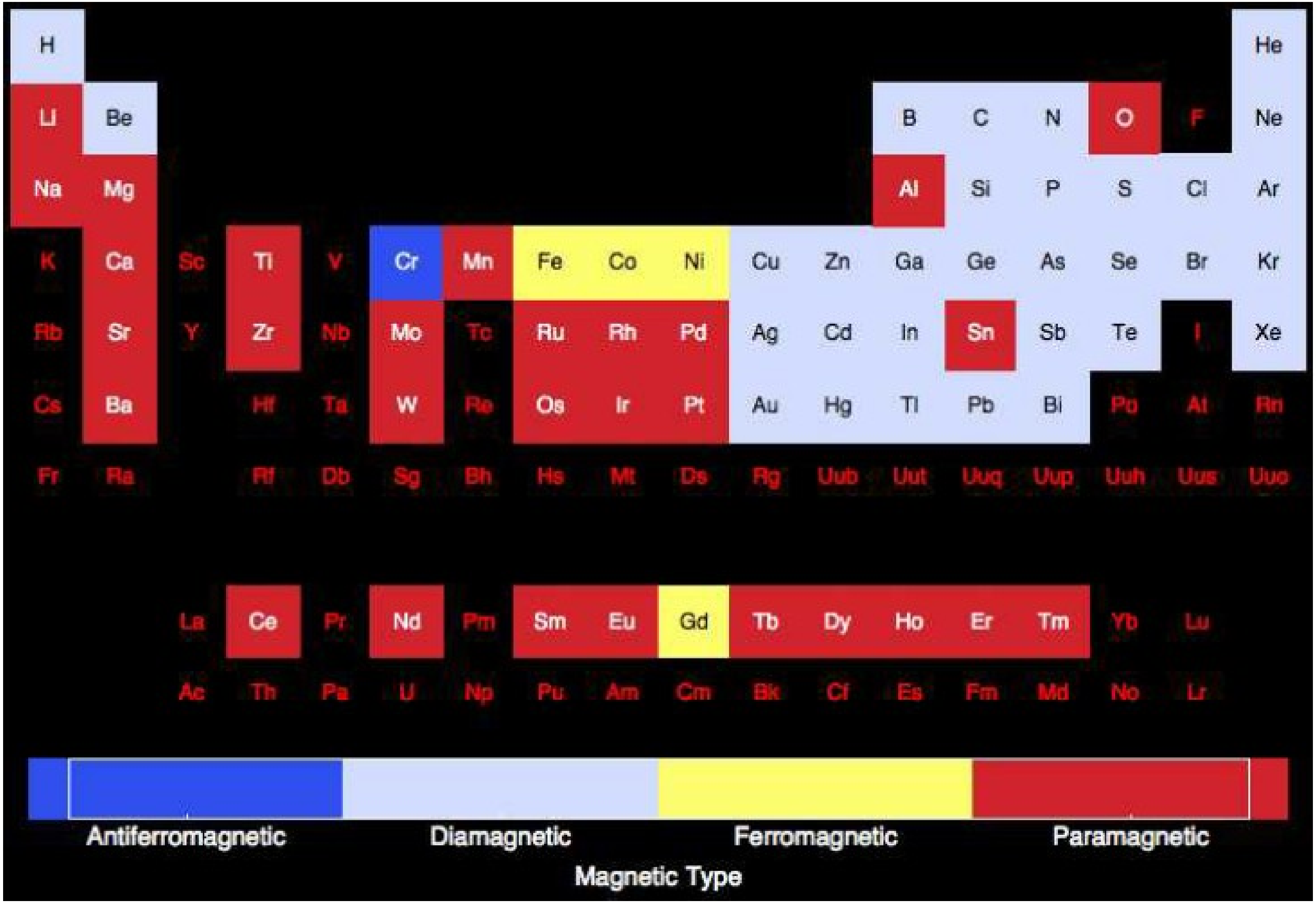
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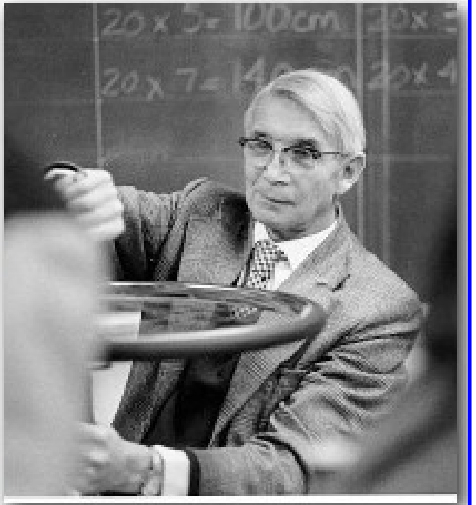
Ac
Th
Pa
U
Np
Pu
Am
Cm
Bk
Cf
Es
Fm
Md
No
Lr
Antiferromagnetic
Diamagnetic
Ferromagnetic
Paramagnetic
Magnetic Type

