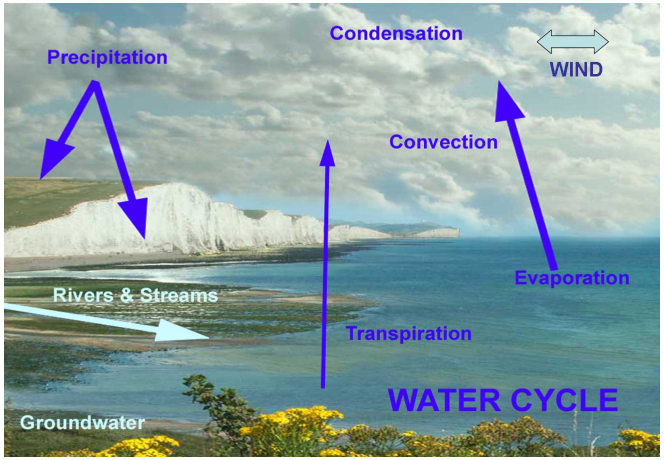
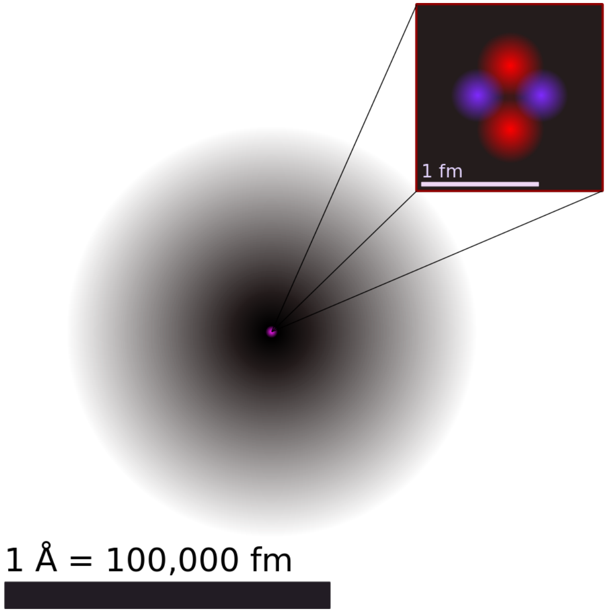
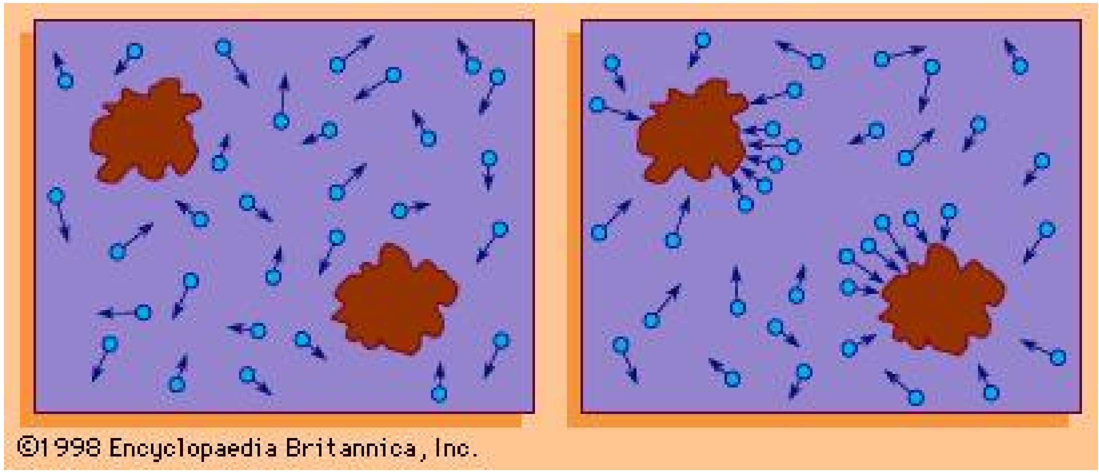
Criticality and the Ising Model



Democritus





Criticality and the Ising Model

The Hamiltonian

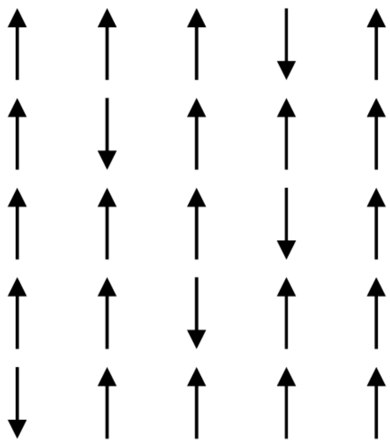
$$\mathcal{H} = -J \sum_{<ij>} s_i s_j - h \sum_i s_i$$

