks from this exercise into the text will work if the latter PDF is downloaded into the same directory/folder as this PDF.