Ernst Ising

May 10, 1900 in Köln-May 11 1998 in Peoria (IL)

- Student of Wilhelm Lenz in Hamburg. PhD 1924. Thesis work on linear chains of coupled magnetic moments. This is known as the Ising model.
- The name 'Ising model' was coined by Rudolf Peierls in his 1936 publication 'On Ising's model of ferromagnetism'.
- He survived World War II but it removed him from research. He learned in 1949 - 25 years after the publication of his model - that his model had become famous.
- Lars Onsager solved the Ising model (zero field) in two dimensions in 1944.

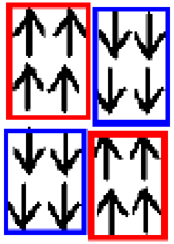


S. G. Brush, History of the Lenz-Ising Model, Rev. Mod. Phys **39**, 883-893 (1962)

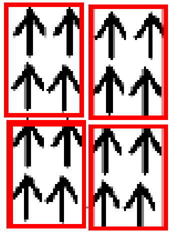
Ferromagnetism

Magnetic domains of a material all line up in one direction

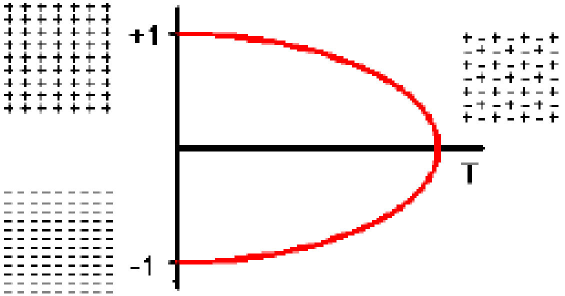
In general, domains do not line up
→ no macroscopic magnetization



Can be forced to line up in one direction



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



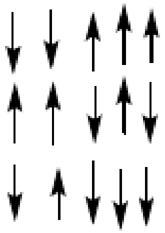
Curie temp - temp at which ferromagnetism disappears
Iron: 1043 K

Critical point
→ 2nd order phase transition

Models

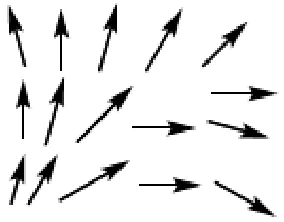
Universality Class – large class of systems whose properties are independent of the dynamic details of the system

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



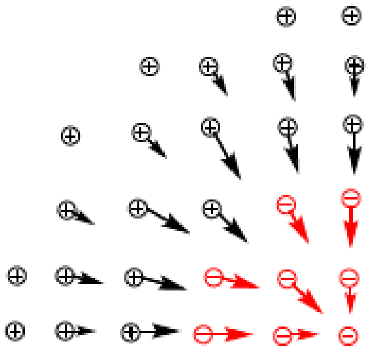
- binary alloys
- binary liquid mixtures
- gas-liquid (atoms and vacancies)

