Ising model and XY model

1 Ising 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*.

1.1 Simulation methods

Our 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.

It uses the *Metropolis* method, im which 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.

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 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 graphs show magnetization and energy of the current configuration.

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 "Hot", 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. 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 "Hot".
   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 at or close to the critical temperature. 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.

2 XY model

In the classical xy-model, the variables are two-dimensional unit vectors $\vec{s}_i$ on each lattice site, equivalent to an angle θ. This model is a limiting case of the Heisenberg spin model. The vectors correspond to the directions of spins (originally quantum mechanical) in a material in which the z-component of spins couples less than the x and y components. (The opposite case leads to the Ising model.)

This model is particularly important in two spatial dimensions, where it shows a peculiar phase transition, the so called *Kosterlitz Thouless* (KT) transition, which is observed experimentally also in *liquid crystals* (LCD displays), *thin films of liquid helium*, *films of superconducters*, probably including the layered *high temperature superconductors*. In addition the model can be mapped to so called SOS (solid on solid) models, describing, e.g. crystal growth and *roughening* transitions.

The energy of a configuration of spins is similar to that of the Ising model,

$$E \;=\; -J \sum_{\text{neighbors } i,j} \vec{s}_i \, \vec{s}_j \;\;=\;\; -J \sum_{\text{neighbors } i,j} \cos(\theta_i - \theta_j) \;\; . \tag{3}$$

Again, each state of the system occurs with probability given by the *Boltzmann factor*

$$p = \frac{1}{Z} \; \exp(-\frac{E}{k_B T}) \; , \tag{4}$$

where T is temperature, k_B the Boltzmann constant, and Z a normalization factor. The energy is *invariant under a global continuous rotation* of all spins, i.e., it possesses a continuous global "$O(2)$" symmetry.

In two spatial dimensions, the *Mermin-Wagner theorem* shows rigorously that such a continuous symmetry cannot be broken spontaneously at any finite temperature. Thus the XY-model *cannot* have an ordered phase at low temperature like the Ising model does. Yet in two dimensions it does show the very peculiar Kosterlitz-Thouless (KT) transition, which is very soft, of infinite order. Above the transition temperature T_{KT}, correlations between spins decay exponentially as usual, with some correlation length ξ. Below the transition temperature, they decay instead like a *power* of distance, with temperature-dependent exponents. Thus in the whole low temperature phase the exponential correlation length is infinite.

The relevant degrees of freedom for this phase transition turn out to be "*vortices*". i.e. points on the lattice around which the spins *wind* an integer number of times. In the low temperature phase, there are few vortices, closely coupled as vortex-antivortex pairs. In the high temperature phase, many vortices are present, in a so called condensed phase or vortex plasma. Another suitable indication of the phase transition is given by the "*spin stiffness*", which measures the response of the system to a twist of a spin on the boundary. The spin-stiffness exhibits a discontinuous jump (!) at the phase transition in an infinite system.

The XY-model can be better understood theoretically by mapping it, exactly, to a completely different looking so called *SOS* (Solid On Solid) model, in which the degrees of freedom are not continuous vectors, but instead discrete height variables at each lattice site. They can be interpreted, e.g., as the height of a crystal surface (measured in atoms), or the height of a layer of material deposited by Molecular Beam Epitaxy (MBE). Fortunately, a closely related SOS model is one of the few models in statistical mechanics which can be

solved *exactly*, in two dimensions. This is the BCSOS or (in yet another guise) the 6-vertex-model, closely related also to the spin $\frac{1}{2}$ quantum Heisenberg XXZ chain. This model turns out to indeed possess the previously conjecture KT transition, which is under full control in this case.

Because of the algebraic decay, and because important effects depend only logarithmically on system size, it is notoriously difficult to obtain the relevant physics of the XY-model directly. For simulations, in order to see the correct asymptotic algebraic decay of correlation functions, lattice sizes exceeding 10000^2 are necessary. The best available numerical results have therefore been obtained indirectly, by matching the behavior of the system on different size lattices (the Renormalization Group flow) to that of the BCSOS model in simulations of systems up to size 512^2.

Our applet shows a simulation of the two-dimensional XY model, using the Metropolis algorithm. For each single-spin-update, a rotation of that spin by a finite angle is proposed, taken from a suitable continuous range. The spins in the applet are displayed in 8 different colors accouding to the octant of their orientation, so that the degree of order of the spin configuration can be easily visualized. *Vortices* and anti-vortices are marked by big colored dots, and one can easily see the proliferation of vortices at high temperature. At low temperature, on the other hand, this simulation takes a fairly long time to reach an equilibrium configuration. Other simulation methods, especially cluster algorithms, help to improve such simulations.