# Magnetism at finite temperature

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Temperature is an important parameter since exchange energies and ordering temperatures are comparable to room temperature

Curie (Néel) temperature: 1044°K in Fe, 70°K in EuO, 2292K in Gd, 525°K in NiO (AF)

Exchange: 0.01eV ≈ 100°K

Magnetocrystalline anisotropy: 1mK to 10K

Shape anisotropy: from 1mK to 1K

External field: 1T ≈ 1°K

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# Outline

- The Heisenberg model in molecular field approximation
- Landau theory of phase transitions
- Beyond mean field:
    - Magnons (spin waves)
    - Ginzburg-Landau theory
    - Critical behavior
    - Role of dimensionality: 1D and 2D systems

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    - Critical behavior
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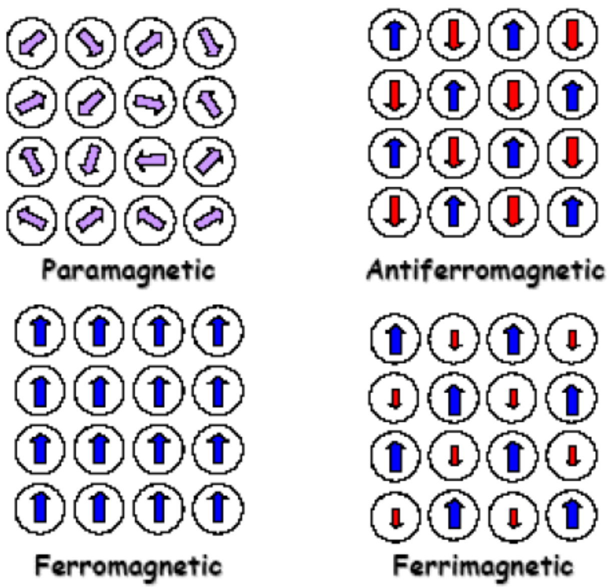
Various microscopic mecanisms for exchange interactions in solids:

-Localized / itinerant spin systems
-Short / long range
-Ferro or antiferro

$$H = -\sum_{ij} J_{ij}\, \vec{S_i}.\vec{S_j}$$

Various types of ordered magnetic structures:




Ferromagnets

| | $T_C$ |
|---|---|
| Fe | 1043 K |
| Co | 1394 K |
| Ni | 631 K |
| Gd | 293 K |

Antiferromagnets

| | $T_N$ |
|---|---|
| CoO | 293K |
| NiO | 523K |

Type of magnetic order depends on the interactions

Also spin glasses, spin liquids… : no long range magnetic order

The various exchange mecanisms can usually be described by an effective exchange hamiltonian: Heisenberg model

$$H = -\sum_{ij} J_{ij}\, \vec{S_i}.\vec{S_j}$$

$J_{ij}$ can be long or short range, positive or negative

$\vec{S_i}$ : classical (vector) or quantum spin

It is an interaction between spins: if the magnetic moment is given by J instead of S (J=L+S), interaction can be rewritten as:

$$\tilde{H} = -\sum_{ij} I_{ij}\, \vec{J_i}.\vec{J_j}$$

If $J = L+S$, and $L+2S = g_J J$, then, $S = (g-1)J$ and $I_{ij} = (g-1)^2 J_{ij}$

In this lecture: no anisotropy effect

K coefficients vary with T as $M^n$

## What is mean field approximation ?

one moment in a magnetic field $H_{ext}$: $M = M_0\, g\left(\frac{\mu H}{k_B T}\right)$

Where the function $g$ is

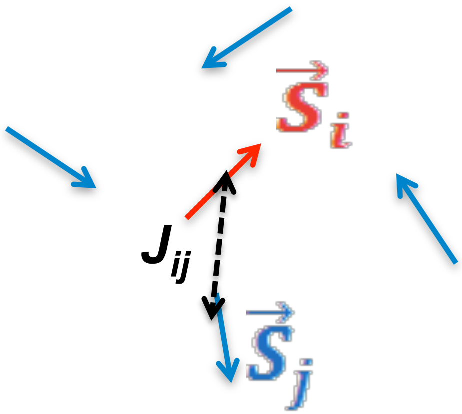
- the Brillouin function (quantum case)
- or the Langevin function (classical spins)

Heisenberg model: $H = -\sum_{ij} J_{ij}\, \vec{S_i}.\vec{S_j}$

Main assumption: $\vec{S_i}$ is replaced by its average $\langle\vec{S_i}\rangle$

$$H = -\sum_{ij} J_{ij}\, \vec{S_i}.\vec{S_j} \Rightarrow H_{MF} = -\sum_{ij} J_{ij}\left[\langle\vec{S_i}\rangle.\vec{S_j} + \langle\vec{S_j}\rangle.\vec{S_i} - \langle\vec{S_i}\rangle.\overrightarrow{\langle S_j\rangle}\right]$$

(similar to molecular field, or Hartree-Fock approximation)




$$H_{MF} = -\sum_{ij} J_{ij} \left[ \langle \vec{S_i} \rangle . \vec{S_j} + \langle \vec{S_j} \rangle . \vec{S_i} - \langle \vec{S_i} \rangle . \overrightarrow{\langle S_j \rangle} \right]$$

$$= -\sum_{ij} 2J_{ij} \; \langle \vec{S_i} \rangle . \vec{S_j} \; + constant$$

field acting on $\vec{S}_i$ due to the other spins $\vec{S}_j$ :

$$h_i = -\sum_{j} J_{ij} \; \langle \vec{S_j} \rangle$$

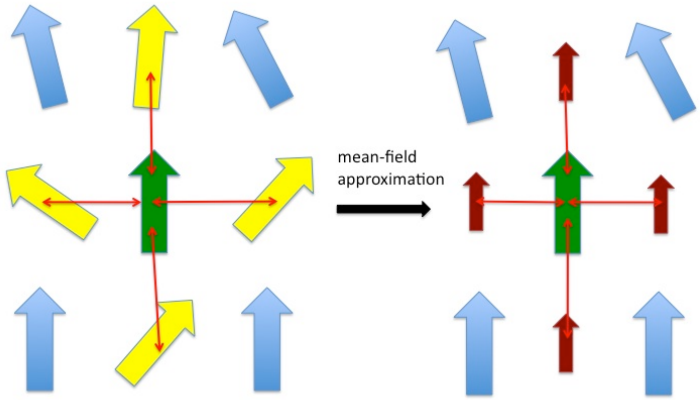
If there is also an external field:

$$h_i = -\sum_{j} J_{ij} \; \langle \vec{S_j} \rangle + \vec{h}_{ext}$$

Initial problem: many-body system of interacting spins

New problem: collection of spins in static local magnetic field

Mean field approximation




The field created by the neighbors is static; i.e. all thermal and quantum fluctuations are neglected. When fluctuations are small, it is a good approximation.

Fluctuations are large

- at high temperature: near $T_c$ (critical behavior) and above $T_c$ (paramagnetic fluctuations)
- in low dimensional systems (1D, 2D)
- Small spin value (quantum fluctuations):effect of spin waves is more important for small S-value

If fluctuations are large, corrections to mean field are important

## The molecular field approximation

$$H = -\sum_{ij} J_{ij}\, \vec{S_i}.\vec{S_j} - \sum_i \vec{S}_i.\vec{h}_{ext}$$

$$\Rightarrow \quad H = -\sum_i \vec{S}_i.(\vec{h}_i + \vec{h}_{ext})$$

Each magnetic moment is in an effective field

$$\vec{h}_{ext} + \sum_j 2J_{ij}\,\langle \vec{S}_j \rangle$$

external field + field created by the neighboring moments

Local magnetization: $M_i = g\mu_B \langle \vec{S}_i \rangle = M_0\, g\left(\frac{\mu H_i}{k_B T}\right)$ (*$g$ is Brillouin or Langevin function*)

Set of coupled equations to determine $\langle \vec{S_i} \rangle$ on each site

In a ferromagnet, it becomes simple since $\langle \vec{S_i} \rangle$ is <u>uniform :</u>

$$\langle \vec{S_i} \rangle = m_F \Rightarrow m_F = m_F\, g\left(\frac{h_{ext} + \alpha m_F}{k_B T}\right), \alpha = 2\sum_j J_{ij}$$

New problem: each spin is in a local field that depands on surroundings

$$h_i = -\sum_j J_{ij} \langle \overrightarrow{S_j} \rangle$$

Hypothesis on the nature of ground state:

Ferromagnetic state: $\langle \overrightarrow{S_\iota} \rangle = S, \langle \overrightarrow{h_\iota} \rangle = h$ (uniform solution)

2 sublattices AF $\langle \overrightarrow{S_\iota} \rangle = \pm S, \langle \overrightarrow{h_\iota} \rangle = \pm h$

Helimagnets: $\langle \overrightarrow{S_\iota} \rangle = \vec{S} e^{iqR_i}, \langle \overrightarrow{h_\iota} \rangle = \vec{h} e^{i(qR_i+\varphi)}$

Receipe: for each solution, solve the selfconsistent equations, calculate S, calculate the corresponding free energy, compare the energy of the various solutions.