Potts Model – vectors point in any direction IN A PLANE



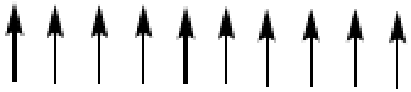
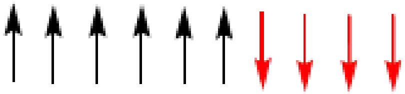
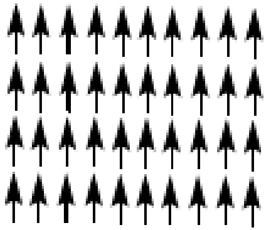
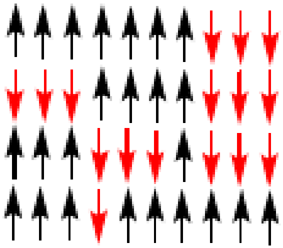
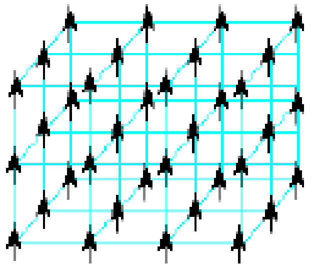
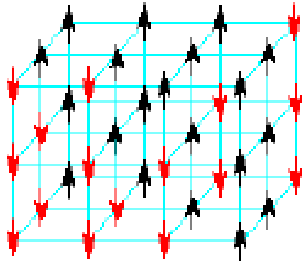
- superfluid helium
- superconducting metals

Heisenberg Model – vectors point in any direction IN SPACE



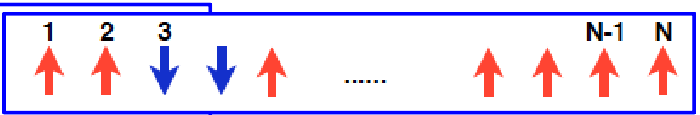
different dimensionality → different universality class

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

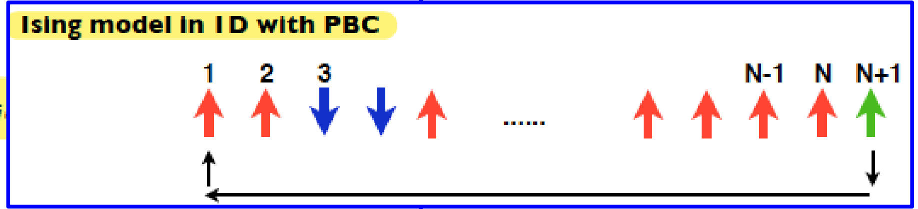
Ising model



A general Ising model is defined as

$$\mathcal{H} = -\sum_i H_i s_i - \sum_{i,j} J_{i,j} s_i s_j - \sum_{i,j,k} J^1_{i,j,k} s_i s_j$$

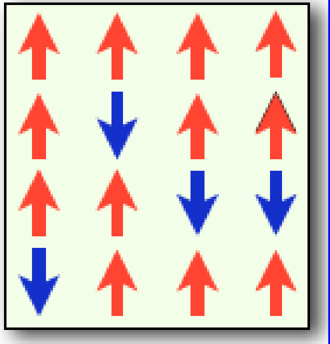
coupling to a field — pair interactions — 3-body interactions



It has the following general properties

- No phase transition at d=1 for T>0
- For $J^1_{ijk}=0$, phase transition(s) for $\sum_{i \neq j} |J_{ij}| < \infty$
- For d>4, mean field results are exact

Ising model in 2D



Lower critical dimension is $d_L = 1$ and the upper critical dimension is $d_U=4$.

Thermodynamics of the Ising model can be obtained from

$$F = -k_B T \ln[\mathrm{Tr}\, e^{-\beta \mathcal{H}}] \quad \text{for example} \quad \langle s_i \rangle = -\left(\frac{\partial F}{\partial H_i}\right)_T$$

The 1-D Case

The partition function, Z, is given by:

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

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

Vith no external magnetic field *m* = 0.

