The Ising Model of Ferromagnetism

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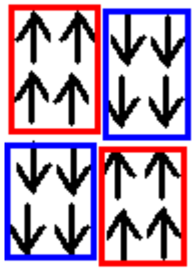
Chem 444 Fall 2006

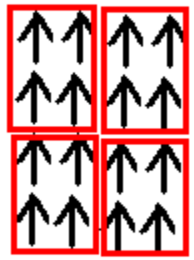
Ferromagnetism

Magnetic domains of a material all line up in one direction

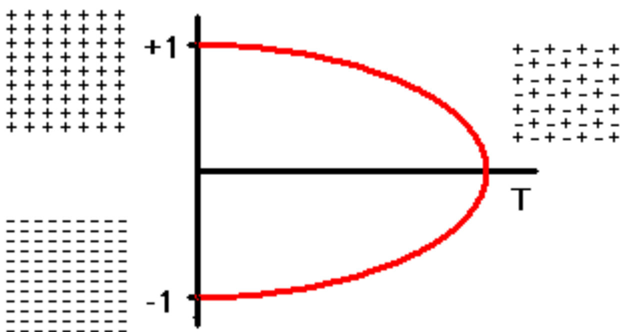
In general, domains do not line up
→ no macroscopic magnetization



Can be forced to line up in one direction



Lowest energy configuration, at low T
→ all spins aligned → 2 configurations (up and down)



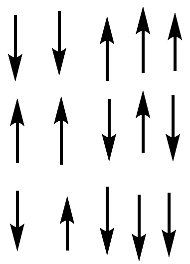
Curie temp - temp at which ferromagnetism disappears
Iron: 1043 K

Critical point
→ 2nd order phase transition

Models

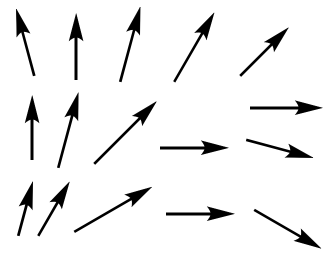
Universality Class – large class of systems whose properties are independent of the dynamic details of the system

Ising Model – vectors point UP OR DOWN *ONLY* → simplest



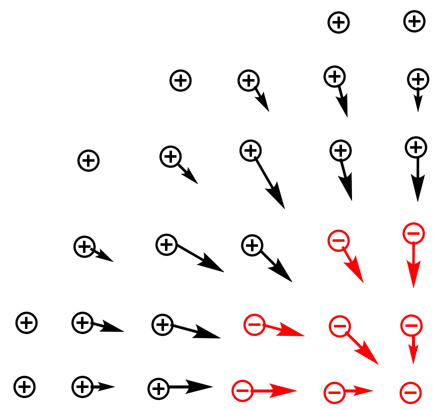
- **binary alloys**
- **binary liquid mixtures**
- **gas-liquid (atoms and vacancies)**