## The molecular field approximation: ferromagnetic solution

Approximation: $S_j$ is replaced by its average $\langle S_j \rangle = S(T)$

If exchange only between nearest neighbors, $h_{eff} = h_{ext} + 2zJS(T)$, (z= number of nearest neighbors)

Simple problem: magnetic moment in a uniform field $h_{eff}$:

$$S(T) = SB_S\left(\frac{g\mu_B(hext + 2zJS(T))}{k_BT}\right)$$

selfconsistent equation for S(T)

($B_S$: Brillouin function for spin S)

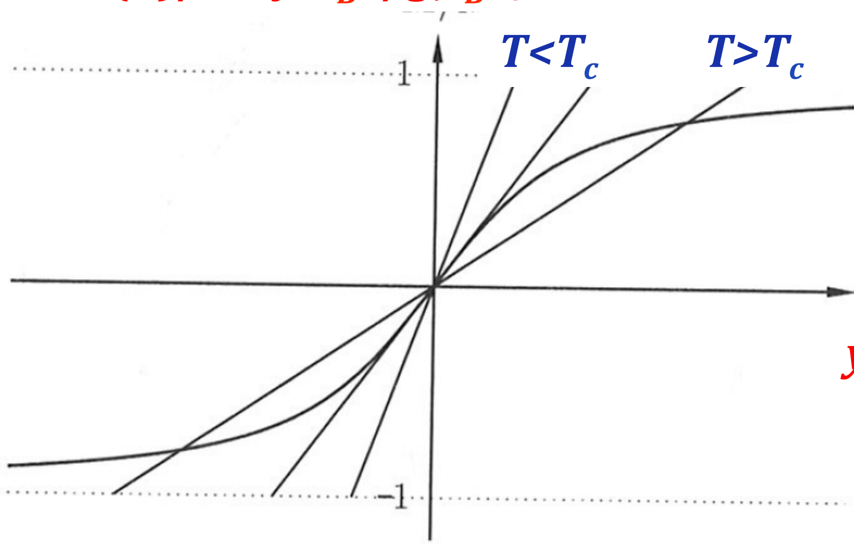
For Antiferromagnet: 2 coupled equations for $S_A$ and $S_B$ (2 sublattices)

(if spins are considered as classical spins: $B_S$ is replaced by Langevin function $L$)

Solution of the mean field equation: $S(T) = SB_S\left(\frac{g\mu_B(h_{ext} + 2zJS(T))}{k_BT}\right)$

If $h_{ext} = 0$

$S(T)/S = y\, k_BT/g\mu_B zJS$




At $T>T_C$: $y=0$
At $T<T_C$: 1 solution $y_0 \neq 0$

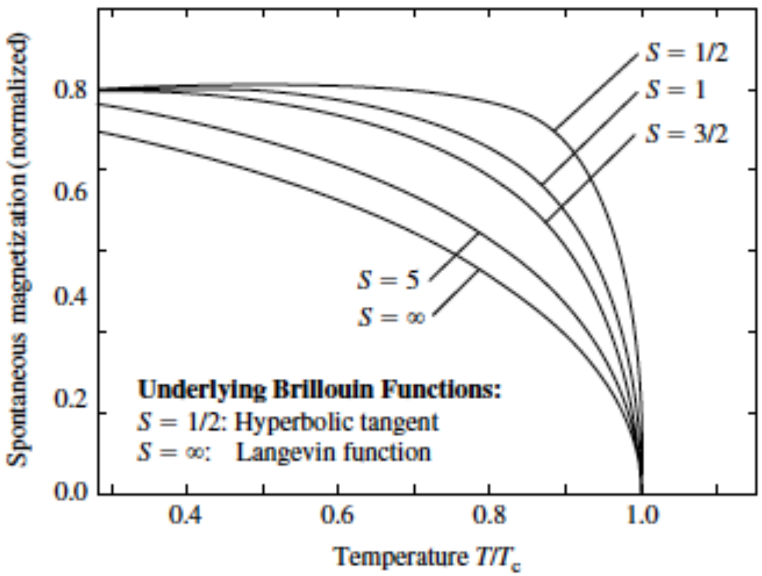
$T_C$ is obtained when $y_0=0$

Calculation of $T_C$:
near $y=0$, $B_S(y) = y\, S(S+1)/3S + \ldots$.

At $T_c$ $S(S+1)/3S = k_BT/g\mu_B zJS$

## Ferromagnet: Order parameter and Curie temperature

$$k_B T_c = \frac{2S(S+1)}{3} \sum_j J_{ij} = \frac{2S(S+1)}{3} zJ$$ (If only nearest neighbor interactions J)



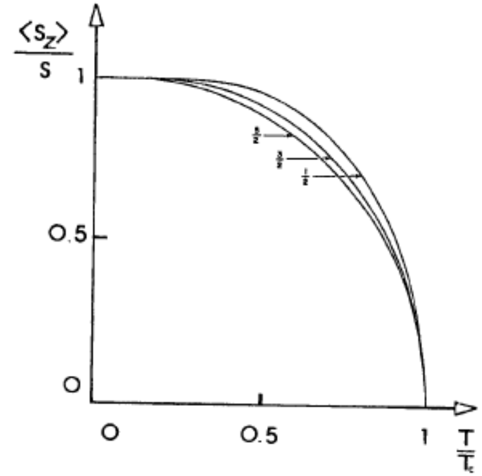

Magnetization is calculated selfconsistently

At low T: $M(T) - M_0 \propto exp\left(-{}^{2T_C}/_{T}\right)$

Near $T_c$: $M(T) \propto (T_c - T)^{1/2}$

Similar calculations for antiferromagnets or ferrimagnets (2 sublattices, 2 selfconsistent parameters $S_A$ and $S_B$);
also with longer range interactions

**Predictions of mean field theories:**




-$T<T_c$ $M(T)$ calculated selfconsistently

- $T_c = 2zJ\, S(S+1)/3k_B$

At low T: exponential decrease of S(T)

Near $T_c$: S(T) vanishes as $(T_c-T)^{1/2}$ (critical exponent $\beta=1/2$)

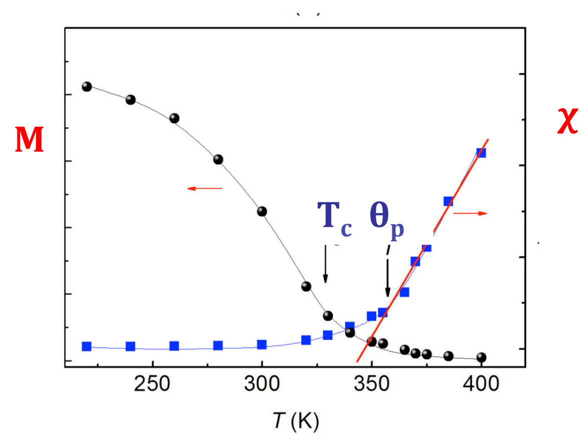
-$T>T_c$ susceptibility: Curie Weiss law

Calculated using $M(T) = SB_S\left(\dfrac{g\mu_B(h_{ext} + 2zJM(T))}{k_B T}\right)$

In the paramagnetic state: $M(T)=\chi\, h_{ext}$. Expansion of the Brillouin function:

**Curie-Weiss law:** $\chi = C/(T-T_c),\, C = S(S+1)/3k_B$ (critical exponent $\gamma = 1$)

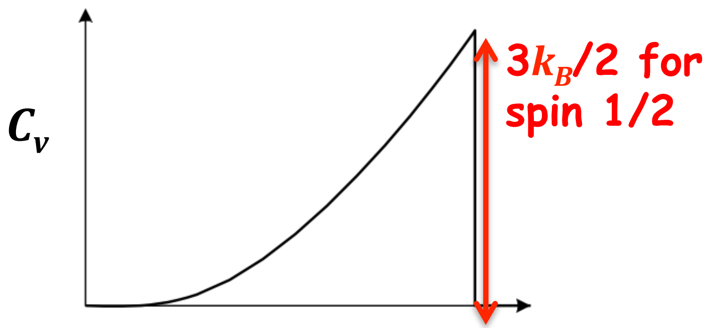
In general, at $T>>T_c$ $\chi = C/(T-\theta_p)$
with $\theta_p \neq T_c$.

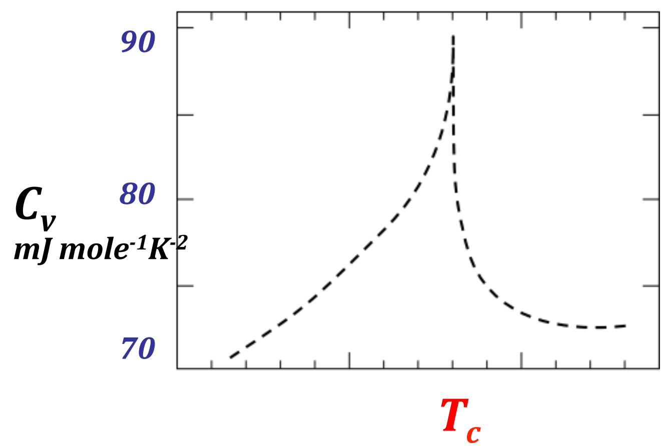


- Specific heat: partition function for one spin in the effective field $h_{eff}$

$$Z = e^{-\beta h_{eff}/2} + e^{+\beta h_{eff}/2}$$

$$F = -k_B T \, LnZ \, , C_v = -T\frac{\partial^2 F}{\partial T^2}$$



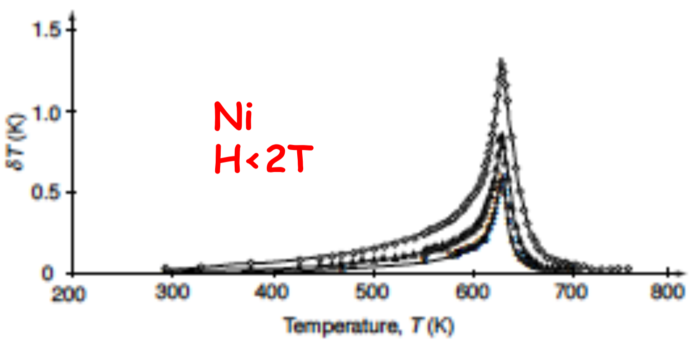

$RbMnF_3$

Discontinuity of $C_v$ at $T_c$: critical exponent $\alpha = 0$

- Magnetocaloric effect:

At $T>T_c$: $\delta Q \propto \frac{TT_c}{(T-T_c)^2}\delta H^2 \, , \delta T \propto \frac{1}{C_M}\frac{T}{T_c}\delta M^2$

At $T<T_c$: $\delta T \propto \frac{1}{C_M}\delta M^2$



Generalization to describe more complex models: antiferromagnets, ferrimagnets,….

