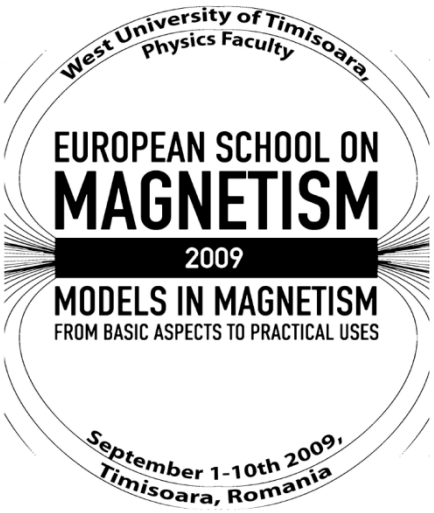
Magnetism at finite temperature: molecular field, phase transitions

-The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

- Mean field for itinerant systems

- Landau theory of phase transitions

- Beyond mean field:
critical exponents
spin waves
Dimensionality effects: absence of phase transition in 1D and 2D models



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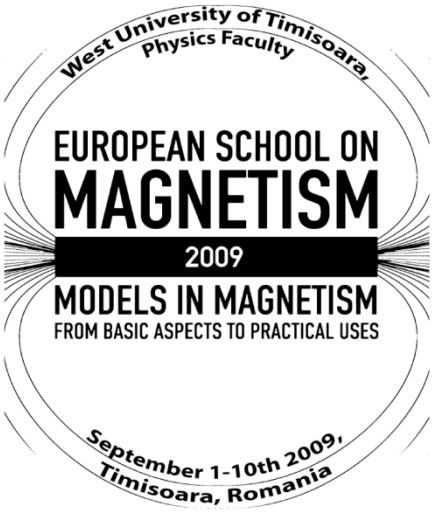


What is mean field approximation?

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

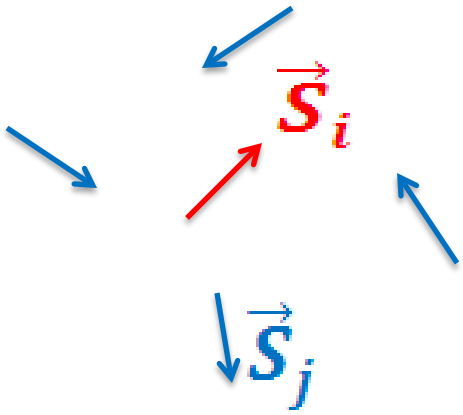
Where the function g is
-the Brillouin function (quantum case)
- or the Langevin function (classical spins)

Heisenberg model: $H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$

Main assumption: $\vec{S}_i$ **is replaced by its average** $\langle \vec{S}_i \rangle$

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \quad \Rightarrow \quad \tilde{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \langle \vec{S}_j \rangle$$

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



$$\tilde{H} = \sum_{ij} J_{ij} \ \vec{S}_i . \langle \vec{S}_j \rangle$$

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

$$\vec{H}_i = \sum_j J_{ij} \ \langle \vec{S}_j \rangle$$

If there is also an external field: $\vec{H}_i = \sum_j J_{ij} \ \langle \vec{S}_j \rangle + \vec{H}_{ext}$

$$M = M_0\, g\left(\frac{\mu H}{kT}\right) \quad \Rightarrow \quad M_i = M_0\, g\left(\frac{\mu H_i}{kT}\right)$$

$$\vec{H}_i = \sum_j J_{ij}\ \langle \vec{S}_j \rangle + \vec{H}_{ext}$$

H_i is a local field due to

-the interaction with neigboring spins (« molecular field »)

-the external field

In a ferromagnet: $\langle \vec{S}_j \rangle$ is constant: $\langle \vec{S}_j \rangle = M/g\mu_B$

⇒ molecular field is the the same on all sites:

$$\vec{H}_{ferro} = \vec{M} \sum_j J_{ij} + \vec{H}_{ext}$$

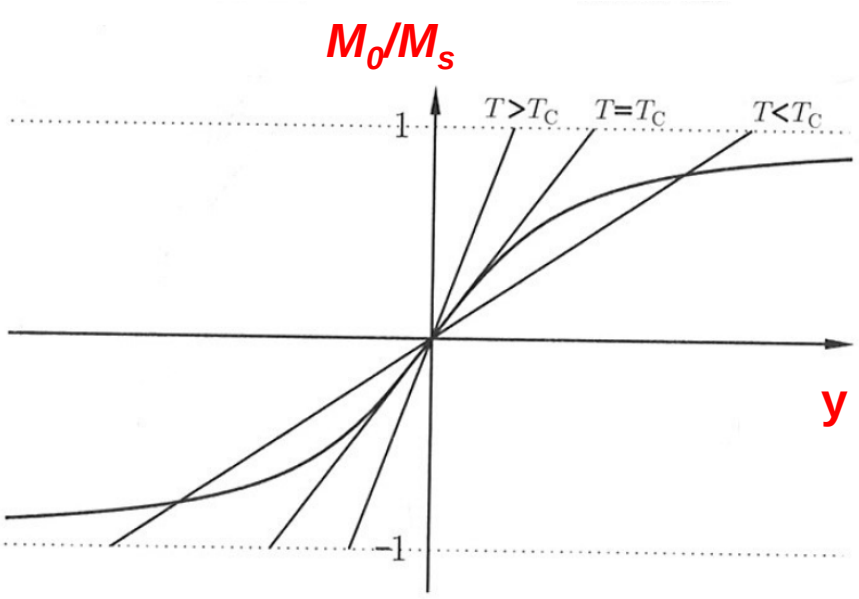
Solution of the mean field equation: $M_i = M_0\, g\left(\frac{\mu H_i}{kT}\right)$