$s_i = \pm 1, \; i = 1, \ldots, N$

$< ij >$ - sum of all nearest neighboring pair of spins

J - coupling constant

h - external field



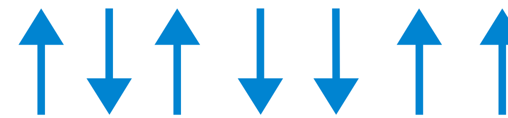
Göran Wahnström, Department of Applied Physics, Chalmers

Criticality and the Ising Model

Wilhelm Lenz

Ernst Ising

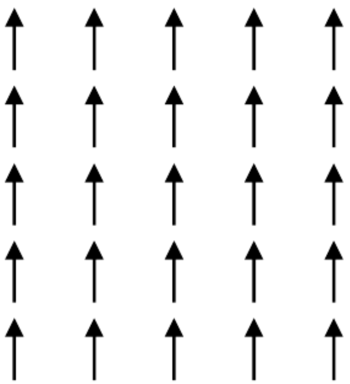
Lars Onsager



- Ising model inveted by W Lenz (1920).
- Solved in 1-D by E Ising (1924): no phase transition in 1-D.
- Solved in 2-D by L Onsager (1944): 2nd order (continuous) phase transition.
- Still unsolved in 3-D.
- In 4 or more dimensions, mean field.
- Paradigm in statistical physics. ~800 papers/year with diverse applications.

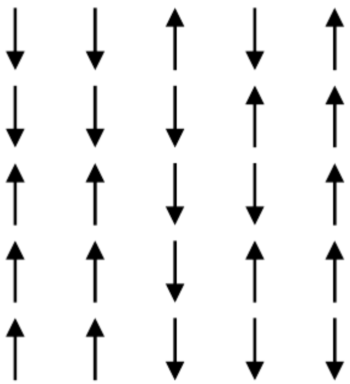
Criticality and the Ising Model

low T



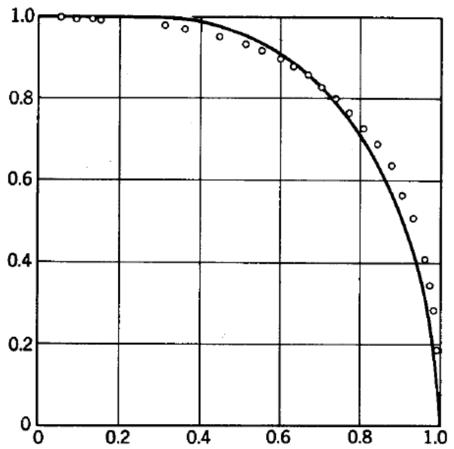
ferromagnetic

high T



paramagnetic

Magnetization



temperature

Criticality and the Ising Model

Canonical ensemble:

The probability for the system to be in microstate ν:

$$P_\nu = \frac{1}{Z}\exp(-\beta E_\nu)$$

where $\beta = 1/k_B T$.

The partition function:

$$Z(\beta, h) = \sum_\nu \exp(-\beta E_\nu)$$

The magnetization

$$M_\nu = \sum_{i=1}^{N} s_i$$

The energy

$$E_\nu = -J \sum_{<ij>} s_i s_j - h \sum_i s_i$$

The mean magnetization

$$M \equiv \langle M_\nu \rangle = \frac{1}{Z}\sum_\nu M_\nu \exp(-\beta E_\nu)$$

The mean energy

$$U \equiv \langle E_\nu \rangle = \frac{1}{Z}\sum_\nu E_\nu \exp(-\beta E_\nu)$$