Crystal field effects

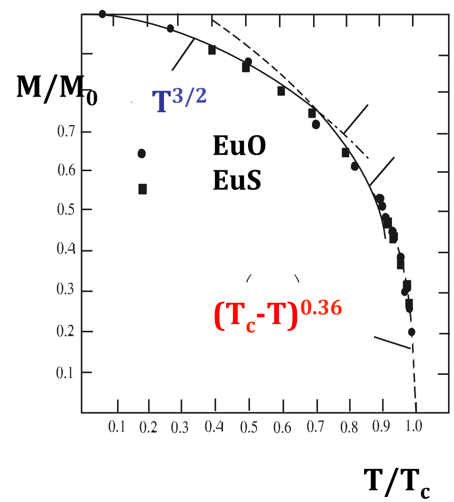
Comparison with experiments: qualitatively correct but:

- Mean field $T_c$ generally too large

- Deviations at low T: $M(T)/M_0 = 1 - AT^{3/2}$ ( in a ferromagnet)
$= 1\text{-}AT^2$ ( in antiferromagnet)

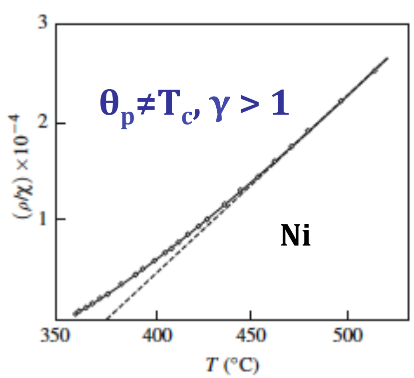
- Deviations near $T_c$:

$M(T)/M_0 = (Tc\text{-}T)^{\beta}$ with $\beta < 0.5$




- Deviations above $T_c$:

$\chi(T) \propto (T - T_c)^{\gamma}$ with $\gamma > 1$



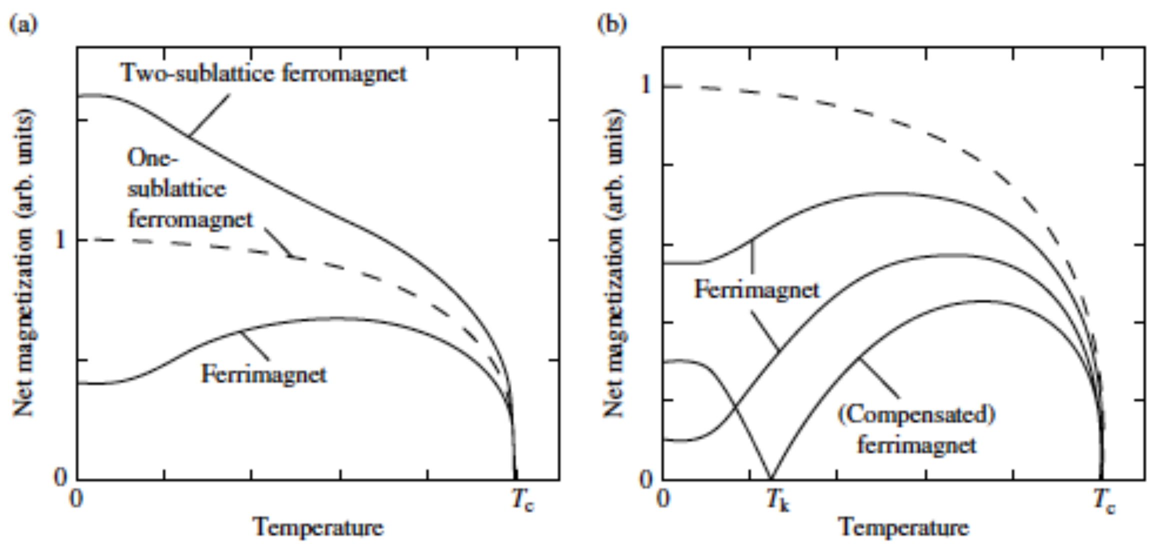
# Mean field magnetization for antiferro, ferrimagnets;..

Several sublattices: A, B, C ……

Molecular field on each sublattice created by the neighbors $H_A$, $H_B$….

$H_A$: $\alpha M_A + \beta M_B + \ldots$

$M_A = B_A\,(g\mu(H_A + H_{ext})/kT)$, $M_B = B_B\,(g\mu(H_B + H_{ext})/kT)$



# Advantages and limitations of mean field approximations

-Simplicity

-Simple calculations of thermodynamic properties

-Various magnetic order: ferro, ferri, AF, helimagnets

-Anisotropy can be taken into account

-1st step to investigate a model.

-Powerful method, can be applied to many problems in physics

But it is necessary to compare various mean field solutions

-At low T: $M(T) - M_0 \approx \exp(-\Delta/kT)$ instead of $T^\alpha$ ($\alpha$=2 or 3/2): possible corrections if spin waves are included

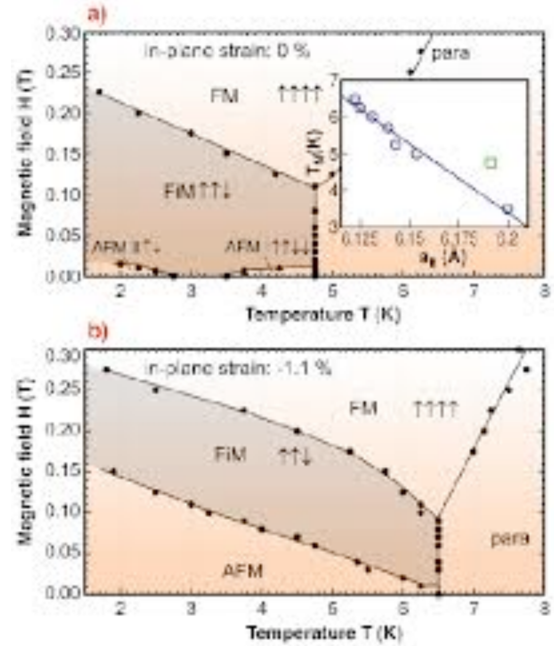
-Near $T_c$ : critical exponents are not correct

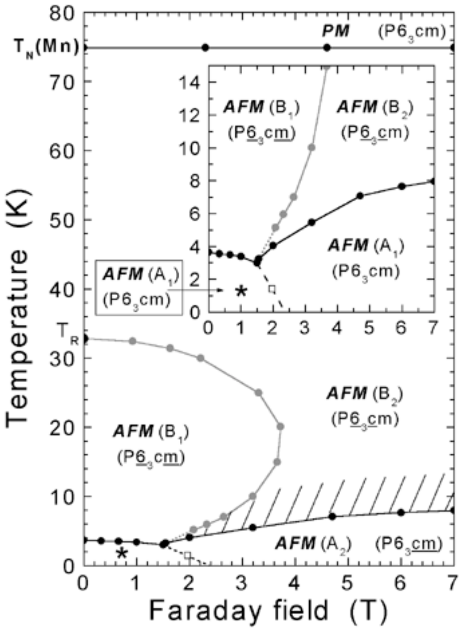
-Overestimation of $T_c$

-Absence of magnetism above $T_c$ (short range correlations are not included)

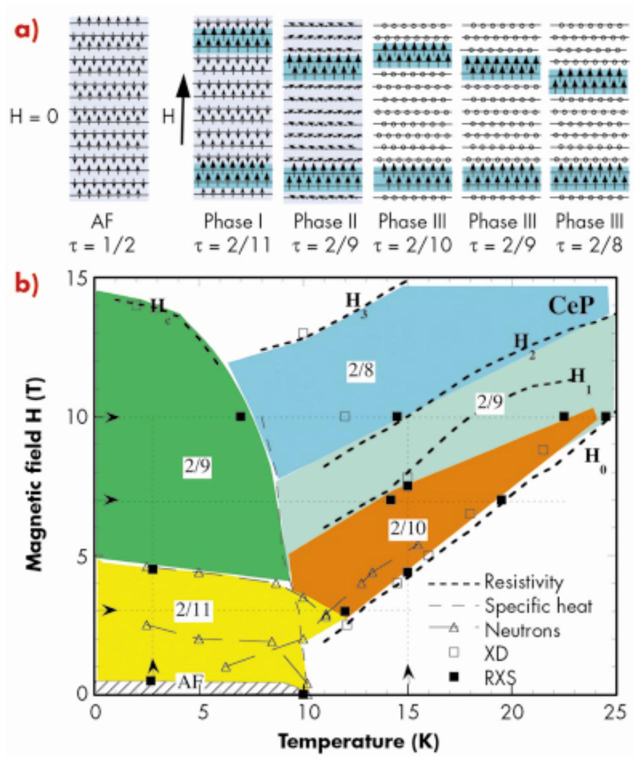
-Dimensionality effects are not described: absence of magnetism for d=1, $T_c$ = 0 for d=2 (Heisenberg case)- In MF $T_c$ is determined by z only

EuSe




HoMnO3




CeP

## Estimation of $T_C$

Mean field: $k_B T_C$ = $2zJ\ S(S+1)/3k_B$ for Heisenberg model
$zJ$ for Ising model

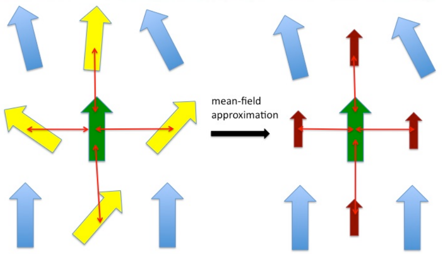
Real $T_c$ is always smaller (even 0 for some models)

$T_c$ for the Ising model:

**Table 5.2** Exact and approximate Curie temperatures for the Ising model (in units of $zJ/k_B$).

| lattice | $d$ | $z$ | mean-field | Oguchi | exact |
|---|---|---|---|---|---|
| linear chain | 1 | 2 | 1 | 0.782 | 0.000 |
| square | 2 | 4 | 1 | 0.944 | 0.567 |
| simple cubic | 3 | 6 | 1 | 0.974 | 0.752 |
| bcc | 3 | 8 | 1 | 0.985 | 0.794 |
| fcc | 3 | 12 | 1 | 0.993 | 0.816 |

Mean field is better if z is large!