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

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

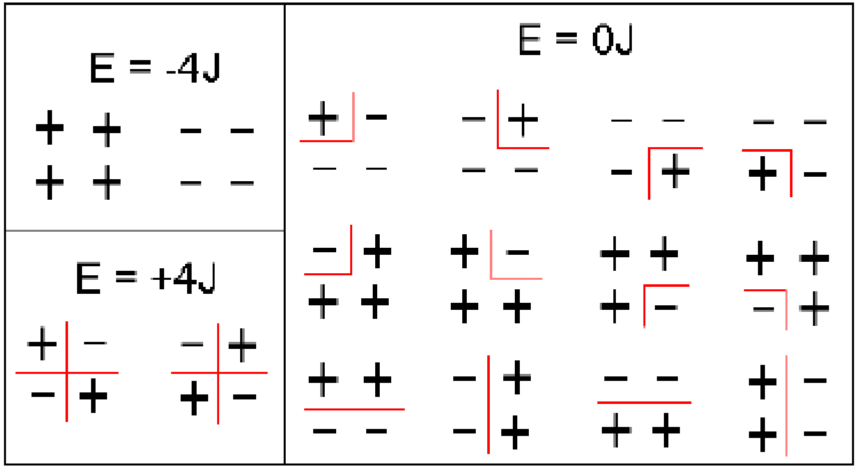
$$Z = \sum_{s_k = \pm 1} \exp\{K \sum_{i=1}^{N} s_i\} = (2\cosh K)^N$$

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.

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

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

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

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

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

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

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

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

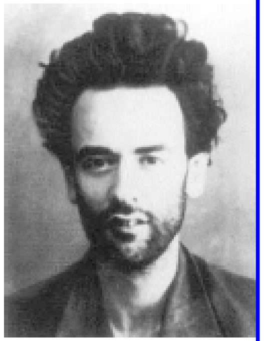
$$k_B T_C = \frac{4J}{\ln\left(3 + 2\sqrt{2}\right)} = \frac{2J}{\ln\left(1 + \sqrt{2}\right)} ; \; 2.269J$$

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

Digression: Lev Davidovich Landau

Lev Davidovich Landau, Jan. 22 1908 in Baku – Apr. 1 1968 Moscow
Nobel Prize 1962 for pioneering theories in condensed matter physics

- Graduated from Leningrad University at the age of 19. He started at the age of 14! After graduating from Leningrad he spent time in Denmark with Bohr. Collaborated and interacted also with Pauli, Peierls and Teller. For his travels he got a Rockefeller fellowship!

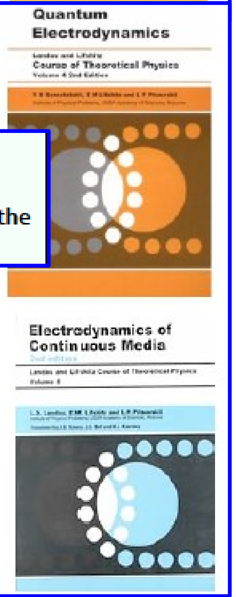


- His work covers basically all of theoretical physics from fluids to quantum field theory.

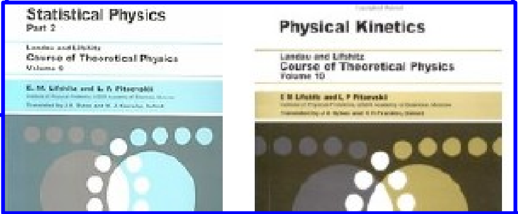
- Was imprisoned by Stalin for a year after being accused to be a German spy. Was freed after Piotr Kapitza threatened to stop his own work unless Landau was released

- On Jan. 7 1962 he suffered a major car accident and was unable to continue his work. For the same reason he was not able to attend the Nobel Prize seremonies.

More reading: Akhiezer, Recollections of Lev Davidovich Landau, *Physics Today* **47**, 35-42 (1994).
Ginzburg, Landau's attitude towards physics and physicists, *Physics Today* **42**, 54-61 (1989).
Khalatnikov, Reminiscences of Landau, *Physics Today* **42**, 34-41 (1989).