Potts Model – vectors point in any direction IN A PLANE



- **superfluid helium**
- **superconducting metals**

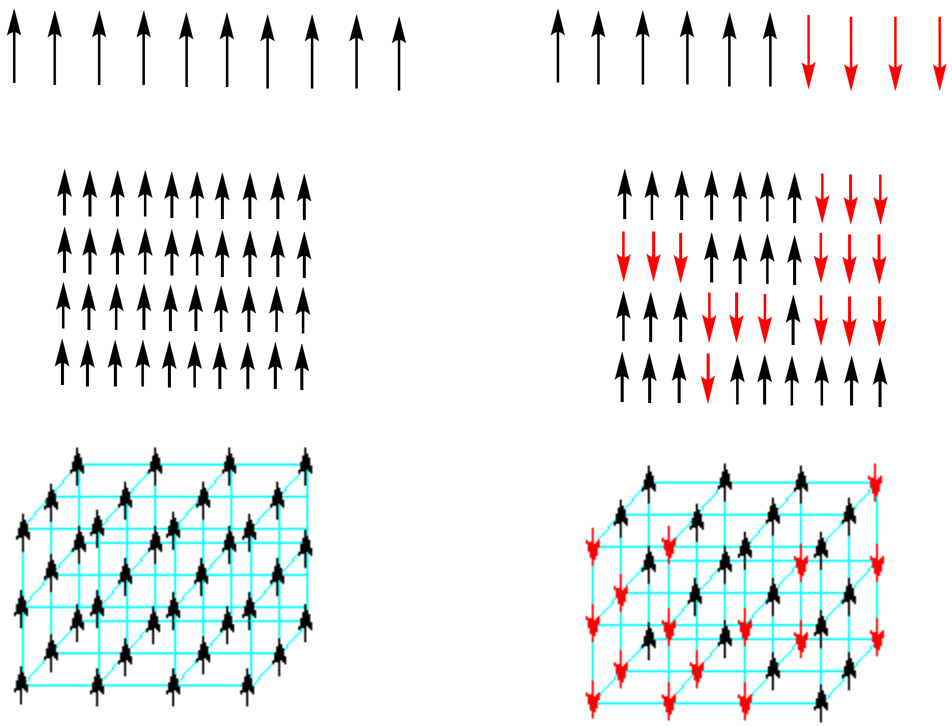
Heisenberg Model – vectors point in any direction IN SPACE



different dimensionality → different universality class

Ising Model

	Low T	High T	Solved
1-D			Ising – 1925
2-D			Onsager – 1944
3-D			Proven computationally intractable - 2000



As T increases, S increases but net magnetization decreases

The 1-D Case

The partition function, Z, is given by:

$$Z = \sum_{\sigma_k = \pm 1} f_L(\sigma_1) \exp\left\{ K \sum_{i=1}^{N} \sigma_i \sigma_{i+1} + m \sum_{i=1}^{N+1} \sigma_i \right\} f_R(\sigma_{N+1})$$

where $K = \dfrac{J}{T}$ and $m = \dfrac{H}{T}$ where H is the magnetic field

With no external magnetic field *m* = 0.

With free boundary conditions $f_L(\sigma) = f_R(\sigma) = 1.$

Make substitution $\sigma_i \sigma_{i+1} = s_i.$

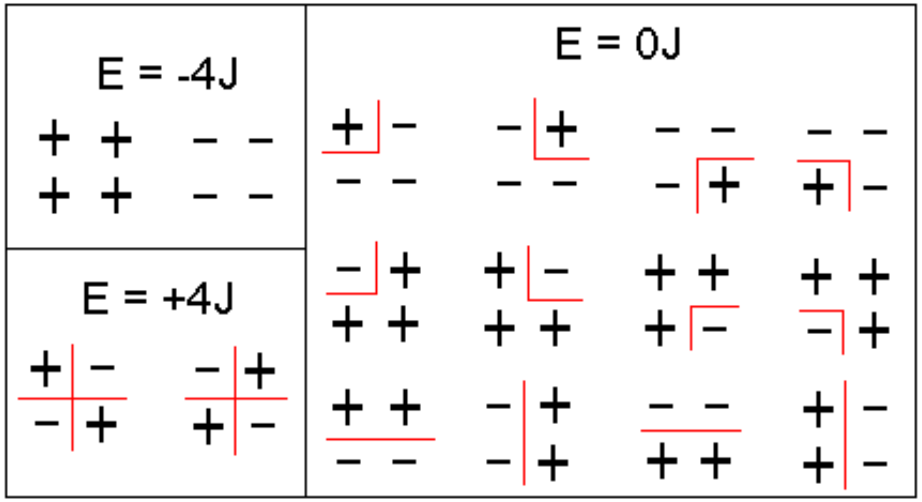
$$Z = \sum_{s_k = \pm 1} \mathrm{e}^{K \sum_{i=1}^{N} s_i} = (2 \cosh K)^N$$

The 1-D Ising model does NOT have a phase transition.

