Exercises

11.4 **Nucleation in the Ising model.**[1] ③

The Ising model (Section 8.1) is not only our archetype for a continuous phase transition; it is also our best model for nucleation (this exercise) and for the dynamics of phase separation (Exercise 11.6).

The Ising model can be used to study the nucleation of one phase inside another. Supercooling water and waiting for an ice crystal nucleus to form can be shown to be quite analogous to changing a magnet from external field $H_{\rm ext} > 0$ to $H_{\rm ext} < 0$ at a temperature $T < T_c$. The analogy with changing the temperature or pressure of H_20 gas and waiting for a raindrop is even better.

Start up the Ising model simulation, available in the computer exercises portion of the book web site [129]. Run at $T = 1.5$ (below T_c) at size 40×40, initialized with all spins up. Set $H_{\rm ext} = -0.3$ and watch the spins. They should eventually flop over to point down, with the new phase starting in a small, roughly circular cluster of spins, which then grows to fill the system.[2]

(a) *Using the graph of magnetization versus time, measure the average time it takes to cross zero (which we will call the time to nucleate the down phase), averaging over ten measurements. (You may want to reduce the graphics refresh rate to speed up the simulation.) Similarly measure the average time to nucleate the down phase for* $H_{\rm ext} = -0.2$. Since the nucleation center can be located at any site on the lattice, the nucleation rate scales with the number of spins in the system. *Calculate, for both fields, the nucleation rate per spin* $\Gamma_{\rm exp}(H)$.

We can use critical droplet theory (Section 11.3) to estimate the nucleation rate. Small droplets of the stable phase will shrink due to surface tension σ; large ones grow due to the free energy difference per unit area $H_{\rm ext}\Delta M(T)$, where ΔM is the magnetization difference between the two states. Presuming that the temperature is high and the droplet large and the times long (so that continuum theories are applicable), one can estimate the critical radius R_c for nucleation.

(b) *Give the formula for the free energy of a flipped cluster of radius* R *as a function of* σ, H, *and* ΔM. *Give formulæ for* R_c *(the critical droplet size where the free energy is a local maximum), the resulting barrier* B *to nucleation, and the predicted rate* $\Gamma_{\rm theory} = \exp(-B/T)$ *(assuming a prefactor of roughly one attempt per sweep per spin). At low temperatures,* $\sigma \sim 2J \equiv 2$ *and* $\Delta M \approx 2$, *since the system is almost fully magnetized and* σ *is the number of broken bonds (*$2J$ *each) per unit length of interface. Make a table with rows for the two fields you simulated and with columns for* H, R_c, B, $\Gamma_{\rm theory}$, *and* $\Gamma_{\rm exp}$ *from (a).*

This should work pretty badly. Is the predicted droplet size large enough (several lattice constants) so that the continuum theory should be valid?

We can test these ideas better by starting with droplets of down-spins (white) in an up background. Use a small system (40×40). You can make such a droplet by setting the spins up and then flipping a circular cluster of spins in the center. After making the circle, store it for re-use. You will want to refresh the display each sweep, since the droplet will grow or shrink rather quickly.

(c) *Start with* $H = -0.2$, $T = 1.5$ *and a down-spin droplet of radius five (diameter of ten), and run ten times. Does it grow more often than it shrinks, or vice versa? (Testing this should be fast.) On the magnetization curve, count the shrinking fraction* f. *Make a table of the values of* H *and* f *you measure. Vary the field* H *until the probabilities roughly match; find the field for* $R_c = 5$ *to within* 0.1. *For what field is the theoretical critical droplet radius* $R_c = 5$ *at* $T = 1.5$*?*

[1] From *Statistical Mechanics: Entropy, Order Parameters, and Complexity* by James P. Sethna, copyright Oxford University Press, 2007, page 253. 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.

[2] The system has periodic boundary conditions, so a cluster which starts near a boundary or corner may falsely look like more than one simultaneous nucleation event.

In part (b) we found that critical droplet theory worked badly for predicting the nucleation rate. In part (c) we found that it worked rather well (within a factor of two) at predicting the relationship between the critical droplet size and the external field. This is mostly because the nucleation rate depends exponentially on the barrier, so a small error in the barrier (or critical droplet radius) makes a big error in the nucleation rate. You will notice that theory papers rarely try to predict rates of reactions. They will almost always instead compare theoretical and experimental barrier heights (or here, critical droplet radii). This avoids embarrassment.

This free energy barrier to nucleation is what allows supercooled liquids and supersaturated vapor to be stable for long periods.