In a ferromagnet:

$$M_i = M_0 = g\left(\frac{\mu(H + zJM_0)}{kT}\right)$$

(*g(x)* **is the Brillouin or Langevin function)**

H=0

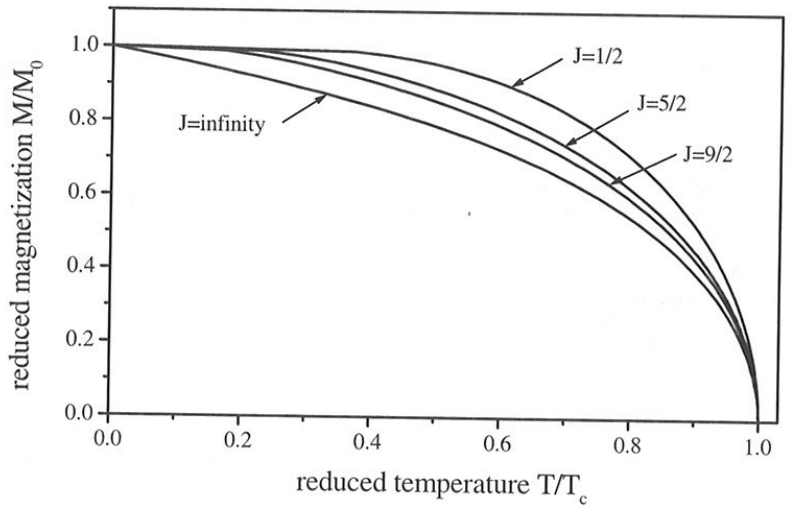


y = μ zJM$_0$/kT

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: $M(T) - M_0 \propto \exp(-2T_c/T)$
Near T_c: $M(T) \propto (T_c - T)^{1/2}$

Similar calculations for antiferromagnets, or longer range interactions

Thermodynamics of a ferromagnet in mean field approximation

-Calculate the partition function *Z* of the system: one spin in an effective field H_{eff} ($H_{eff} = H_{ext} + zJM_0$)

For S= ½:

$E_{\downarrow} = +g\mu_B H_{eff}/2$

$E_{\uparrow} = -g\mu_B H_{eff}/2$

$$Z = e^{-E_{\uparrow}/kT} + e^{-E_{\downarrow}/kT}$$

-Free energy: $F = -kT\,LnZ$

⇒ Susceptibility $\chi = -\partial^2 F/\partial H^2$

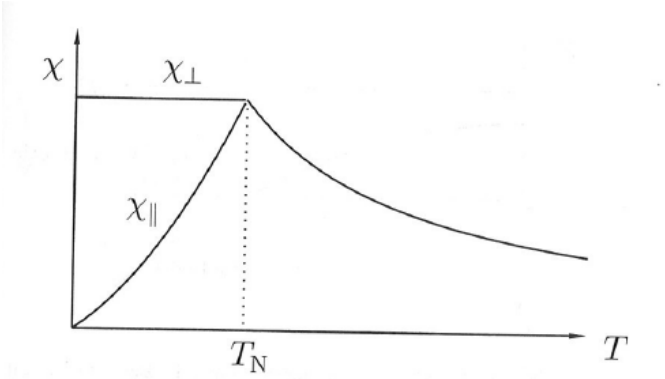
$$\chi = \frac{C}{T - T_c}, C = \frac{(g\mu_B)^2}{3k} S(S+1)$$

⇒ Curie –Weiss law above T_c:

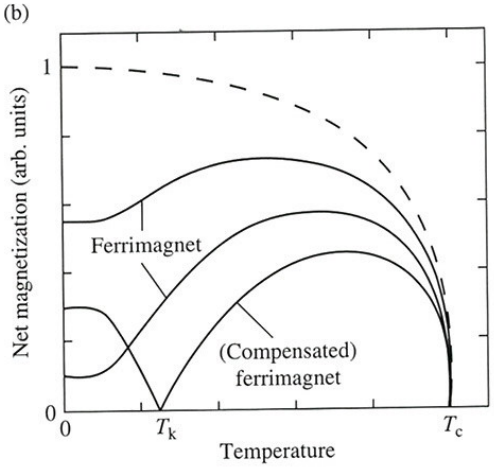
⇒specific heat: $C_v = -T\,\partial^2 F/\partial T^2$

⇒ Discontinuity at T_c : $\Delta C_v = 3k_B/2$

Same calculation can be done for an antiferrromagnet with 2 sublattices: H_i is site-dependent (H_A and H_B)



Also ferrimagnetism, helicoidal order, commensurate and incommensurate orderings…



Free energy and thermodynamics: F = free energy of a moment in an effective field

$$\vec{H}_i = \sum_j J_{ij} \langle \vec{S}_j \rangle + \vec{H}_{ext}$$

General case: - interactions J_{ij} between 1st, 2nd, 3rd ….
- Any kind of Bravais lattice (1 magnetic site per unit cell)

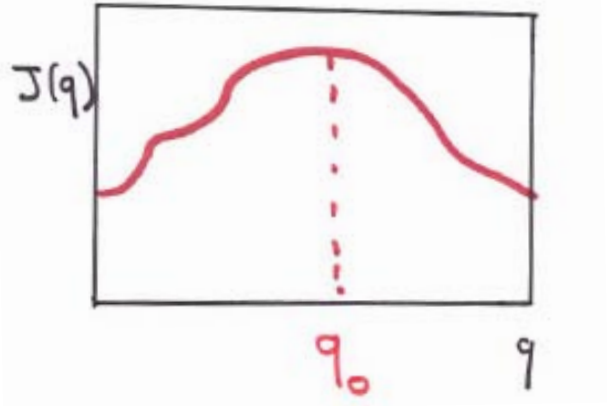
Energy: $$E = -\sum_{i,j} J(R_i - R_j)\langle \vec{S}_i . \vec{S}_j \rangle$$

In mean field approximation: $$E = -\sum_{i,j} J(R_i - R_j)\langle \vec{S}_i \rangle . \langle \vec{S}_j \rangle$$

Fourier transforms: $$J(q) = \frac{1}{N}\sum_{j} e^{iq(R_i - R_j)} J(R_i - R_j)$$

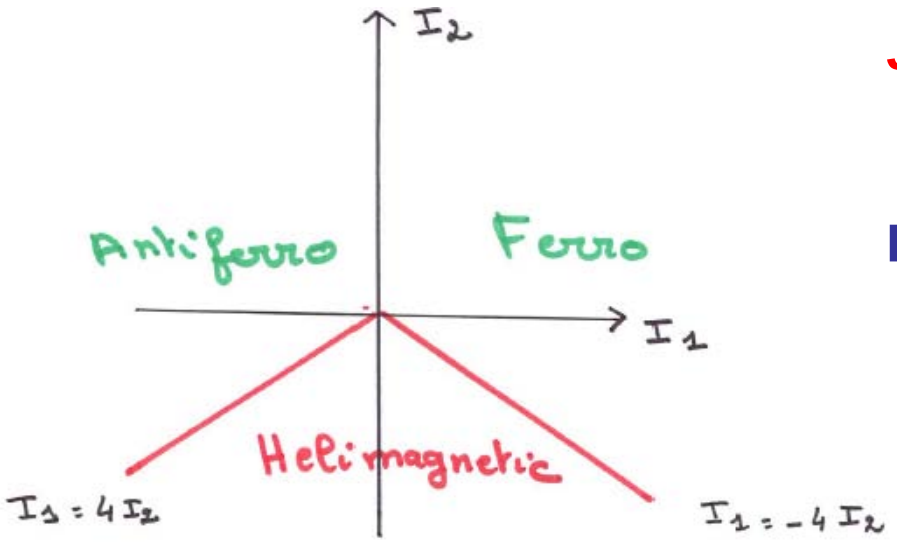
$$\vec{S}(q) = \frac{1}{N}\sum_{i} \langle \vec{S}_i \rangle e^{iqR_i}$$

$$\Rightarrow \quad E = -\sum_{q} J(q) S(q) . S(-q)$$



Energy is minimum at q_0 for which J(q) is maximum

The phase diagram for the 1D chain:



$J(q) = - J_1 \cos qa - J_2 \cos 2qa$

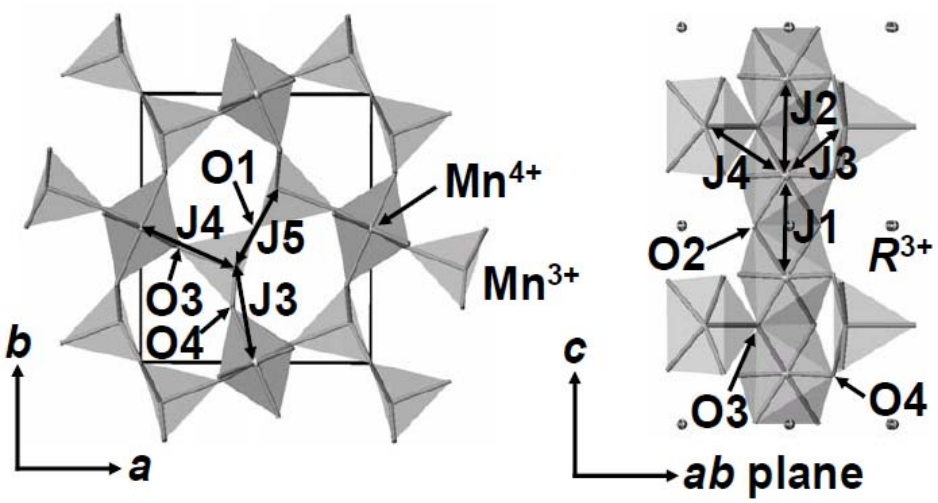
Extrema of J(q):

- q = 0 (ferro)
- $q = \pi/a$ (antiferro)
- $\cos qa = -J_1/4J_2$ (if $|J_1/4J_2| \leq 1$)

-The helimagnetic state is stabilized in the frustrated region ($J_2 < 0$)

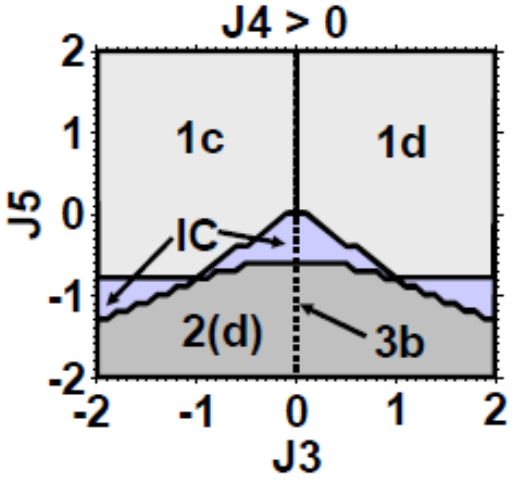
-It is in general incommensurate with the lattice periodicity

Example: multiferroics RMn_2O_5



4 commensurate structures

IC: incommensurate orderings



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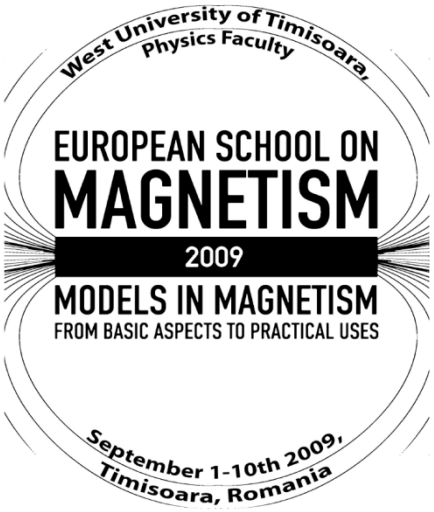
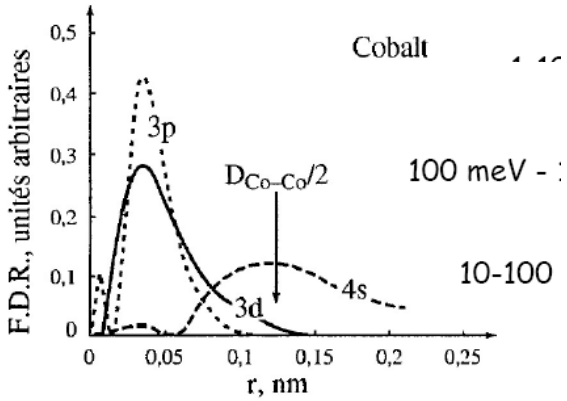


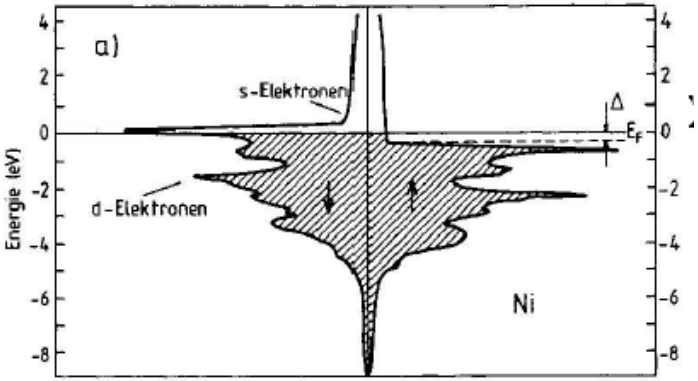
Itinerant magnetic systems



In 3d: overlap of 3d wave functions of nearest neighbors atoms: metallic systems

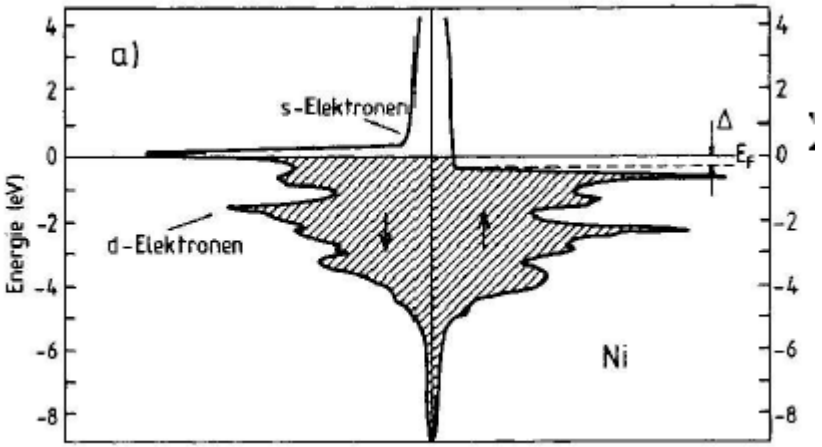
⇒Competition between magnetic and kinetic energy: itinerant magnetism