The 2-D Case

The energy is given by $E = -J\sum_{\langle i,j \rangle} s_i s_j$

For a 2 x 2 lattice there are $2^4 = 16$ configurations



Energy, E, is proportional to the length of the boundaries; the more boundaries, the higher (more positive) the energy.

In 1-D case, E ~ # of walls

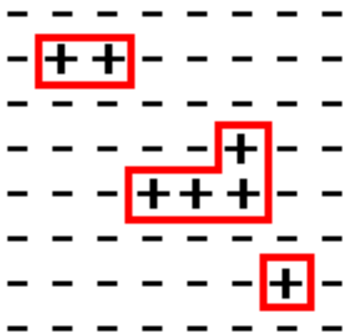
In 3-D case, E ~ area of boundary

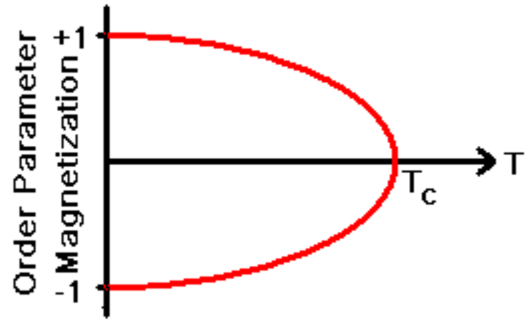
The upper bound on the entropy, S, is $k_B \ln 3$ per unit length.

The system wants to minimize F = E – TS.
At low T, the lowest energy configuration dominates.
At high T, the highest entropy configuration dominates.