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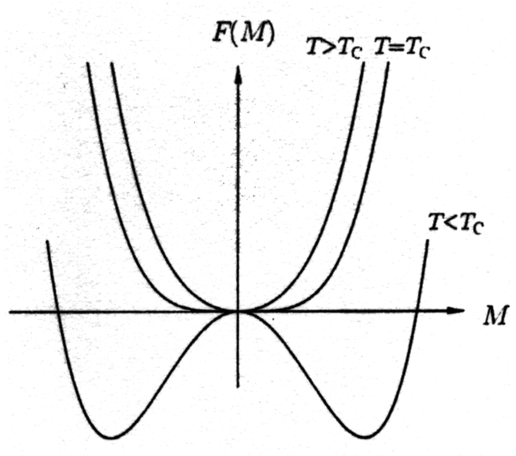
## Landau expansion for 2nd order phase transition

Free energy near $T_c$ can be expanded in powers of M:

$$F(M, h_{ext}, T) = F_0 + \frac{1}{2}aM^2 + \frac{1}{4}bM^4 + \frac{1}{6}cM^6 + \cdots - Mh_{ext}$$




- a, b and c can be calculated for each model (Heisenberg, Hubbard.... )

- They depend on the microscopic parameters: $J_{ij}$, U, band structure…

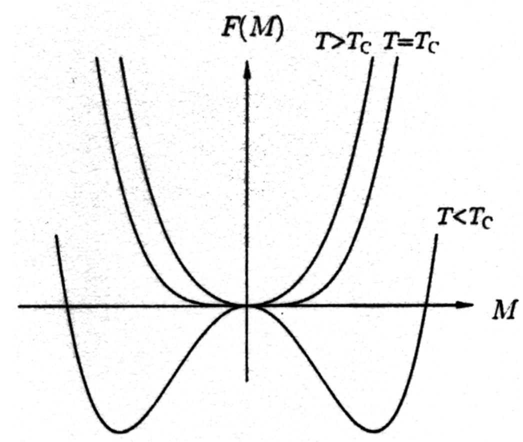
- They depend on temperature

⇒ magnetization, specific heat, susceptibility above $T_c$ can be obtained from F(M,H,T)

## Different situations depending on the coefficients (c >0)

$$F(M, h_{ext}, T) = F_0 + \frac{1}{2}aM^2 + \frac{1}{4}bM^4 + \frac{1}{6}cM^6 + \cdots - Mh_{ext}$$

Magnetization for $h_{ext}$=0 is determined by :




$$M(a + bM^2 + cM^4) = 0$$

1) a>0, and $b^2$ -4ac <0: M = 0
(no magnetic order)

2) a <0 (and $b^2$ -4ac >0): M ≠ 0

→ $T_c$ is determined by a($T_c$) = 0 ⇒ a = $a_0$ (T-$T_c$)

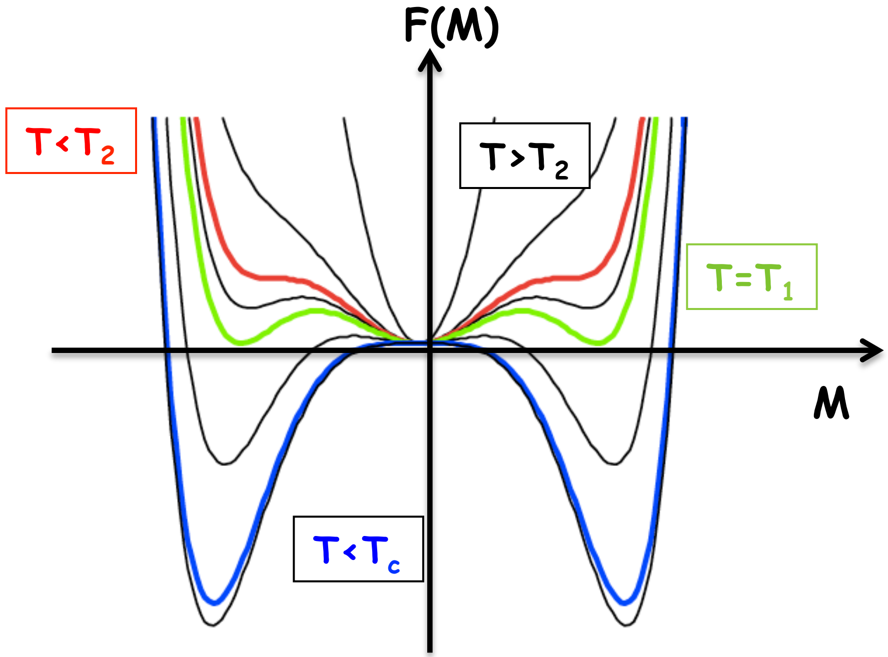
And M(T) = $(a_0/b)^{1/2}$ $(T_c-T)^{1/2}$

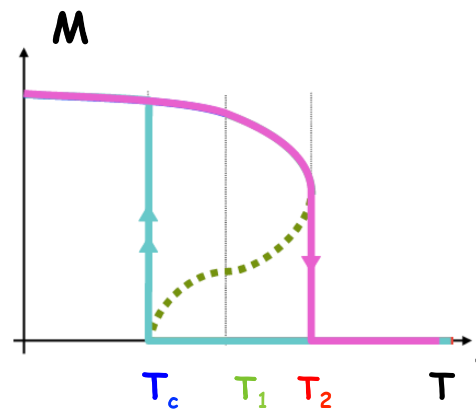
Above $T_c$: if $h_{ext}$≠ 0 , $h_{ext} = aM$

⇒ Curie Weiss law: M/$h_{ext}$ = 1/$a_0$ (T-$T_c$)

$$M(a + bM^2 + cM^4) = 0$$

a > 0 and $b^2$ -4ac >0 : 1st order transition is possible




$T<T_2$: 2 minima M=0 and M=m; F(m) > F(0) ⟶ stable minimum for M=0

$T=T_1$: F(m)=F(0)

$T<T_1$: 2 minima but F(m)<F(0) ⟶ stable solution M= m

$T<T_c$ : 1 minimum m (a changes sign at $T_c$)

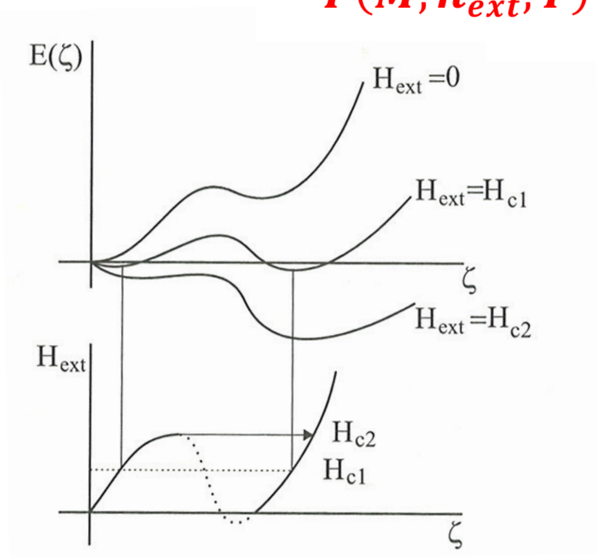
Transition occurs at $T_1$ (> $T_c$) – 2 minima for $T_c<T<T_1$

Hysteresis for $T_c<T<T_1$

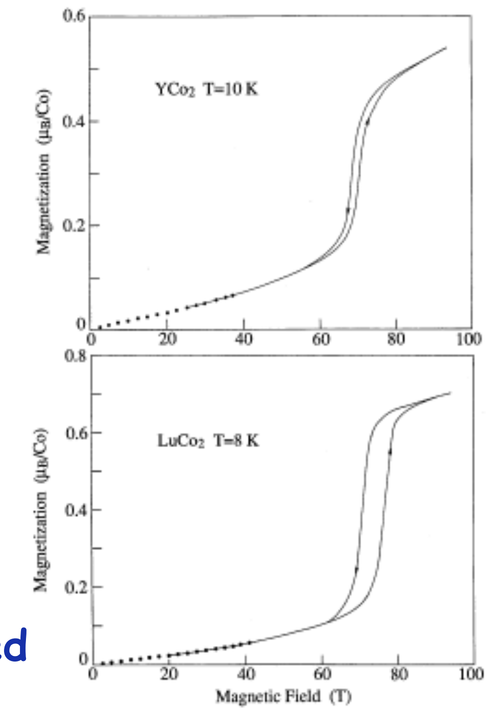
1st order transition under magnetic field: <u>metamagnetism</u>

Occurs if $a > 0$ and $b^2 - 4ac > 0$

$$F(M, h_{ext}, T) = F_0 + \frac{1}{2} a M^2 + \frac{1}{4} b M^4 + \frac{1}{6} c M^6 + \cdots - M h_{ext}$$




$\Rightarrow$




This may occur if the Fermi level is located in a minimum of DOS

# Thermodynamic properties within Landau theory

$$F(M,h_{ext},T) = F_0 + \frac{1}{2}aM^2 + \frac{1}{4}bM^4 + \frac{1}{6}cM^6 + \cdots - Mh_{ext}$$

If $a = a_0 (T - T_c)$

Near $T_c$: $M \propto (T-T_c)^{1/2}$ $(T<T_c)$ , $\chi \propto 1/((T_c-T)$ $(T>T_c)$

Specific heat jump at $T_c$: $a_0 T_c / b$

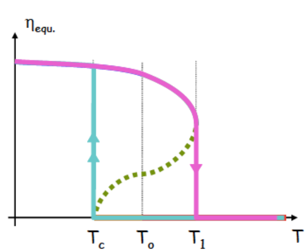
At $T_c$ $M \propto {h_{ext}}^{1/3}$

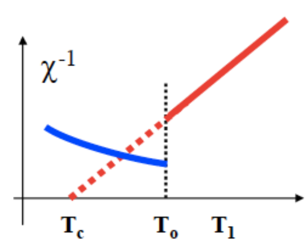
Critical exponents

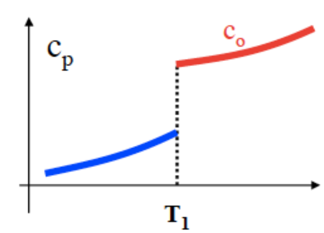
$\beta = \frac{1}{2}$, $\gamma = 1$, $\alpha = 0$, $\delta = 3$