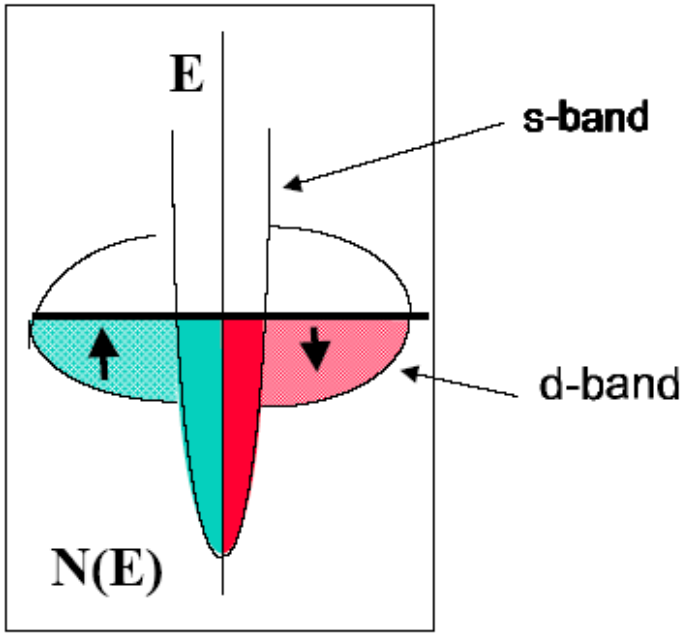
Itinerant spin systems: magnetic moment is due to electrons in partially filled bands (3d band of transition metals)



Magnetism of 3d metals: due to itinerant 3 d electrons

Band structure of Ni





d electrons form a narrow band (few eV)

Description of d electrons: Hubbard model

-band energy + Local Coulomb repulsion with U≈W (few eV)

$$\sum_{k\sigma} \varepsilon_k n_{k\sigma} \qquad U n_{i\downarrow} n_{i\downarrow}$$

(+ longer range interactions)

One band : degeneracy of the 3d band neglected

Coulomb repulsion: electrostatic interactions between electrons $V(r) = -\frac{e^2}{r}$

In solids this interaction is screened by the other charges:

$$V(r) = -\frac{e^2\, exp(-qr)}{r}$$

In metals 1/q is very small (< interatomic distance). ⇒ Only short range interactions are important

Local Coulomb repulsion: $Un_{i\uparrow}n_{i\downarrow}$

Hubbard model: $H = \sum_{k,\sigma} \varepsilon_k\, n_{k,\sigma} + U \sum_i n_{i\uparrow}\, n_{i\downarrow}$

⇒ from Pauli paramagnet to itinerant magnet and localized magnetic systems with increasing U

Mean field approximation on the term $Un_{i\downarrow}n_{i\downarrow}$:

$$Un_{i\uparrow}n_{i\downarrow} = U/4(n_{i\uparrow}+n_{i\downarrow})^2 - U/4(n_{i\uparrow}-n_{i\downarrow})^2$$

1st term: $\frac{U}{4}(n_{i\uparrow}+n_{i\downarrow})^2 = \frac{U}{4}n_i{}^2$ **Charge fluctuations are small**

⇒ constant potential

2nd term: $-\frac{U}{4}(n_{i\uparrow}-n_{i\downarrow})^2 = -US_{iz}{}^2$

Mean field approximation on the 2nd term:

$-US_{iz}{}^2 \approx -2US_{iz} < S_{iz} > +U\langle S_{iz}\rangle^2$ **where** $S_{iz} = (n_{i\uparrow}-n_{i\downarrow})/2$

This 2nd term induces a spin-dependent potential on each site:

$$V_{i\sigma} = -\sigma U/2\langle n_{i\uparrow}-n_{i\downarrow}\rangle$$

Itinerant ferromagnetism: Stoner model at T=0

Description of 3d metals: narrow band + Coulomb interactions

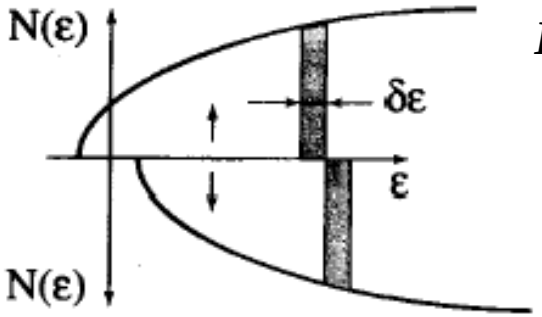
Local Coulomb repulsion: $Un_{i\uparrow}n_{i\downarrow}$

U favors magnetic state

Hartree-Fock approximation:

$$H = \sum_{k,\sigma} (\varepsilon_k + V_\sigma)\, n_{k,\sigma}$$

with: $V_{i\sigma} = -\sigma U/2\langle n_{i\uparrow} - n_{i\downarrow}\rangle$



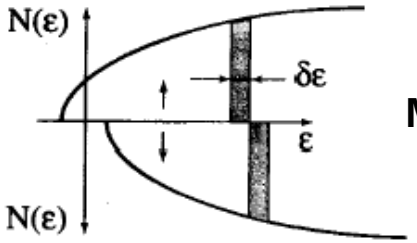
$$E_M = Un_\uparrow n_\downarrow = U\left(\frac{N}{2} + \rho(\varepsilon_F)\delta\varepsilon\right)\left(\frac{N}{2} - \rho(\varepsilon_F)\delta\varepsilon\right)$$

$$= \mathrm{U}\frac{\mathrm{N}^2}{4} - \mathrm{U}(\rho(\varepsilon_F)\delta\varepsilon)^2$$