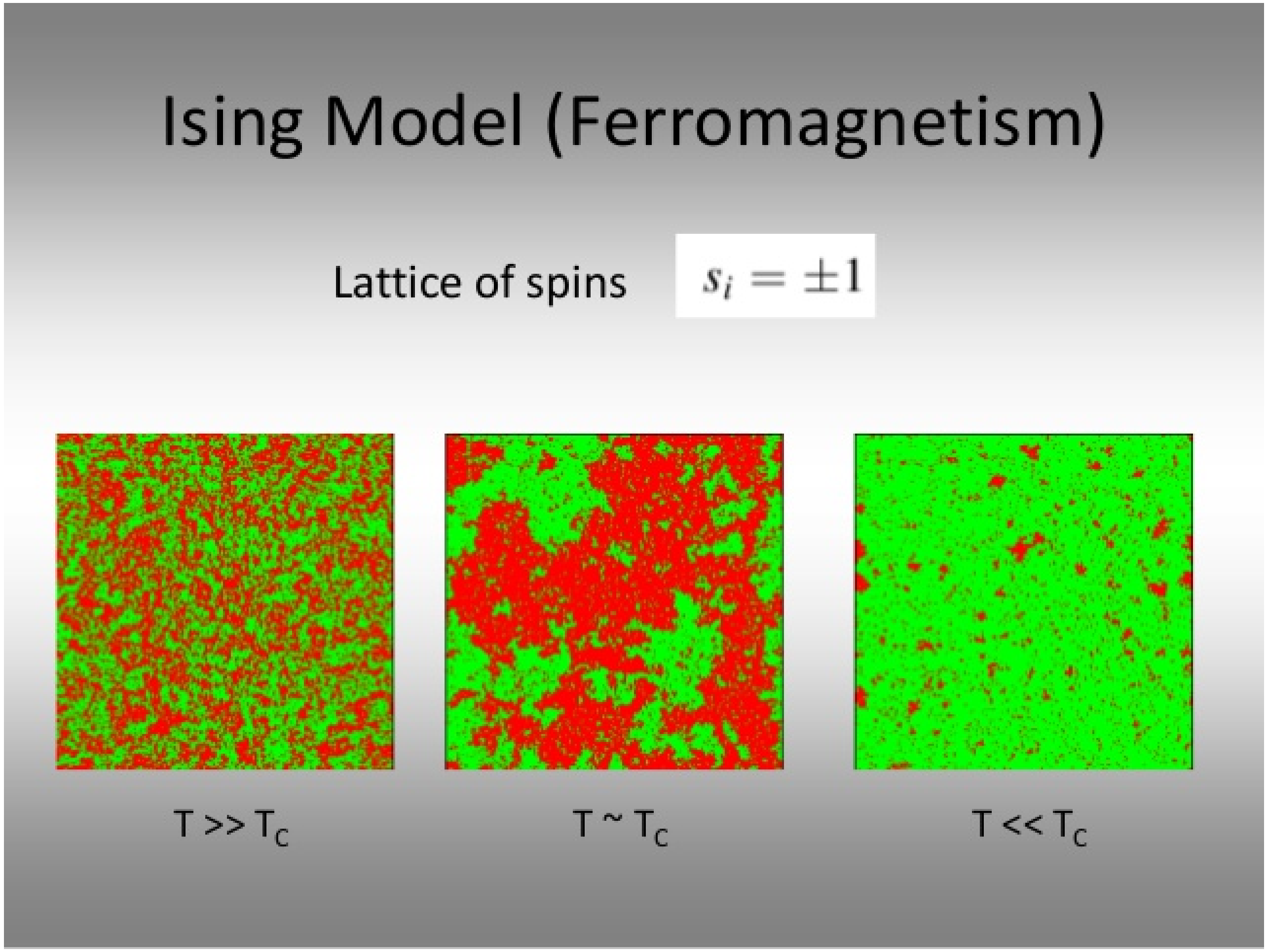
The isothermal susceptibility

$$\chi_T \equiv \left(\frac{\partial M}{\partial h}\right)_T = \frac{1}{k_B T}\left[\left\langle M_\nu^2 \right\rangle - \langle M_\nu \rangle^2\right]$$

The heat capacity at constant field

$$C_h \equiv \left(\frac{\partial U}{\partial T}\right)_h = \frac{1}{k_B T^2}\left[\left\langle E_\nu^2 \right\rangle - \langle E_\nu \rangle^2\right]$$

Criticality and the Ising Model



10. 1. The mean-field approximation

Recall that the Ising configurational energy is

$$E(\{S_i\}) = -h\sum_i S_i - J\sum_{<ij>} S_i S_j \tag{1}$$

Consider all contributions involving spin j

$$\epsilon(S_j) = -hS_j - JS_j \sum_k^{n.n} S_k \tag{2}$$

where the sum is over nearest neighbours (n.n.) k of site j.

