ISING MODEL

One of the most celebrated and enduring models of statistical mechanics is the Ising model [2]. Consider a regular two-dimensional square lattice of size L. At each site i, there is a spin that can point either up, $s_i = +1$, or down, $s_i = -1$, coloured white and black, respectively, in the animation. The energy associated with a configuration of $N = L \times L$ spins $\{s_i\}$ is given by

$$E_{\{s_i\}} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_{i=1}^{N} s_i, \tag{1}$$

where the first sum runs over nearest-neighbour spins only, J is the coupling constant that measures the strength of the interaction between nearest neighbour spins, and H is the strength of the externally applied magnetic field. For simplicity in the following, let us consider zero external field, $H = 0$, and this is indeed the case in the animation.

The first term in the above expression indicates that spin alignment lowers the energy of the system. However, temperature adds a randomising element and will tend to break up patches of aligned spins. In equilibrium, the system will assume a configuration such that the free energy

$$F = \langle E \rangle - TS \tag{2}$$

is minimised, where $\langle E \rangle$ is the average energy, T is the temperature and S is the entropy. When the temperature is large, the entropic second term dominates the free energy, and the spins are effectively pointing up and down randomly. In the animation, this is reminiscent of an untuned TV set. Conversely, if the temperature is very small the free energy is dominated by the configurational first term, and the spins all align in the same direction. Since the external field is assumed to be zero, the spins may align either up or down with equal preference – ultimately one direction will be chosen.

It is interesting to consider what happens for intermediate temperatures. One way of quantifying the competition between the configurational and entropic terms of the free energy is to introduce an order parameter, namely the magnetisation per spin, defined by

$$m = \left\langle \frac{1}{N} \sum_{i=1}^{N} s_i \right\rangle, \tag{3}$$

which ranges between $+1$ (all spins pointing up) and -1 (all spins pointing down). As you have probably guessed by now, the magnetisation undergoes a continuous phase transition at some critical value of temperature T_c in zero external field. Below this temperature, the spins are aligned such that a net (non-zero) magnetisation persists. Above this temperature, the magnetisation is zero. Of course, in a finite system there are always fluctuations, and the magnetisation will never settle precisely on the value dictated by the minimum of the free energy. In the animation, the instantaneous magnetisation

$$m_{\{s_i\}} = \frac{1}{N} \sum_{i=1}^{N} s_i \tag{4}$$

is given on the left and is continually updated in time.

What will be evident visually in the animation is that as the critical temperature is approached (say, from above), patches of aligned spins start to form, rather like droplets. These structures are clearly not random, and reflect the fact that the correlations among spins are heightened at the critical temperature. The system is delicately poised between an ordered up-spin phase, and an ordered down-spin phase. A little below the critical temperature the system is deep within one phase or the other. Again, since the system is finite it is always possible that the system flips between phases, even if it is below the critical temperature. However, the time for making such flips rapidly increases as the temperature is cooled further below T_c.

Finally, it is worth remarking on how the Ising model is simulated. Equation (1) for the configurational energy of the spins is not an equation of motion. In other words, it cannot be integrated in time to work out the future evolution of all the individual spins. In the animation, the system is made to evolve dynamically in such a way that, if one waits long enough, it visits spin configurations with a frequency that is consistent with Equation (1), that is, with the correct Boltzmann weight. This is the idea behind Monte-Carlo simulations of the Ising model, and the particular algorithm used in the animation is the so-called Metropolis algorithm [3]. For further details see [4, 1].

References

[1] D. P. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics*, 2nd ed., Cambridge University Press, Cambridge, UK, 2005.

[2] W. Lenz, *Beitrag zum Verständnis der Magnetischen Erscheinungen in festen Körpern*, Phys. Z. **21** (1920), 613–615.

[3] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *Equation of state calculations by fast computing machines*, J. Chem. Phys. **21** (1953), 1087–1092.

[4] M. E. J. Newman and G. T. Barkema, *Monte Carlo Methods in Statistical Physics*, Clarendon Press, Oxford, 1999.