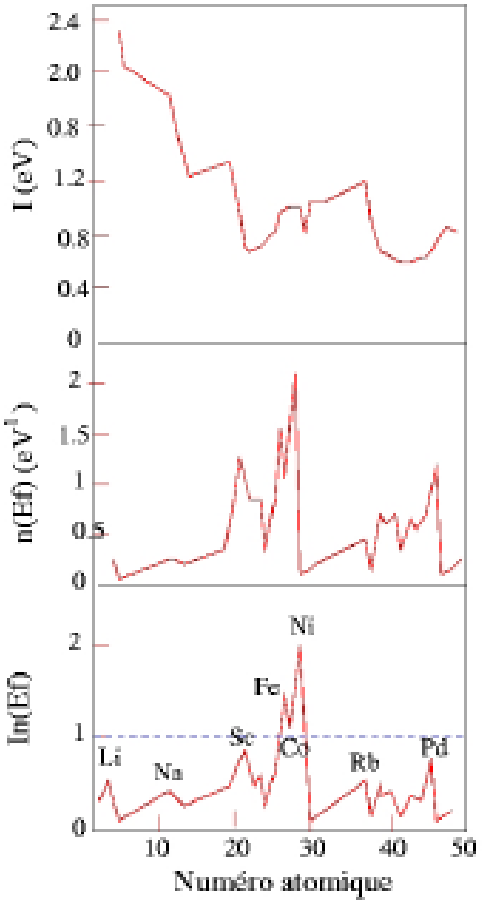
$$\Delta E_c = \rho(\varepsilon_F)(\delta\varepsilon)^2$$

Total energy variation:

$$\Delta E_t = \Delta E_M + \Delta E_c = \rho(\varepsilon_F)\delta\varepsilon^2(1 - U\rho(\varepsilon_F))$$



$M = 2\mu_B\, \rho(\varepsilon_F)\, \delta\varepsilon$



⇒ Stoner criterion :

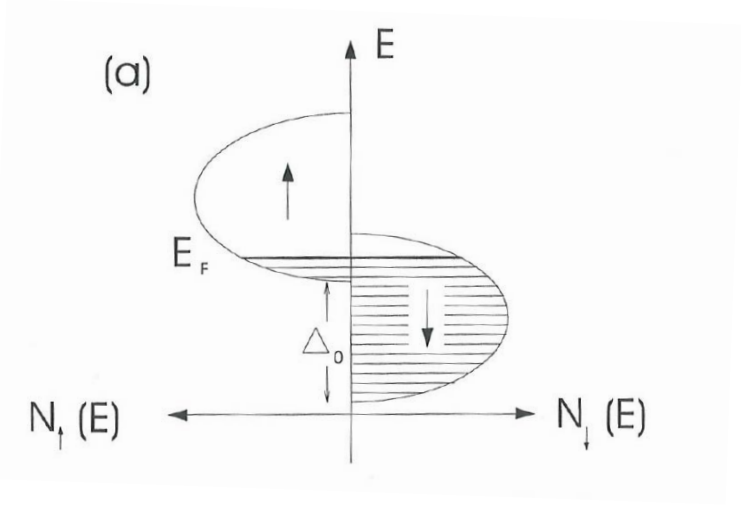
-If $1\text{-}U\rho(\varepsilon_F) < 0$: magnetic state is stable (ferromagnetism)

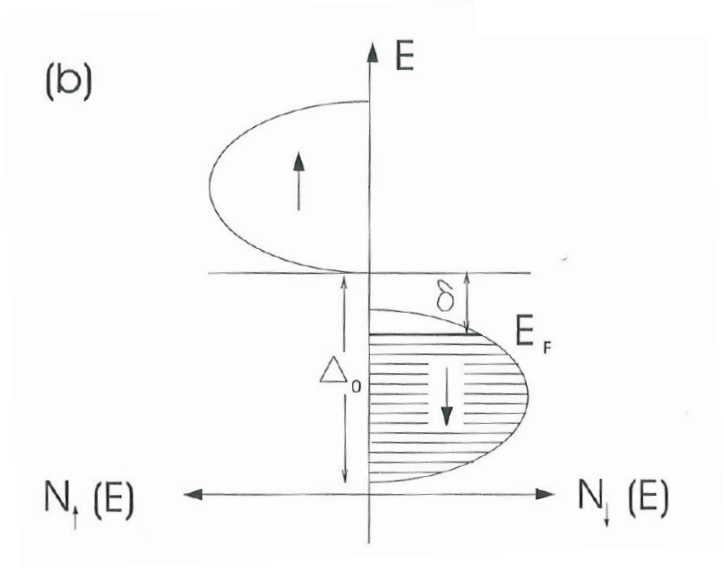
-If $1\text{-}U\rho(\varepsilon_F) > 0$: paramagnetic state

Magnetic moments are non-integer
For pure transition metals:
Fe → $m_0 \approx 2.2\ \mu_B$ / atom
Co → $m_0 \approx 1.8\ \mu_B$ / atom
Ni → $m_0 \approx 0.64\ \mu_B$ / atom

Weak vs strong ferromagnets

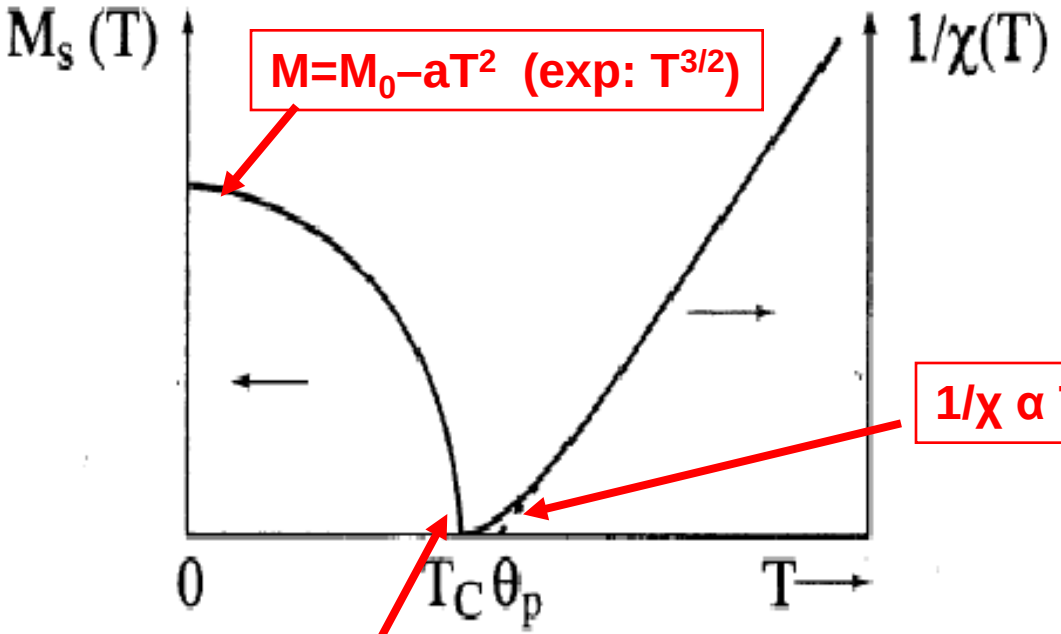
W.F: both spin directions at E_F (Fe)