➔ Mean field exponents

1st order transition: discontinuity of M, susceptibility, specific heat



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# Improving the mean field approximation: Ginzburg_Landau theory

In Landau theory M(T) =0 at $T>T_c$

But near $T_c$, large fluctuations of M ($\langle M \rangle = 0$ , but $\langle M^2 \rangle \neq 0$)

Ginzburg-Landau theory: takes into account spatial fluctuations of M

M ➔ M(r)

Ginzburg-Landau free energy:

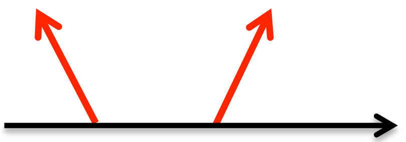
$$F(M, h_{ext}, T) - F_0 = \iiint d^3r \left(\frac{1}{2} aM(r)^2 + \frac{1}{4} bM(r)^4 + + \frac{1}{2} g\left|\vec{\nabla} M(r)\right|^2 - M(r)h_{ext}\right)$$

If $M(r)=M_0+m(r)$ with $m(r) \ll M_0$,

$$\Delta F = \sum_{q \neq 0} \left(gq^2 + a + 3bM_0{}^2\right)\left|m_q\right|^2$$

## Why a $(\nabla M)^2$ contribution?

If variation of M(r) is « smooth »:




$S_iS_j = S^2 \cos(\theta_i - \theta_j) \approx S^2(1 - (\theta_i - \theta_j)^2/2)$

Contribution to exchange energy:

$$J(R_i - R_j)S^2\,(\theta_i - \theta_j)^2/2 \approx A\,(\partial\theta/\partial x)^2$$ in the continuum limit

If $M(r) = M_0\,(\cos\theta(x), \sin\theta(x), 0)$ (1D model)

$\Rightarrow \nabla M = M_0\,\partial\theta/\partial x\,(-\sin\theta(x), \cos\theta(x), 0)$ and $(\nabla M)^2 = M_0{}^2\,(\partial\theta/\partial x)^2$

The $(\nabla M)^2$ is justified if spatial fluctuations are small

Fourier transform: $M(r) = \sum_q M(q)e^{iqr} \Rightarrow \vec{\nabla}M(r) = \sum_q qM(q)e^{iqr}$

# Improving the mean field approximation: Ginzburg_Landau theory

In Landau theory M(T) =0 at $T>T_c$

But near $T_c$, large fluctuations of M ($\langle M \rangle = 0$ , but $\langle M^2 \rangle \neq 0$)

Ginzburg-Landau theory: takes into account spatial fluctuations of M

M ➔ M(r)

Ginzburg-Landau free energy:

$$F(M, h_{ext}, T) - F_0 = \iiint d^3r \left(\frac{1}{2} a M(r)^2 + \frac{1}{4} b M(r)^4 + + \frac{1}{2} g \left|\vec{\nabla} M(r)\right|^2 - M(r) h_{ext}\right)$$

If $M(r)=M_0+m(r)$ with $m(r) \ll M_0$,

$$\Delta F = \sum_{q \neq 0} \left(g q^2 + a + 3 b {M_0}^2\right) \left|m_q\right|^2$$

Additional contribution to the free energy $\Delta F = \sum_{q \neq 0} (gq^2 + a + 3bM_0{}^2)|m_q|^2$

→ contribution to susceptibility, specific heat … $\Delta C_v \propto (T-T_c)^{-1/2}$

Correlation length ξ

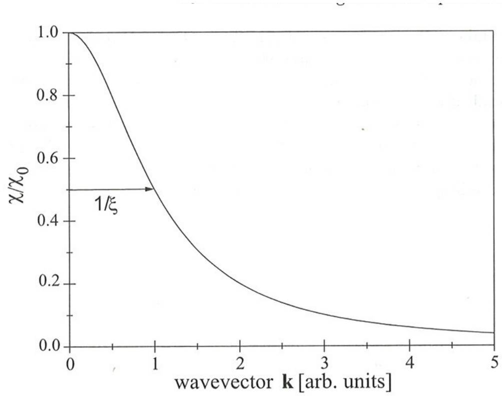
$$\langle |m_q|^2 \rangle \propto \frac{kT}{q^2 + 1/\xi^2} \quad \text{with} \quad \xi \propto \sqrt{\frac{gT_c}{T - T_c}}$$

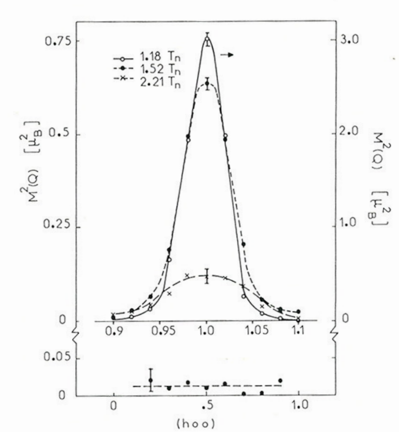
(Orstein-Zernike Critical exponent ν=1/2)

in real space: $\langle m(r).m(r') \rangle \propto exp(-(r-r')/\xi)$

Small q fluctuations are large

q=0 fluctuations and correlation length diverge at $T_c$




ξ can be measured with neutrons

Landau Ginzburg: spatial fluctuations (Landau Lifhitz Gilbert: dynamic)

Valid only if : $1 >> |T-T_c|/T_c >> AT_c^2$ (Ginzburg criterion)

Near $T_c$: better description of critical behavior.

→ Description of phase transitions: sophisticated techniques (renormalization group) – Universality of the critical behavior at 2nd order phase transitions

Define the order parameter M

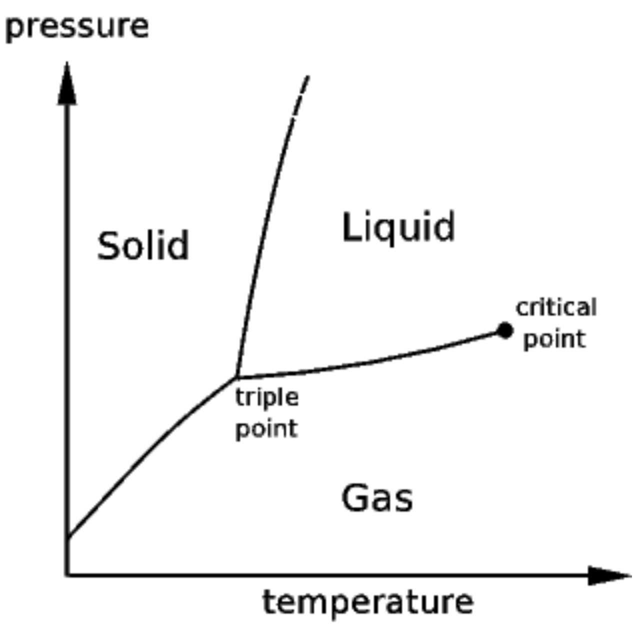
if $t = (T-Tc)/Tc$, and $h = \mu H/kTc$

| | values in M. F. approximation |
| --- | --- |
| $M(T) \sim t^{\beta}$ (h=0) | $\beta=1/2$ |
| $M(h) \sim h^{1/\delta}$ (t=0) | $\delta = 3$ |
| $\chi(T) \sim t^{-\gamma}$ | $\gamma = 1$ |
| $\zeta(T) \sim t^{-\nu}$ | |
| $C(T) \sim t^{-\alpha}$ | $\alpha = 0$ |
| $S(k) \sim k^{-2+\eta}$ (t=0) | |

# Outline

- The Heisenberg model in molecular field approximation
- Landau theory of phase transitions
- Beyond mean field:
  - Magnons (spin waves)
  - Ginzburg-Landau theory
  - Critical behavior
  - Role of dimensionality: 1D and 2D systems

# Magnetic transition is an example of phase transitions

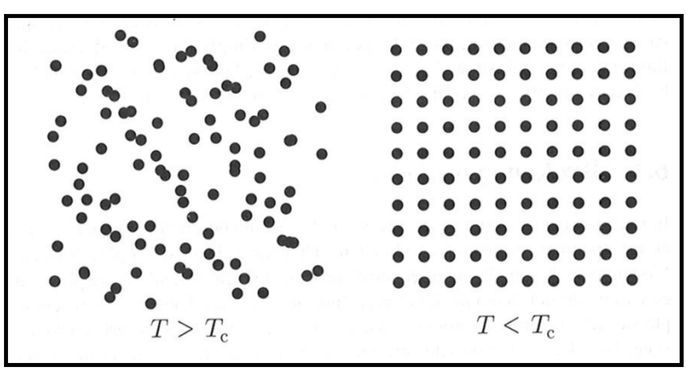


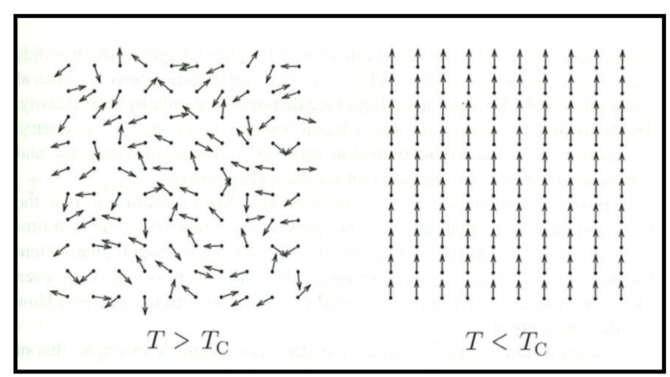

-Liquid-solid transition: spontaneous symmetry breaking at $T_c$

-Order parameter (spatial)

-A liquid has more symmetries than a solid: complete translational and rotational invariance