Landau and Lifshitz started in 1930's and the 10 volume series was completed in 1979 by Lifshitz. They received the 1962 Lenin Prize for the "Course of Theoretical Physics".



Landau's revolutionary ideas

- **Superfluidity:** Landau considered the quantized states o of the **whole liquid** instead of single atoms. That was a re idea and using it Landau was able to explain superfluidity.
- **Superconductivity:** Even before the BCS theory, Ginzburg and Landau suggested a phenomenological theory of superconductivity based on Landau's earlier theory of continuous phase transitions. When it was published, the GL theory received only limited attention. This changed dramatically in 1959, when L.P. Gorkov showed rigorously that close to T_c the GL theory and the BCS theory become equivalent. Furthermore, two years before Gorkov, A. Abrikosov predicted the possibility of two different kinds of superconductors by using the GL theory!
- Landau's theory of phase transitions.
- If we sum up the leading ideas we end up with two things: **the importance of symmetry and symmetry breaking, and the existence of an order parameter.**

The order parameter characterizes the system the following way:

$\Psi = 0$ in the disordered state (above T_c),

Ψ is ***small*** and ***finite*** in the ordered state ($T<T_c$).

1. It is possible to define an order parameter.
2. It is possible to describe the system with a free energy.
3. The free energy must be consistent with the high temperature symmetry properties of the system. Mathematically speaking, the Hamiltonian must commute with the symmetry group of the high temperature phase (note: discrete & continuous).
4. The free energy must be analytic. In addition, the expansion coefficients must be regular functions of the temperature.

Symmetry

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4. The free energy must be analytic. In addition, the expansion coefficients must be regular functions of the temperature.

Close to T_c the free energy can be expanded in powers of the order parameter

free energy — order parameter. must be small

$$F(\Psi) = \sum_{n=0}^{\infty} a_{2n}\Psi^{2n}$$

expansion coefficients are phenomenological parameters that depend on T and microscopics

Order parameter must be small for the expansion to converge.

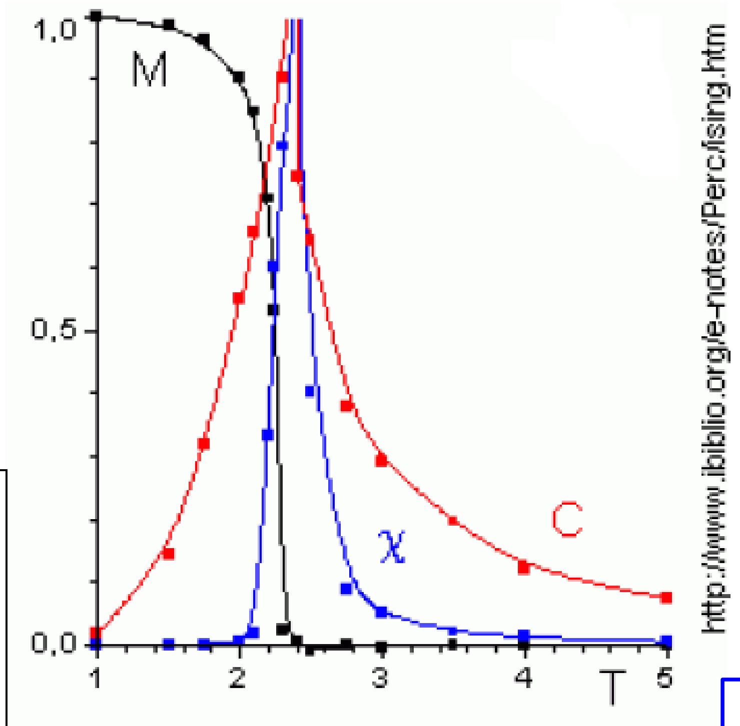
Order parameters

system	order parameter
liquid-gas	density
ferromagnetic	magnetization
superconducting	condensate wave function
liquid crystal	degree of molecular alignemnt
binary mixture (methanol-n-hexane)	concentration of either substance
helix-coil	number of helix base pairs
XY-model	magnetization (Mx,My)
$BaTiO_3$	polarization
crystal	density wave
liquid crystal	director

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.