SF: only 1 spin directions at E_F
Gap in the spin flip excitations (Co and Ni)

Itinerant systems: Stoner theory at finite temperature:



Order of magnitudes for Tc:
Fe: 1040 (Stoner: 4400-6000)
Co: 1400 (Stoner: 3300-4800)
Ni: 630 (Stoner: 1700-2900)

More on Hubbard model and itinerant magnetism: next talk ! (M. Lavagna)

There are few exact results for the Hubbard model:

$$H = \sum_{k,\sigma} \varepsilon_k \, n_{k,\sigma} + U \sum_i n_{i\uparrow} \, n_{i\downarrow}$$

Stoner criterion for ferromagnetism: $1\text{-}U\rho(\varepsilon_F) < 0$ **?**

- U cannot be too large (screening effects)

-But almost all these exact results do not give a ferromagnetic ground state, even for large U (see also the arguments given by T. Dietl)

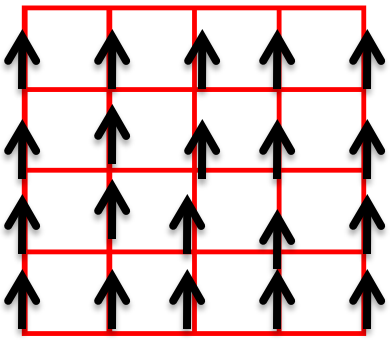
Orbital degeneracy (Hund's coupling) and s-d interactions are very important for stabilizing ferromagnetism)

Why is mean field not good for large U?

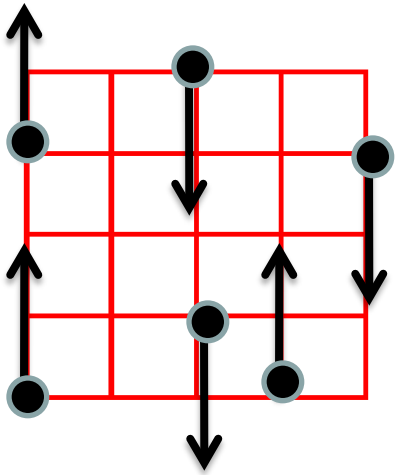
If the number of electrons is small: uniform potential on all sites

$V_{i\sigma} = -\sigma U/2\langle n_{i\uparrow} - n_{i\downarrow}\rangle$ **and the electrons density is the same on all sites.**

However it could be more favorable to « maintain » the electrons far from each other, so that they almost not interact . This is not described by mean field



In mean field : small moments evrywhere



Large U: large moments, well separated

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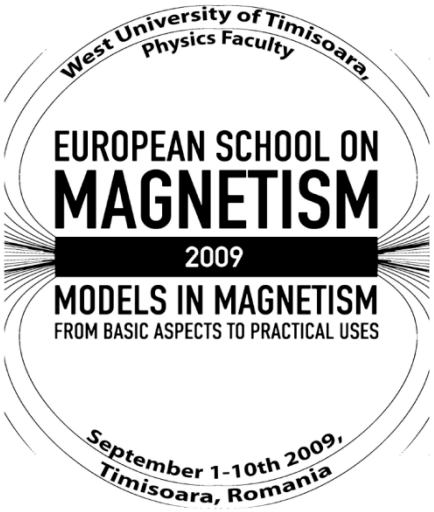
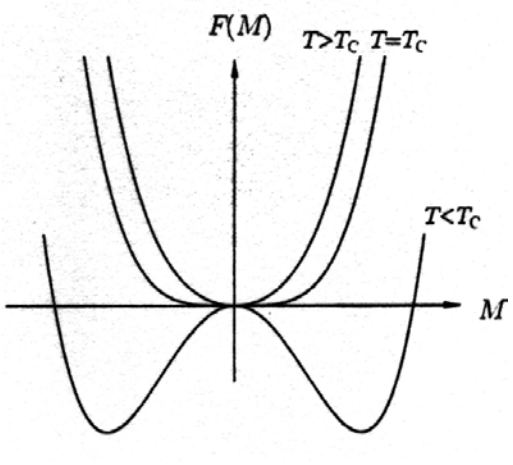


Landau expansion for 2nd order phase transition

Free energy near Tc can be expanded in powers of M:

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



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

- They depend on the microscopic parameters: J_{ij} or U and band structure

- They depend on temperature

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

Different situations as a function of the sign of coefficients (c >0)

Magnetization is determined by : $aM + bM^3 + cM^5 = H$

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

2) H=0, a <0 (and b^2 -4ac >0): M≠0

Usually T_c is determined by $a(T_c) = 0 \Rightarrow a = a_0 (T-T_c)$

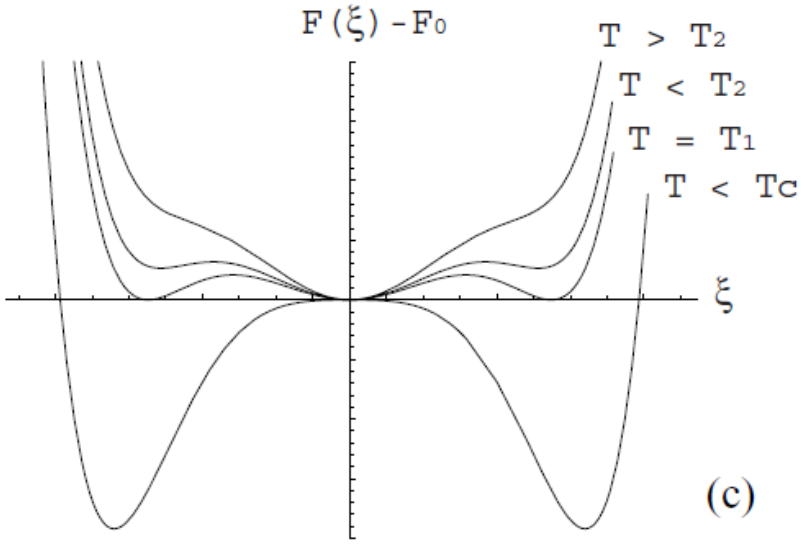
And $M(T) = (a_0/b)^{1/2} (T_c-T)^{1/2}$

