Exercises

8.2 Ising fluctuations and susceptibilities.¹ (Computation) ③

The partition function for the Ising model is $Z = \sum_{n} \exp(-\beta E_n)$, where the states *n* run over all 2^N possible configurations of the Ising spins (eqn 8.1), and the free energy $F = -kT \log Z$.

(a) Show that the average of the magnetization M equals $-(\partial F/\partial H)|_T$. (Hint: Write out the sum for the partition function and take the derivative.) Derive the formula for the susceptibility $\chi_0 = (\partial M/\partial H)|_T$ in terms of $\langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2$. (Hint: Remember our derivation of formula 6.13 $\langle (E - \langle E \rangle)^2 \rangle = k_B T^2 C$.)

Download an Ising model simulation from the computational exercises section of the book web site [129]. Notice that the program outputs averages of several quantities: $\langle |m| \rangle$, $\langle (m - \langle m \rangle)^2 \rangle$, $\langle e \rangle$, $\langle (e - \langle e \rangle)^2 \rangle$. In simulations, it is standard to measure e = E/N and m = M/N per spin (so that the plots do not depend upon system size); you will need to rescale properties appropriately to make comparisons with formulæ written for the energy and magnetization of the system as a whole. You can change the system size and decrease the graphics refresh rate (number of sweeps per draw) to speed your averaging. Make sure to equilibrate before starting to average!

(b) Correlations and susceptibilities: numerical. Check the formulæ for C and χ from part (a) at H = 0 and T = 3, by measuring the fluctuations and the averages, and then changing by $\Delta H = 0.02$ or $\Delta T = 0.1$ and measuring the averages again. Check them also for T = 2, where $\langle M \rangle \neq 0.^2$

There are systematic series expansions for the Ising

model at high and low temperatures, using Feynman diagrams (see Section 3.3). The first terms of these expansions are both famous and illuminating. *Low-temperature expansion for the magnetization*. At low temperatures we can assume all spins flip alone, ignoring clusters.

(c) What is the energy for flipping a spin antiparallel to its neighbors? Equilibrate at a relatively low temperature T = 1.0, and measure the magnetization. Notice that the primary excitations are single spin flips. In the low-temperature approximation that the flipped spins are dilute (so we may ignore the possibility that two flipped spins touch or overlap), write a formula for the magnetization. (Remember, each flipped spin changes the magnetization by 2.) Check your prediction against the simulation. (Hint: See eqn 8.19.)

The magnetization (and the specific heat) are exponentially small at low temperatures because there is an *energy gap* to spin excitations in the Ising model,³ just as there is a gap to charge excitations in a semiconductor or an insulator.

High-temperature expansion for the susceptibility. At high temperatures, we can ignore the coupling to the neighboring spins.

(d) Calculate a formula for the susceptibility of a free spin coupled to an external field. Compare it to the susceptibility you measure at high temperature T = 100 for the Ising model, say, $\Delta M/\Delta H$ with $\Delta H = 1$. (Why is H = 1 a small field in this case?)

Your formula for the high-temperature susceptibility is known more generally as Curie's law.

¹From *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.

²Be sure to wait until the state is equilibrated before you start! Below T_c this means the state should not have red and black 'domains', but be all in one ground state. You may need to apply a weak external field for a while to remove stripes at low temperatures.

 3 Not all real magnets have a gap; if there is a spin rotation symmetry, one can have gapless *spin waves*, which are like sound waves except twisting the magnetization rather than wiggling the atoms.