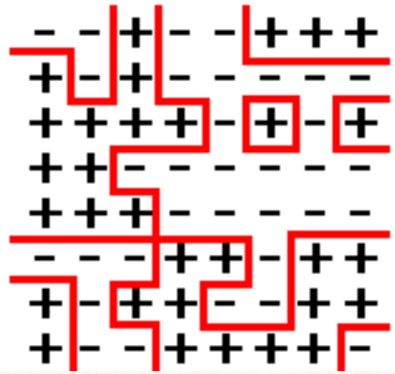
Phase Diagrams

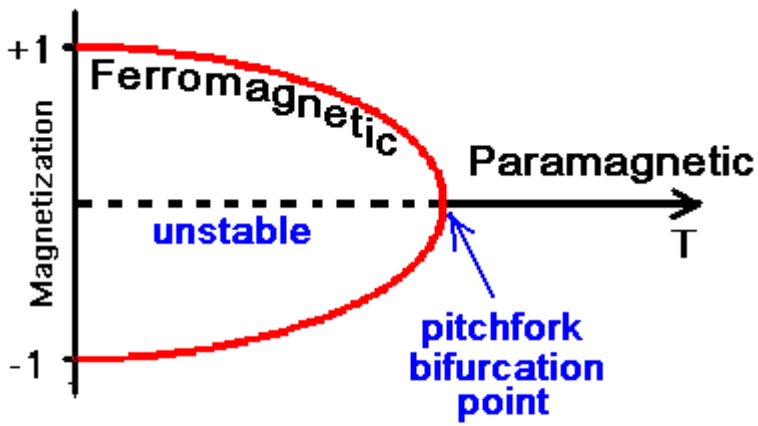
Low T





High T





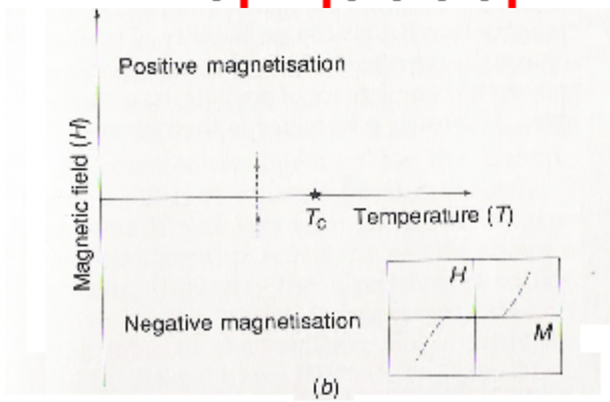


Figure 8.1. (*b*) The critical point of a magnet. Below a critical temperature T_c a magnet possesses a magnetic moment. The direction of the magnetic moment can be switched by a magnetic field, H. Along the line of zero magnetic field different phases, distinguished by the direction of the magnetic moment, coexist. As the magnetic field is varied at constant temperature (the grey path) the orientation of the magnetisation, M, is reversed at the line of phase coexistence (inset). The line of coexistence ends at T_c where the magnetic moment vanishes, and the different phases merge into a single paramagnetic phase.

Davies, "The New Physics" 1989, p 237

The 2-D Case - What is T_c?

From Onsager: $2\tanh^2(2\beta J) = 1$

$$\tanh x = \frac{e^{2x}-1}{e^{2x}+1}$$

let $2\beta J = x$ then $2\tanh^2 x = 1$

$$2\left(\frac{e^{2x}-1}{e^{2x}+1}\right)^2 = 2\frac{e^{4x}-2e^{2x}+1}{e^{4x}+2e^{2x}+1} = 1$$

$$2e^{4x} - 4e^{2x} + 2 = e^{4x} + e^{2x} + 1$$

$$e^{4x} - 6e^{2x} + 1 = 0$$

let $e^{2x} = y$ then $y^2 - 6y + 1 = 0$

quad formula yields $y = 3 \pm 2\sqrt{2}$ so

$$e^{2x} = 3 \pm 2\sqrt{2}$$

$$x = \frac{1}{2}\ln\left(3 \pm 2\sqrt{2}\right) \text{ so}$$

$$2\beta J = \frac{1}{2}\ln\left(3 \pm 2\sqrt{2}\right)$$

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$$\frac{2J}{k_B T} = \frac{1}{2}\ln\left(3 \pm 2\sqrt{2}\right)$$

$$k_B T = \frac{4J}{\ln\left(3 \pm 2\sqrt{2}\right)} \quad \text{but } 3 - 2\sqrt{2} < 1$$

which would lead to negative T
so only positive answer is correct

$$k_B T_C = \frac{4J}{\ln\left(3 + 2\sqrt{2}\right)} = \frac{2J}{\ln\left(1 + \sqrt{2}\right)}; \quad 2.269J$$

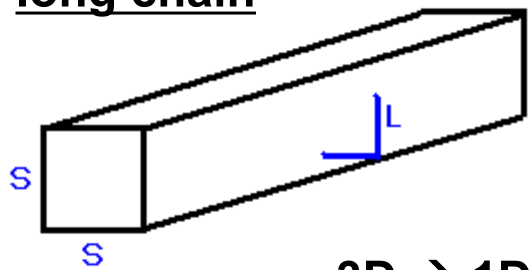
$$\boxed{k_B T_c = 2.269J}$$

What happens at T_c?

Correlation length – distance over which the effects of a disturbance spread.