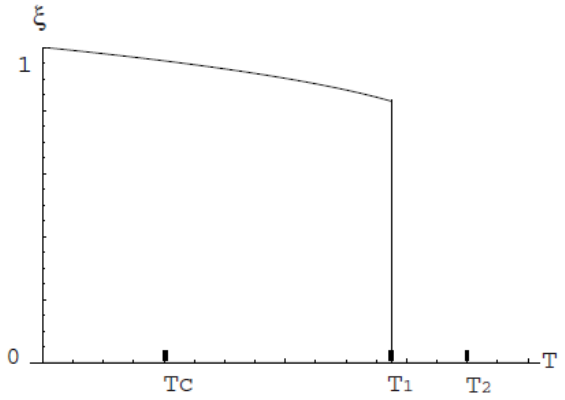
Above Tc: $M/H = 1/a = 1/a_0 (T-T_c)$ ⇒ Curie Weiss law

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

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

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





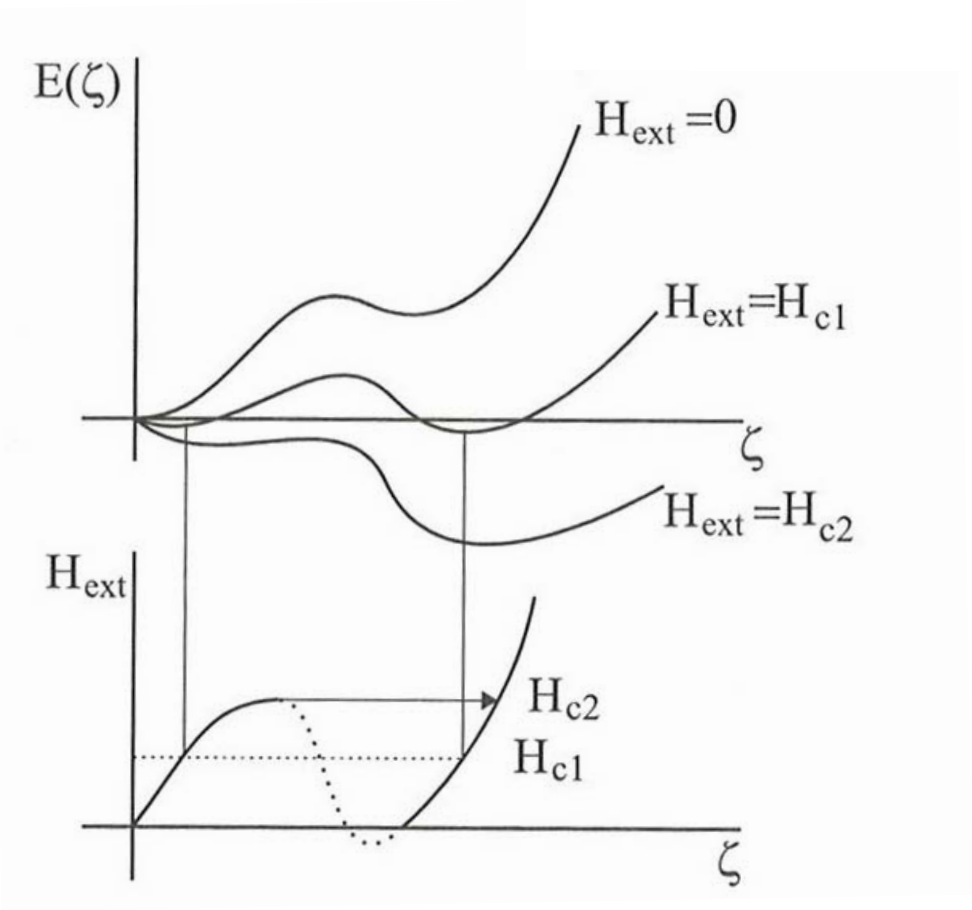
- 1st order transition at T_c: discontinuity of M(T)

- Expansion of F in powers of M is not justified if ΔM is large

- No critical phenomena

1st order transituion under magnetic field: metamagnetism

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



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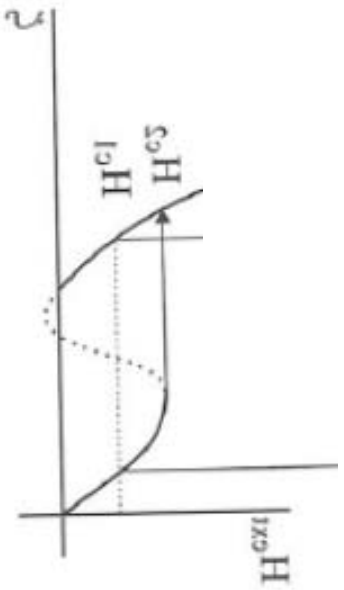


Advantages and limitations of mean field approximations

-Simplicity (localized and itinerant systems)

-Simple calculations of thermodynamic properties

-Physical origin of the magnetic order

-1st step to investigate a model.

-Extension to antiferromagnetism, itinerant models, …..

-At low T: M(T) - $M_0 \approx \exp(-\Delta/kT)$ instead of T^{α} (α=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 not described: absence of magnetism for d=1, T_c = 0 for d=2 (Heisenberg case)

-Size effect : MF predicts magnetic order in finite systems

Estimation of T_C

Mean field: $k_B T_C = zJ$

Real Tc is always smaller (event 0 for some models)

Tc 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!

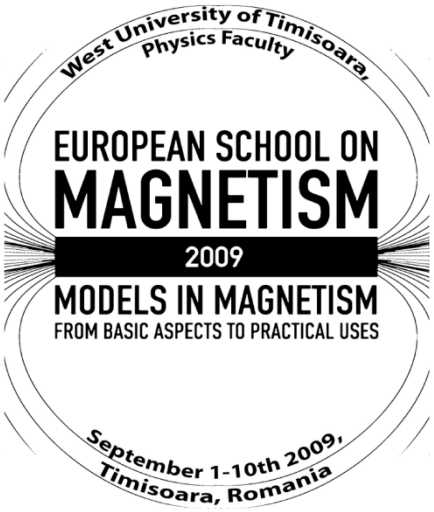
Magnetism at finite temperature: molecular field, phase transitions

-The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

- Mean field for itinerant systems

- Landau theory of phase transitions

- Beyond mean field:
  critical exponents
  spin waves
  Dimensionality effects: absence of phase transition in 1D and 2D models



Improving the mean field approximation

-**Phenomenological fit of Landau expansion**

-**Low T: spin waves**

-**Spin fluctuations theories**

-**Description of critical phenomena**

Mean field results can be tested with

- numerical results (Monte Carlo),

- or expansions…

- exact results in a few cases

Improving the mean field approximation

-**Phenomenological fit of Landau expansion**

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-**Short range correlations**

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At low temperature: thermal variation is dominated by spin waves

Collective excitations of magnetic moments:

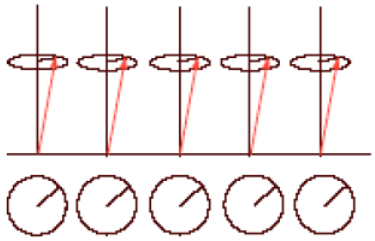
Ground state: ↑↑↑↑↑....