We now *approximate* this contribution by replacing the S_k by their mean value

$$\epsilon_{mf}(S_j) = -hS_j - JS_j \sum_k^{n.n} \langle S_k\rangle = -h_{mf} S_j \tag{3}$$

where

$$h_{mf} = h + Jzm \tag{4}$$

and m, the magnetisation per spin, is just the mean value of any given spin

$$m = \frac{1}{N}\sum_i \langle S_i\rangle = \langle S_k\rangle \quad \forall k \tag{5}$$

Thus the mean field approximation is to replace the configurational energy (1) by the energy of a non-interacting system of spins each experiencing a field h_{mf}. For this problem we can write down the single-spin Boltzmann distribution straightaway

$$p(S_j) = \frac{\mathrm{e}^{-\beta\epsilon_{mf}(S_j)}}{\sum_{S_j=\pm 1} \mathrm{e}^{-\beta\epsilon_{mf}(S_j)}} = \frac{\mathrm{e}^{\beta h_{mf} S_j}}{\mathrm{e}^{\beta h_{mf}} + \mathrm{e}^{-\beta h_{mf}}} \tag{6}$$

However, we still have a *consistency* condition to fulfil: the value of the magnetisation m predicted by (6) should be equal to the value of m used in the expression for h_{mf} (4). Thus we require

$$\begin{aligned} m &= \sum_{S_j=\pm 1} p(S_j) S_j \\ &= \frac{\mathrm{e}^{\beta h_{mf}} - \mathrm{e}^{-\beta h_{mf}}}{\mathrm{e}^{\beta h_{mf}} + \mathrm{e}^{-\beta h_{mf}}} = \tanh(\beta h_{mf}) \end{aligned} \tag{7}$$

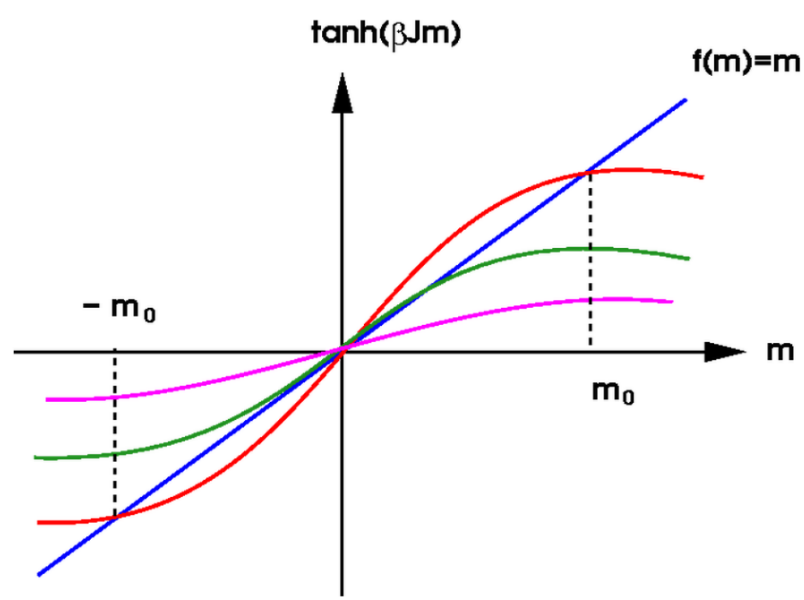
and we arrive at the mean-field equation for the magnetisation

$$\boxed{m = \tanh(\beta h + \beta J z m)} \tag{8}$$

First we will consider the case $h = 0$ (zero applied field). The solutions of

$$m = \tanh(\beta J z m) \tag{9}$$

are best understood graphically. We see that for low β (high T) the only solution is $m = 0$



whereas for high β (low T) there are three possible solutions $m = 0$ and $m = \pm|m|$. The solutions with $|m| > 0$ appear when the the slope of the tanh function at the origin is greater than one

$$\frac{d}{dm} \tanh(\beta J z m)\bigg|_{m=0} > 1 \tag{10}$$

Using the expansion of tanh for small argument

$$\tanh x \simeq x - \frac{x^3}{3} \tag{11}$$

(actually we only need the first term at this point), we find the condition (10) is