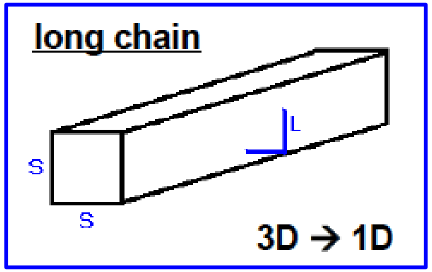
2nd Order Phase Transition

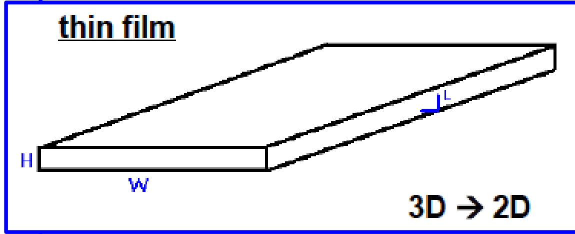
Magnetization, M, (order parameter) – 1st derivative of free energy – continuous

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





2D magnetization

$$P \qquad h$$

$$V \qquad -M = -Nm$$

$$\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial P} \qquad \chi = \frac{\partial m}{\partial h}$$

$$A = A(N, V, T) \qquad A = A(N, M, T)$$

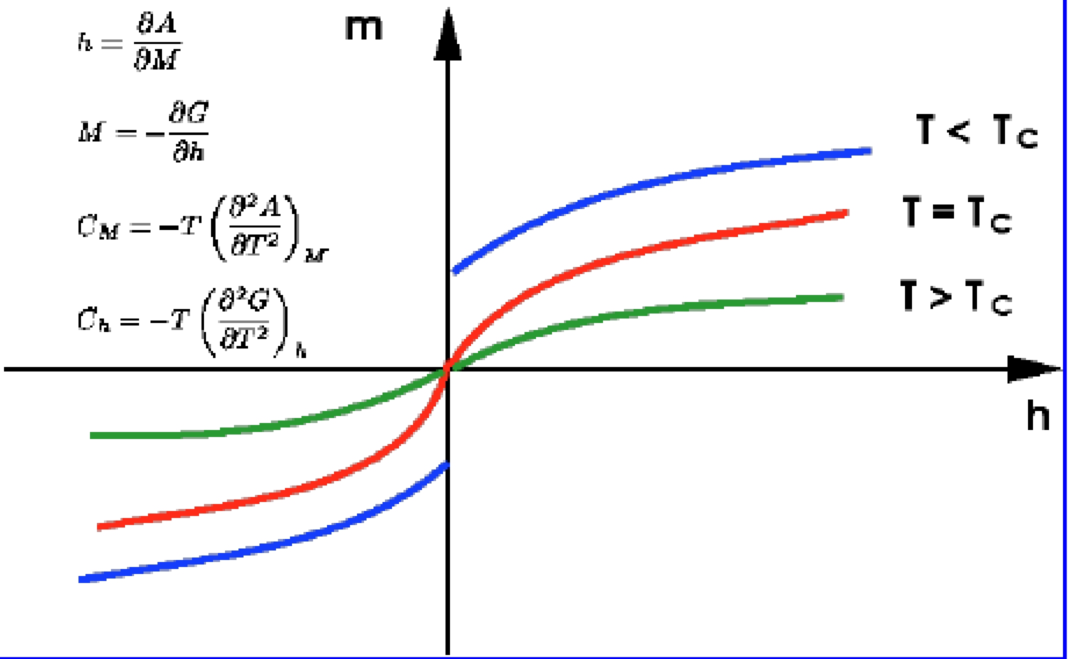
$$G = A + PV(P) \qquad G = A - hM(h)$$

$$P = -\frac{\partial A}{\partial V} \qquad h = \frac{\partial A}{\partial M}$$

$$V = \frac{\partial G}{\partial P} \qquad M = -\frac{\partial G}{\partial h}$$

$$C_V = -T\left(\frac{\partial^2 A}{\partial T^2}\right)_V \qquad C_M = -T\left(\frac{\partial^2 A}{\partial T^2}\right)_M$$

$$C_P = -T\left(\frac{\partial^2 G}{\partial T^2}\right)_P \qquad C_h = -T\left(\frac{\partial^2 G}{\partial T^2}\right)_h$$