-Para-ferromagnetic transition is similar



## Different types of phase transitions:

| Phenomenon | High $T$ Phase | Low $T$ Phase | Order parameter | Excitations | Rigidity phenomenon | Defects |
|---|---|---|---|---|---|---|
| crystal | liquid | solid | $\rho_{\mathbf{G}}$ | phonons | rigidity | dislocations, grain boundaries |
| ferromagnet | paramagnet | ferromagnet | $\mathbf{M}$ | magnons | permanent magnetism | domain walls |
| antiferromagnet | paramagnet | antiferromagnet | $\mathbf{M}$ (on sublattice) | magnons | (rather subtle) | domain walls |
| nematic (liquid crystal) | liquid | oriented liquid | $S = \langle \frac{1}{2}(3\cos^2\theta - 1)\rangle$ | director fluctuations | various | disclinations, point defects |
| ferroelectric | non-polar crystal | polar crystal | $\mathbf{P}$ | soft modes | ferroelectric hysteresis | domain walls |
| superconductor | normal metal | superconductor | $\|\psi\|e^{i\phi}$ | – | superconductivity | flux lines |

# Critical exponents

they depend on

- the model (Heisenberg, X-Y, Ising…)
- the dimensionality of the system

$$M(T) \propto (T_c - T)^{\beta} \;, \propto \chi(T) \propto (T - T_c)^{-\gamma}$$

| | D=1 | D=2 | D=3 | Mean field |
|---|---|---|---|---|
| Heisenberg | No ordering | No ordering | 0.36, 1.39 | $\beta = 1/2$<br>$\gamma = 1$ |
| X-Y | No ordering | **Kosterlitz-Thouless**<br>$\chi \sim \exp(a/t^{1/2})$ | γ<br>0.35, 1.32 | $\beta = 1/2$<br>$\gamma = 1$ |
| Ising | $T_C = 0$<br>$\chi \sim \exp(-a/T)$ | 1/8, 7/4 | 0.32, 1.24 | $\beta = 1/2$<br>$\gamma = 1$ |

$$\alpha + 2\beta + \gamma = 2 \;;\; D\nu = 2 - \alpha$$

## Critical exponents

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- the dimensionality of the system

$$M(T) \propto (T_c - T)^{\beta} \quad , \propto \chi(T) \propto (T - T_c)^{-\gamma}$$

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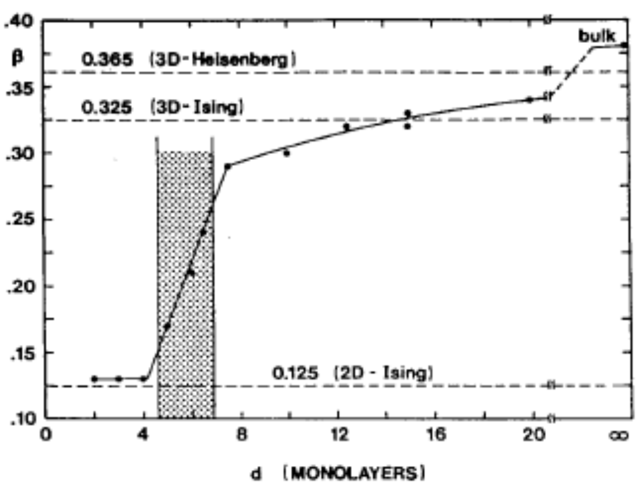
| Ising | $T_C = 0$<br>$\chi \sim \exp(-a/T)$ | 1/8, 7/4 | 0.32, 1.24 | |

Deviations from mean field indicate short range correlations near $T_c$

# Comparison with experiments

| | Mean field | Experiment | 2D Ising | 3D Ising | 3D Heisenberg |
|---|---|---|---|---|---|
| $\chi(T) \propto (T-T_C)^{-\gamma}$ | 1 | 1.3–1.4 | 7/4 | 1.24 | 1.39 |
| $M(T) \propto (T_C-T)^{\beta}$ | 1/2 | $\approx 1/3$ | 1/8 | 0.324 | 0.362 |
| $C(T) \propto \lvert T-T_C \rvert^{-\alpha}$ | 0 | −0.1–0.1 | log | 0.110 | −0.115 |
| $M(B, T=T_C) \propto \lvert B \rvert^{1/\delta}$ | 3 | $\approx 5$ | 15 | 4.82 | 4.82 |

## Critical exponents depend on the dimensionality




critical exponenent β in thin Ni films on W:

- at 6 monolayers transition from 2- to 3-dimensional behavior
- crossover from Ising to Heisenberg due to anisotropy

**(K. Baberschke)**

(K. Baberschke)

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## Improving mean field at low T: spin waves

**1 dimensional model with ferromagnetic nearest neighbor exchange**

$$H = -2\sum_i J\,\vec{S}_i.\vec{S}_{i+1} = -2J\sum_i S_i^z S_{i+1}^z - J\left(\sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)$$

Ground state: ↑↑↑↑↑ Energy: -NJ/2

Excited state
with 1 reversed spin ↑↑↓↑↑ Not an eignenstate of H
(eigenstate of $-2J\sum_i S_i^z S_{i+1}^z$)

$\Psi_i$: wave function with spin reversed on site i

$$-J\left(\sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)$$

➔ The spin flip will propagate on sites i-1 and i+1

$$H\psi_i = -J(\Psi_{i-1} + \Psi_{i+1}) + (-NJ/2 + J)\,\Psi_i$$

$$H\,\psi_i = -J(\Psi_{i-1} + \Psi_{i+1}) + (-NJ/2 + J)\,\Psi_i$$

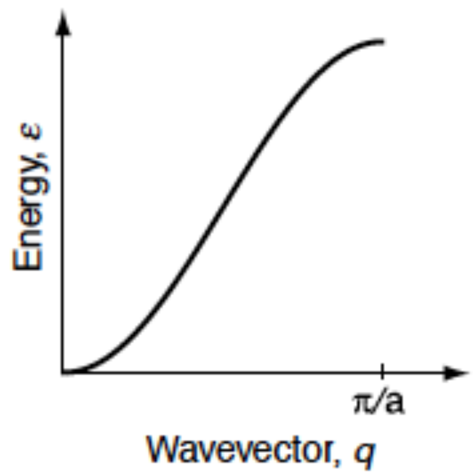
Fourier transform: $\Psi(q) = \sum \exp(iqR_i)\,\Psi_i$

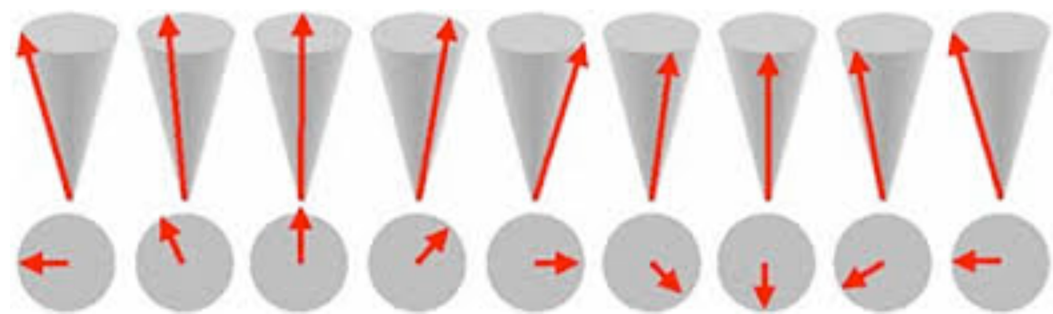
$$H\,\Psi(q) = -NJ/2\,\Psi(q) + J(1-\cos qa)\,\Psi(q)$$

This is an eigenstate (no longer true for states with more spin flips)

Excitation energy: $E(q) = J(1-\cos qa) \approx Ja^2/2\;q^2$

Low energy excitations



$$\langle \vec{S}_i . \vec{S}_{i+1} \rangle \propto \cos qa$$

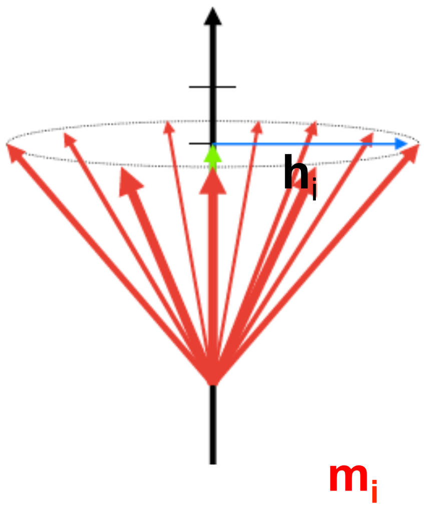
# « Classical » spin waves

Local field $h_i$ on each site: $h_i = J(m_{i-1} + m_{i+1})$

Moment on site i: precession in field $h_i$

$dm_i/dt = -\gamma m_i \times h_i$ ($\gamma$ gyromagnetic factor)

$dm_i/dt = -\gamma J\, m_i \times (m_{i-1} + m_{i+1})$




1. Fourier transform (time and space) → $m_i(t) = m_0\, e^{i\omega t}\, e^{iqR}$
2. Linearization of dm/dt
3. Similar to previous approach $\omega(q) = \gamma J(1-\cos qa)$

## Spin waves in antiferromagnets

$$H = -2\sum_i J\,\vec{S}_i\cdot\vec{S}_{i+1} = -2J\sum_i S_i^z S_{i+1}^z - J\left(\sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)$$