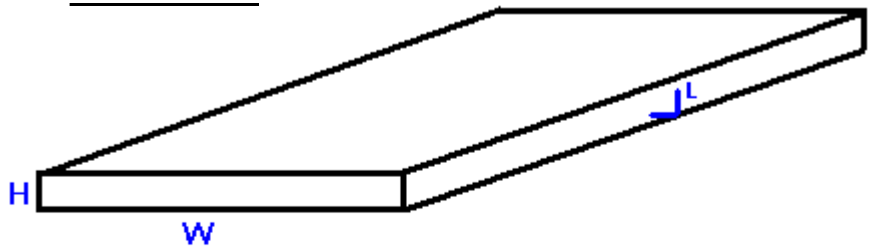
<u>Approaching from high side of Tc</u>

<u>long chain</u>



3D → 1D

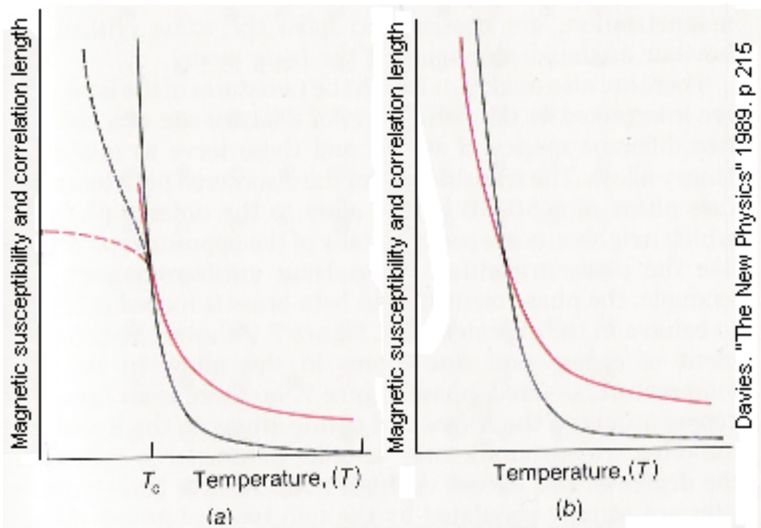
<u>thin film</u>



3D → 2D

Correlation length increases without bound (diverges) at Tc; becomes comparable to wavelength of light (critical opalescence).

Magnetic susceptibility – ratio of induced magnetic moment to applied magnetic field; also diverges at Tc.

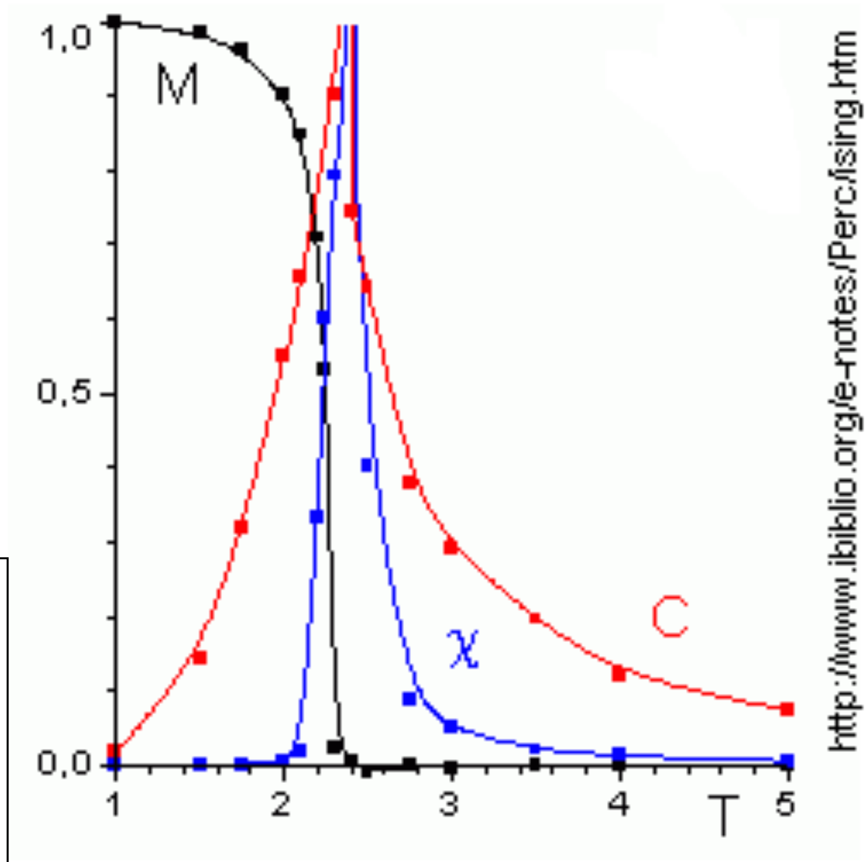


Magnetic susceptibility (black) and correlation lengths (red) for (a) a finite cube (dashed lines) compared with the infinite three-dimensional system (solid lines), and (b) a bar of square cross-section.