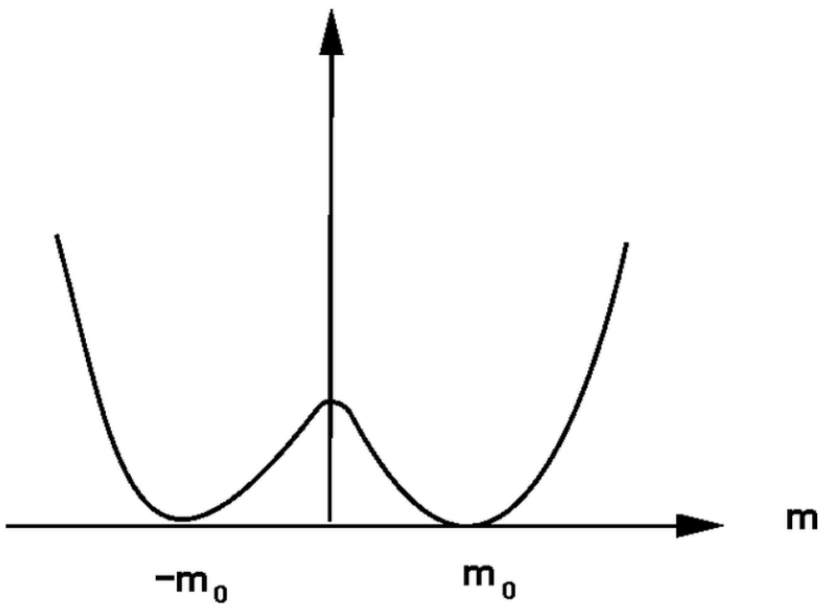
$$\beta J z > 1$$

which gives, remembering $\beta = 1/kT$,

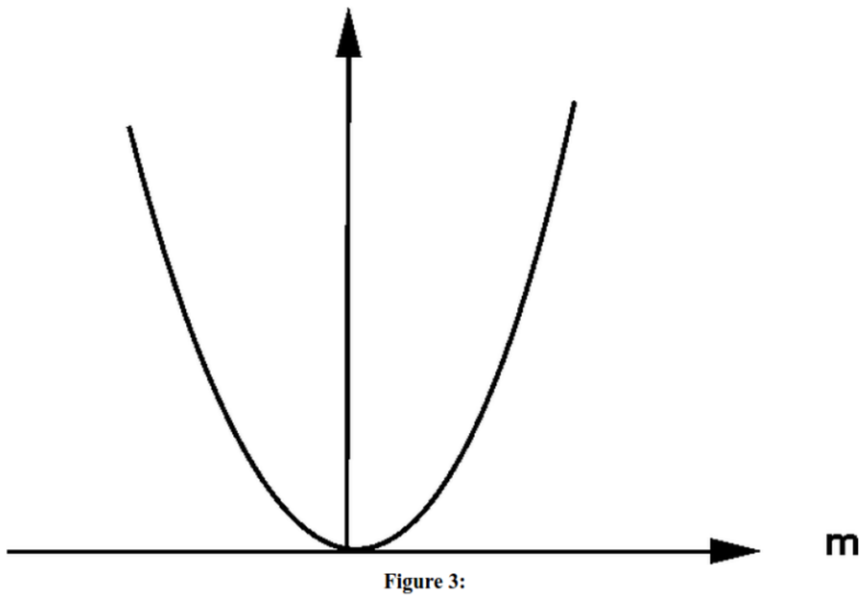
$$\boxed{T_c = \frac{zJ}{k}} \tag{12}$$

Thus for $T > T_c$ only the paramagnetic $m = 0$ solution is available, whereas for $T < T_c$ we also have the ferromagnetic solutions $\pm|m|$. These are the physical solutions for $T < T_c$ as we shall see in the next subsection.

Criticality and the Ising Model



T<Tc



T>Tc

Criticality and the Ising Model

Metropolis algorithm (Monte Carlo)

1. Set the desired temperature T and external field h.

2. Initialize the system, *e.g.* use a random configuration or a configuration from a previous simulation.

3. Perform the desired number of Monte Carlo sweeps through the lattice.

4. Exclude the first configurations (let the system equilibrate).

5. Compute average quantities from subsequent configurations and estimate the error from statistically independent configurations.

3a. Make a trial change, e.g. by flipping a randomly chosen spin.

3b. Determine the change in energy ΔE

3c. If $\Delta E \leq 0$ accept the new configuration

3d. If $\Delta E > 0$ generate a random number r between 0 and 1, and if

$$\exp(-\Delta E/k_B T) \geq r$$

accept the new configuration, otherwise count the old configuration once more.