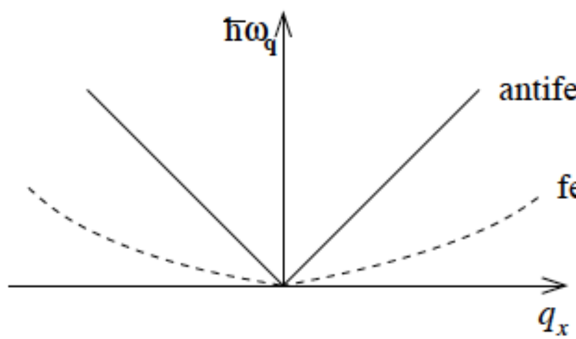
↓↑↓↑↓↑↓ **Not an eigenstate**

$$S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+$$

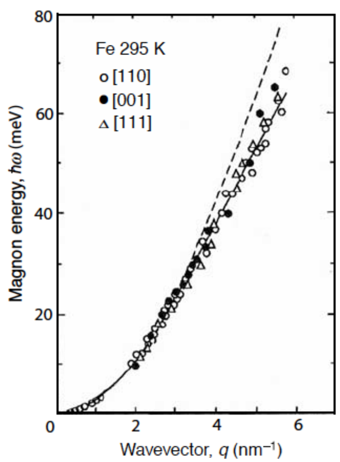
↓↑ ➡ ↑↓

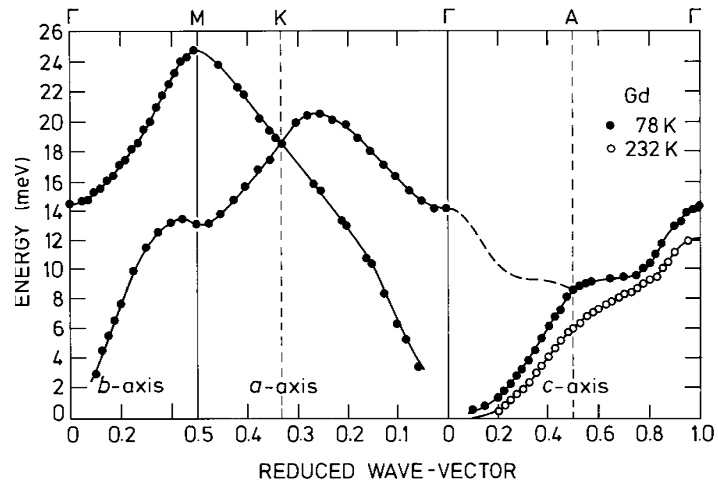
**More complicated calculations**

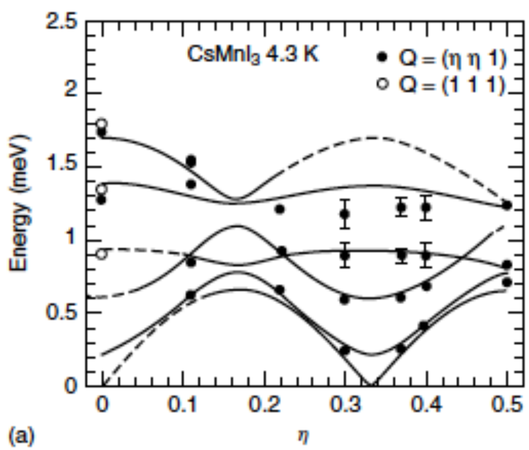
**E(q) = J|sinqa|**



# Examples of spin wave spectra (inelastic neutrons)



# Magnons: low T properties

In ferromagnets:at low k: $E(k) \approx zJM\,S(ka)^2 = k^2$

In antiferromagnets: $E(k) \approx zJM\,ka$

Magnetization at low T : $M(T) = M_0$ – number of excited magnons

Magnons obey Bose-Einstein statistics $N_{sw} = \sum_k < n_k > = \sum_k \frac{1}{e^{E(k)/T} - 1}$

$$\langle S \rangle \approx S - \sum_k n_B(\omega_k) \qquad \sum_k \longrightarrow \int dk^d = \int dk \, \frac{k^{d-1}}{(2\pi)^d}$$

At low T, in 3D systems: <u>for a ferromagnet:</u> $M(T) = M_0 - A(k_B T/D)^{3/2}$

for AF (sublattice magnetization): $M(T) = M_0 - B(kT/C)^2$

(mean field $\exp(-A/k_B T)$)

Estimation of $T_c$ from spin waves:

$$\langle S \rangle \approx S - \sum_k n_B(\omega_k)$$

$T_c$ is determined by, <S> =0 → value for $T_c$ smaller by a factor 10 compared to mean field ($2zS(S+1)/3k_B$)

Specific heat: magnons contribute to energy

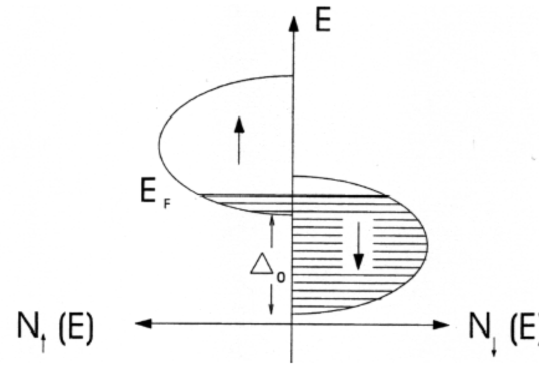
$\Delta E = \sum \omega_k n_B(\omega_k) \rightarrow C_v \propto T^2$ (Ferro) or $T$ (AF)

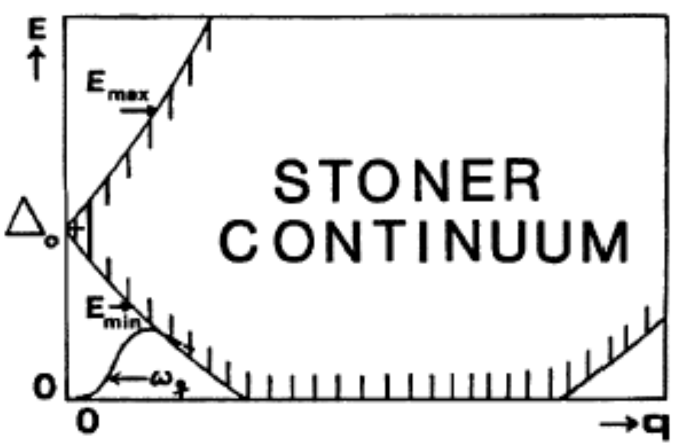
(mean field: $\exp(-A/k_BT)$)

## Spin waves also exist in itinerant ferromagnets:

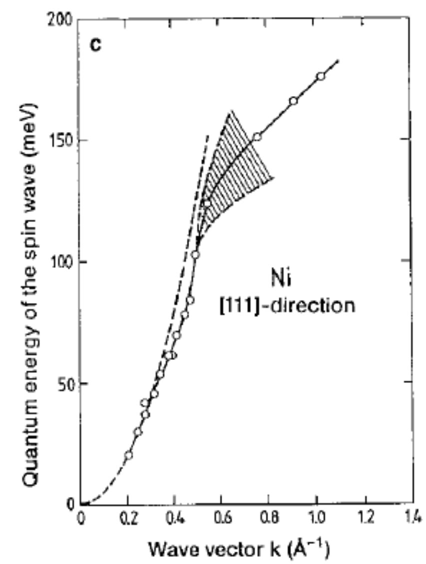
2 types of excitations:

- Stoner excitations: transition from a filled ↑ state to an empty ↓ state: gap Δ at q=0;
- Collective excitations: spin waves




Magnetic excitations in Ni ($\Delta_0 \approx 100$meV)



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## Dimensionality effect

$$\langle S \rangle \approx S - \sum_k n_B(\omega_k) \qquad \sum_k \longrightarrow \int dk^d = \int dk \, \frac{k^{d-1}}{(2\pi)^d}$$

In ferromagnets: $\omega_k = Dk^2$

$$\int \frac{q^{d-1}}{exp(Dq^2/k_BT) - 1} \qquad \text{becomes } (x=Dq^2/kT): \qquad T^{d/2} \int \frac{x^{d/2-1}}{exp(x) - 1} dx$$

At T≠0 integral is divergent for d=1 or 2

➔ No ferromagnetism in 1 and 2 dimensions at T>0

In AF: $\omega_k = Ck$ : integral is divergent in 1 dimension

Mermin-Wagner theorem: For Heisenberg model, no long range order in 1 and 2 dimensional systems at $T>0$

- Magnetism is possible at $T=0$

- Valid only in the absence of anisotropy

Anisotropy may stabilize ferromagnetism in 2-D systems
(surfaces and thin films)

Mermin-Wagner theorem does not apply to Ising or XY models

## Heisenberg spins with anisotropy

Uniaxial anisotropy: $-KS_i^{z^2}$

easy axis: K > 0: spin wave gap at 0°K $\varepsilon(k) = 2S[J(0) - J(q) + K]$

Variation of magnetic moment at T ≠ 0: M(T)-M(0) = $N_{SW}$

In 2D; no divergence of NSW: at low T: $N_{SW} \propto T\exp\left(-\frac{A}{T}\right)$

Easy plane anisotropy: K<0 $\varepsilon(k) = \sqrt{Dk^2(Dk^2 + 2|K|} \propto k$

No spin gap; $N_{SW}$ is divergent at finite T. Order at T=0?

Anisotropy may stabilize ferromagnetism in 2-D systems

Ising model in 1D systems (Mermin-Wagner does not apply)

$$H = -\sum_{i,j} J_{ij} S_i \, S_j$$ with $S_i = \pm 1$

Describes many physical situations: A-B alloy, magnetic system with infinite uniaxial anisotropy, lattice-gas transition ….