Itinerant magnetism & Stoner criterion

$$I N^0(\epsilon_F) > 1$$

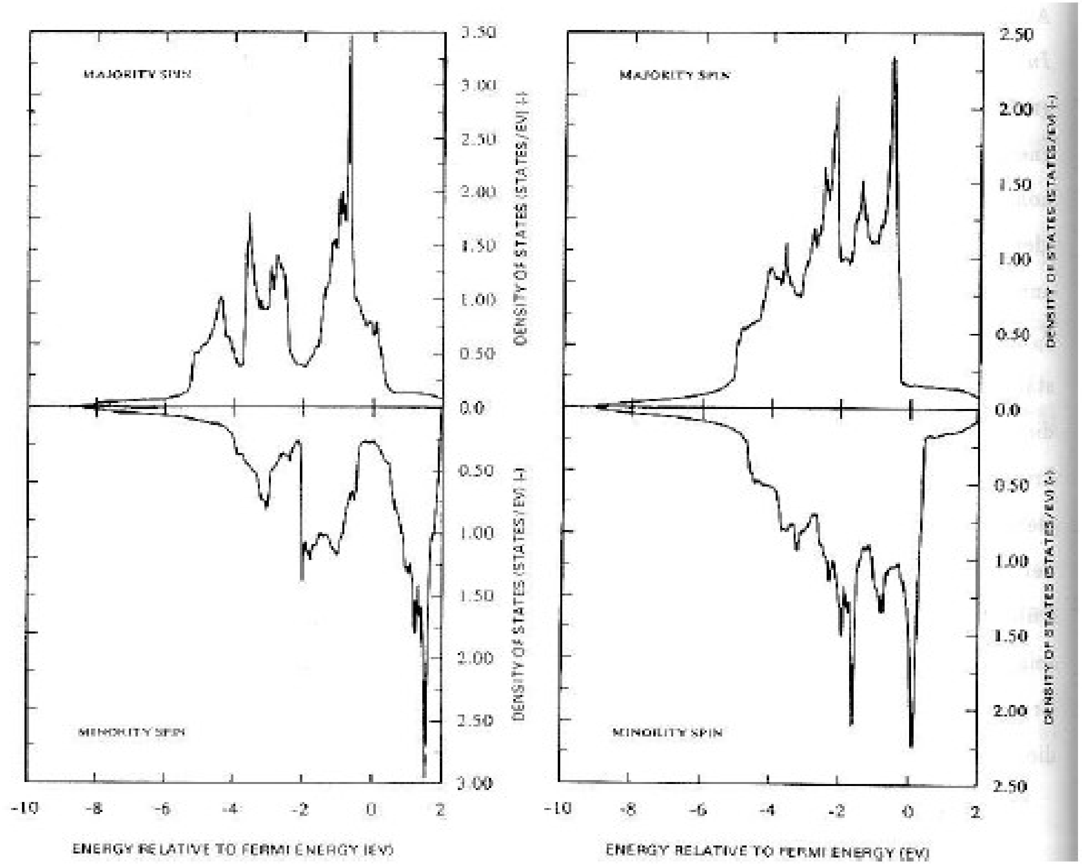


Figure 8.15: Spin-resolved density of states (DOS) for bulk Fe and Ni in DFT-LSDA [from V.L. Moruzzi, J.F. Janak and A.R. Williams, *Calculated electronic properties of metals*, Pergamon Press (1978)].