Specific heat, C, diverges at Tc.

Magnetization, M, is continuous.

Entropy, S, is continuous.



Order parameter, M (magnetization); specific heat, C; and magnetic susceptibility, X, near the critical point for the 2D Ising Model where Tc = 2.269.

2nd Order Phase Transition

Magnetization, M, (order parameter) – 1st derivative of free energy – continuous

Entropy, S – 1st derivative of free energy – continuous

Specific heat, C – 2nd derivative of free energy – discontinuous

Magnetic susceptibility, X – 2nd derivative of free energy – discontinuous

Critical Exponents

Reduced Temperature, t

$$t \equiv \frac{T - T_C}{T_C}$$

Specific heat $C \propto |t|^{-\alpha}$

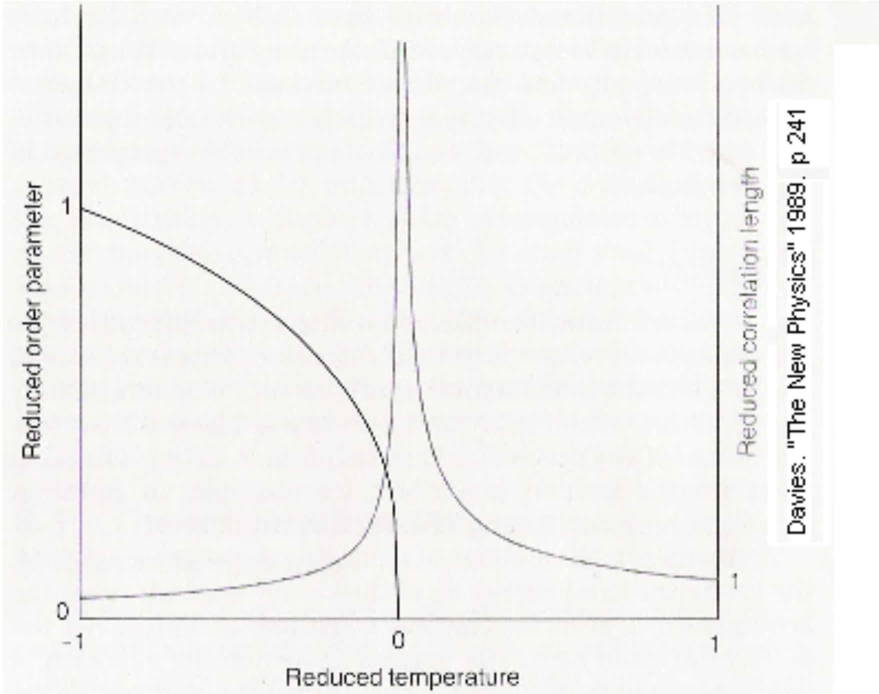
Magnetization $M \propto |t|^{\beta}$

Magnetic susceptibility $\chi \propto |t|^{-\gamma}$

Correlation length $\xi \propto |t|^{-\nu}$

$$\alpha = 0 \text{ (log divergence)}$$

$$\beta = \frac{1}{8} \quad \gamma = \frac{7}{4} \quad \nu = 1$$



Critical behavior of the order parameter an the correlation length. The order parameter vanishes with the power β of the reduced temperature t as the critical point is approached along the line of phase coexistance. The correlation length diverges with the power ν of the reduced temperature.

The exponents display critical point universality (don't depend on details of the model). This explains the success of the Ising model in providing a quantitative description of real magnets.