Ising chain: $H = -\sum_{i=1}^{N-1} J_i \, S_i \, S_{i+1}$ Exactly solvable $Z_N(T) = 2^N \prod_{i=1}^{N-1} \cosh\left(\frac{J_i}{k_B T}\right)$

No phase transition: F=U-TS

U is minimized if all spins are aligned: ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ U=NJ, S=0

1 defect: ↑ ↑ ↑ ↑ ↑ ↑ ↓ ↓ ↓ ↓

Energy cost: $\Delta U = 2J$, $\Delta S = k\ln\Omega = k\ln N$ $\Delta F = 2J - kT\ln N$

if T≠0, defects are alsways favored by entropy ➡ no order (in 2D $T_c \neq 0$)

## Examples of 2D systems:

- Compounds with in-plane interactions >> interplane interactions

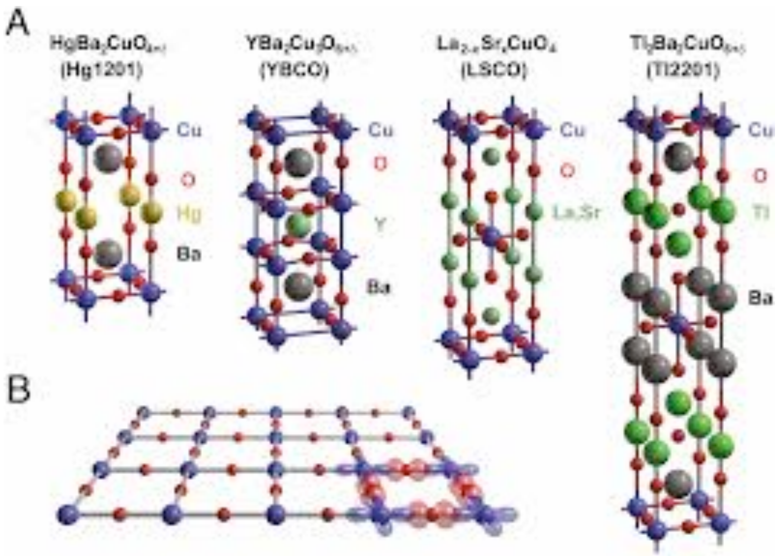
examples: $La_2CuO_4$……

- Ultrathin films : 2d character if
  - $d < 2\pi/k_F$ 0.2 -2 nm
  - d<exchange length: depends on the nature of exchange: 0.2 – 10 nm

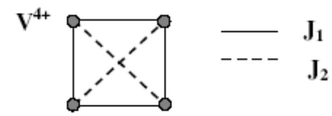
- Surfaces of bulk materials

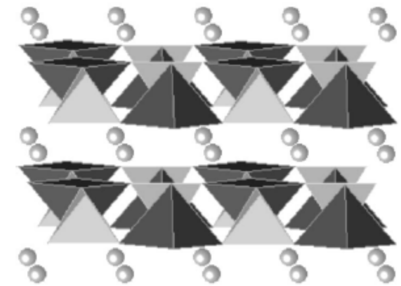
- Superlattices F/NM: interlayer interactions

# Some low dimensional systems



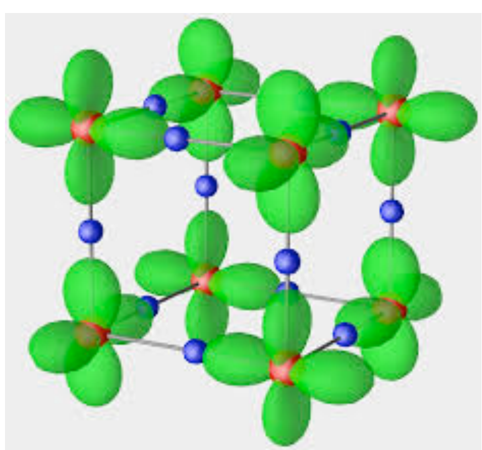

cuprates



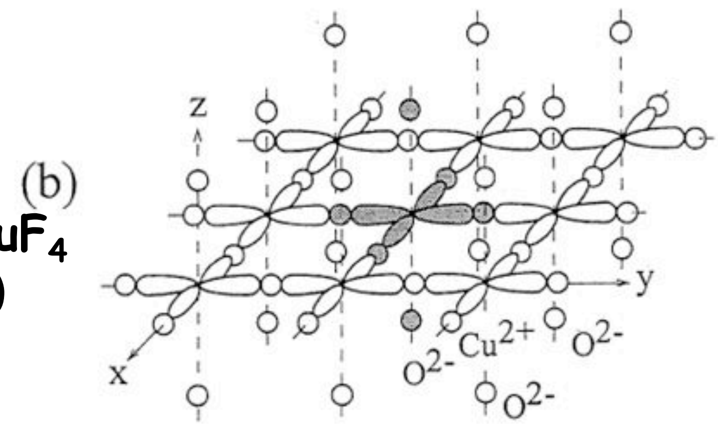



$Li_2VO(Si,Ge)O_4$

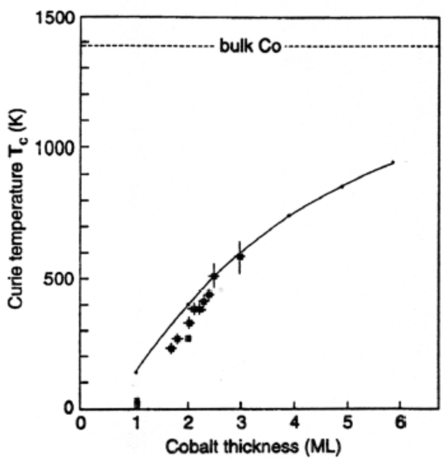
$KCuF_3$
(1D)



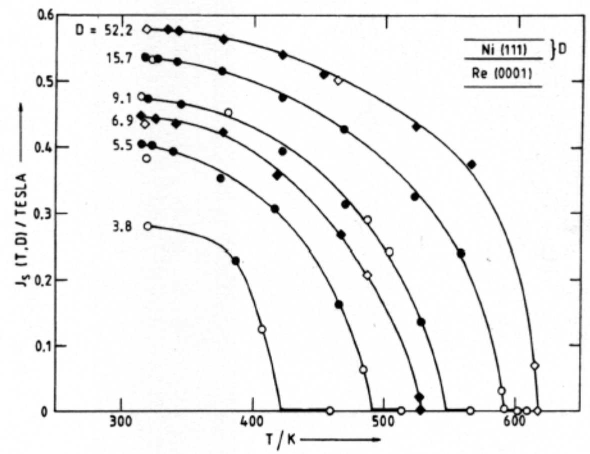
$K2CuF_4$
(2D)



# Reduction of Curie temperature




$T_c$ for Co thin films

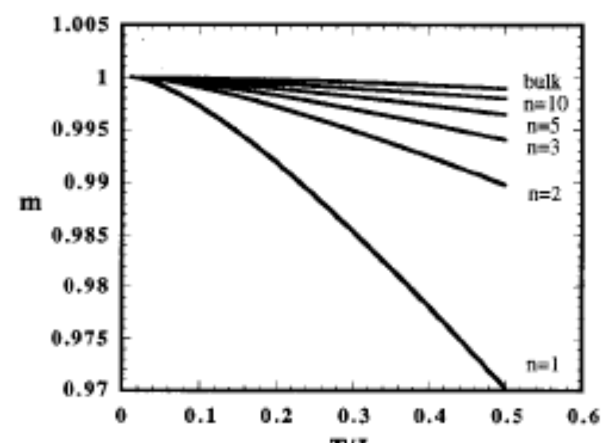



Magnetization of Ni films

In 2D: - no order if no anisotropy

- with anisotropy: reduced $T_c$

(reduction of nb of nearest neighbors )




M(T) for different thickness (theory)

## From 3D to 2D behavior:

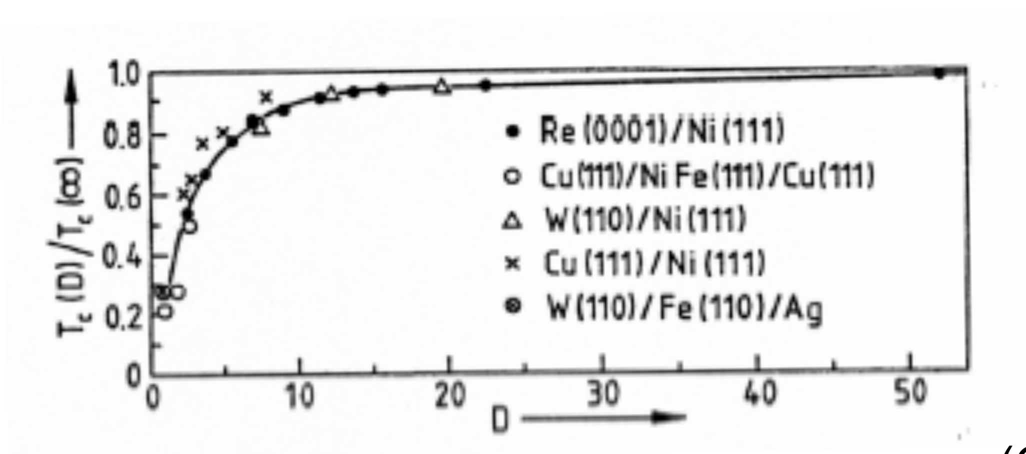
- In 3D systems correlation length diverges at Tc: $$\xi = \xi_0 \left| \frac{T - T_C}{T_C} \right|^{-\nu}$$

- Crossover from 2D to 3D when the thickness $d \approx \xi$

- Asymptotic form for Tc:

$$\frac{T_C(\infty) - T_C(d)}{T_C(d)} = \left( \frac{d}{\xi_0} \right)^{-\frac{1}{\nu}}$$

**(Heisenberg: $\nu$= 0.7  Ising: 0.6)**




**Experimentally: $\nu \approx 0.7$**
**Close to Heisenberg**

(Gradmann, 1993)

## Summary

-Mean field approximation is easy to handle. Allows to compare easily different types of orderings

-In many cases (3D systems) is gives the correct qualitative ground state

-Temperature variation:

- at low T: spin waves
- $T_c$ too large, critical exponents not correct (short range fluctuations)

- Mean field wrong in low dimension systems

## Some general reference books

S. Blundell: Magnetism in Condensed Matter (Oxford University Press, 2001)
J.M.D. Coey: Magnetism and Magnetic materials (Cambridge University Press 2009)
R. Skomski: Simple models of Magnetism (Oxford University Press, 2008)

## More advanced books

D.I. Khomskii: Basic aspects of the quantum theory of magnetism (Cambridge University Press 2010) (in particular: Phase transitions, Landau and Ginzburg Landau theory, magnons)
N. Majilis: The quantum theory of magnetism (World scientific 2007) (in particular Molecular field approximation, magnons
P. Mohn: Magnetism in the solid state (Springer, 2006) (most devoted to itinerant magnetism; see also J. Kübler in 'Handbook of Magnetism and Magnetic materials', vol1 )
D.P. Landau: Phase transitions in 'Handbook of Magnetism and Magnetic materials', vol1 (Wiley 2007)
I.A. Zaliznyak: Spin waves in bulk materials in 'Handbook of Magnetism and Magnetic materials', vol1 (Wiley 2007)