The Ising model

Model

The Ising model is one of the simplest and most fundamental models of statistical mechanics. It can be used to describe such diverse phenomena as *magnets; liquid/gas coexistence; alloys of two metals*; and many others, even outside of physics.

Each such system can be described by elementary variables $\mathbf{s}_i$, usually called "*spins*" with 2 possible values $s_i = \pm 1$. The 2 values stand for, e.g., an elementary magnet pointing *up* or *down*; a piece of *liquid* or *gas*; an atom of metal A or B; etc.). These variables usually live on the sites i of some lattice. One associates an energy

$$E \;=\; -\,J \sum_{\text{neighbors } i,j} s_i\, s_j \tag{1}$$

with each configuration of spins, where J is some constant. Each state of the system occurs with probability given by the *Boltzmann factor*

$$p = \frac{1}{Z}\; \exp(-\frac{E}{k_B T})\;, \tag{2}$$

where T is temperature, k_B the Boltzmann constant, and Z a normalization factor.

Even though the Ising model is drastically simplified from realistic situations, it is able to describe, often quantitatively, the occurence of *order* at low temperatures and *disorder* at high temperatures, and especially the *phase transition* between those situation, in which spin correlations over very large length scales become essential.

The Ising model can be solved exactly only in the simplest cases (in one spatial dimension, and on a two-dimensional square lattice). In most cases of practical interest, one has to resort to either *analytical approximations* like series expansions for high or for low temperature, or to *numerical techniques* like *Markov Chain Monte Carlo simulations*.

Simulation methods

Our Mathlab simulation demonstrates essential features of the Ising model. It implements a Markov Chain Monte Carlo with *importance sampling*, in which configurations of spins are generated iteratively, and eventually appear with Boltzmann probabiliy. It uses one of two methods.

In the *Metropolis* method, the spins are changed one by one, with appropriate probabilities depending on their neighbors. With this method the fluctuations of spins are clearly visible, but it can take very many iterations before a statistically independent new spin configuration is reached.

With *cluster updates*, big regions of equal spins are *constructed stochastically*, again with probabilities depending on the current values of spins. The spins in these clusters are then flipped together. While each update with this method is fairly slow, new independent spin configurations are reached within one or a few iterations.

Interactive simulation

The simulation shows the two-dimensional Ising model. Every little box of the spin field represents one of the two possible states $s_i = \pm 1$. The constants J and k_B are omitted.

You can control the temperature either by typing a positive real number into the temperature field (followed by a TAB) or by adjusting the slide rule with the mouse. The critical temperature of the model is $T_{crit} = \frac{2}{ln(1+\sqrt{2})} = 2.269...$ The magnetization is simply the mean of all spins.

You can also adjust the lattice size, the initial magnetization, and the number of iterations (updating each spin once) to be performed before the simulation pauses. The currently chosen update algorithm is shown on the right.

The first and third graphs show magnetization and energy of the current configuration. For each temperature, the other two graphs display the *average* magnetization and average energy of the configurations generated so far. The exact results (for infinite size lattices) are denoted by the green line.

After the simulation pauses, it can be resumed at the same temperature, or the current averages can be accepted as an estimate for the true result, or the average accumulated so far can be discarded.

Observe the following:

1. Set the temperature to be well above the critical temperature (2.26...). You will see that the spin arrangement converges to a nearly random arrangement, independent of the starting state: "Cold", or "Warm", and fluctuates quickly. Hence, above the critical temperature, there is a single thermodynamic state, with zero magnetization. At infinite temperature the spin arrangement is truly random.

2. Start well below the critical temperature with initial state "Cold".
   All the spins will start with equal value. *Use the Metropolis method*. You will see that just a few small clusters of opposite spins appear, and there is a non-zero magnetization. The analogouous situation would occur if initially all spins were reversed. Hence, below the critical temperature, there are two thermodynamic states (the "up spin" state with positive magnetization and the "down spin" state negative magnetization). With the Metropolis method the system stays in one or the other depending on how the spins are initialized.

3. Start well below the critical temperature with initial state "Warm".
   Use the Metropolis method. You see that the system initially cannot make up its mind whether to go into the "up spin" or "down spin" state. Large clusters of each spin form. Eventually, if you let the simulation run for a long time, one of the states will win. Which one wins depends on the random thermal fluctuations. There is equal probability for it to be in the "up spin" or "down spin" state.

4. Start well below the critical temperature with the *cluster method*. You see that now the system moves easily between the two states with mostly positive and with mostly negative magnetization. (The metropolis method would need an enormously long time to do the same). The initial state does not matter with the cluster method.

5. Start at or close to the critical temperature. *Use the Metropolis method.* You will see large clusters of spins with the same orientation, which fluctuate only very slowly. The typical size of these clusters is the so called *correlation length* ξ which is maximal at the critical temperature, where it would diverge on an infinitely large system.

   The slow fluctuation of spins with the Metropolis method is called *critical slowing down*. Fluctuations of spins travel through the lattice locally in this method, like in a random walk. Therefore they are associated with a time scale of $\tau \simeq \xi^2$ iterations. The system thus keeps a long memory of its initial state, and many iterations must be discarded before useful averages can be taken. These then need many iterations to converge, especially on large systems.

6. Start at or close to the critical temperature. *Use the cluster method.* While each iteration with this method takes longer than with Metropolis, the generated spin configurations quickly become independent of each other, so that much fewer iterations are needed and overall, results converge much more quickly.