Spin wave: linear combination of : ↑↑↓↑↑

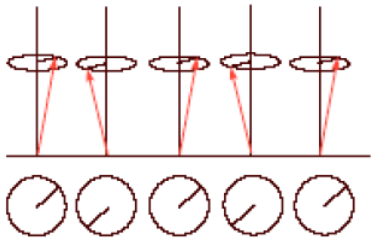
This is not an eigenstate : $S_i^+ S_i^-$ induces correlated spin flips

Energy of spin waves: $E(k) = h\omega(k) = 2S(I(0) - I(k))$

$$I(k) = \sum_{ij} I(r_i - r_j) e^{ik(r_i - r_j)}$$

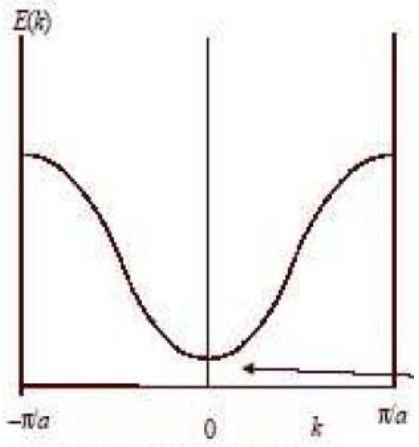


k = 0



k = π/a

Spin waves excitations: low energy cost



At low k: $E(k) \approx 2zJ\,(1 - (ka)^2/2)$

In antiferromagents: spin wave energies
$E(k) \alpha \sin(ka)$

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

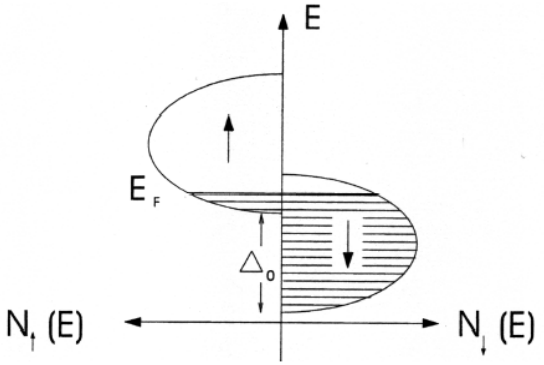
$$N_{sw} = \sum_k < n_k > = \sum_k \frac{1}{e^{E(k)/T} - 1}$$

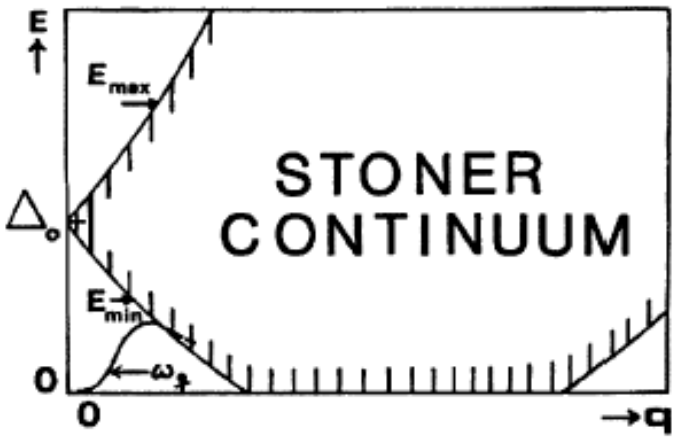
$\Rightarrow$ **in a ferromagnet: magnetization $M(T)/M_0 = 1 - AT^{3/2}$**
in antiferromagnet: $1 - AT^2$

If gap in the spin wave spectrum (i.e. anisotropy), behavior is different: $\exp(-\Delta/T)$

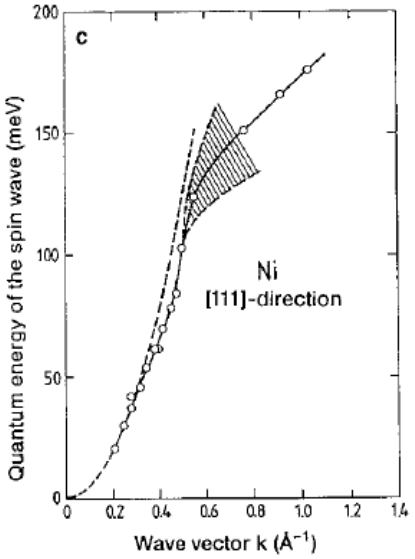
Spin waves also exist in itinerant ferromagnets:

2 types of excitations:
-Stoner excitations: transition from a
-filled ↑ state to an empty ↓ state: gap Δ_0 at q=0; continuum at q ≠ 0
-Collective excitations: spin waves





Magnetic excitations in Ni (Δ_0≈100meV)



Spin waves: talk by W. Wulfheckel on Monday 7th

Improving the mean field approximation

-**Phenomenological fit of Landau expansion**

-**Low T: spin waves**

-**Spin fluctuations theories**

-**Description of critical phenomena**

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Spatial spin fluctuations in Landau – Ginzburg model

Near T_c: large fluctuations of M.

$$F = \int dr \frac{1}{2} a\, M(r)^2 + \frac{g}{2} \left(\vec{\nabla} M(r) \right)^2 - M(r).H_{ext}$$

$M(r) = M_0 + m(r)$

Small fluctuations can be included in the free energy:

$$\langle |m(q)|^2 \rangle \sim k_B T/(gq^2 + a + 3bM_0^2)$$

Fluctuations of small q are large

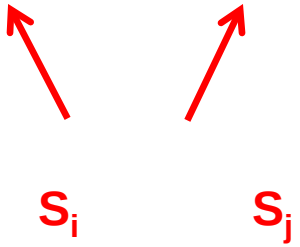
Above Tc: $M_0 = 0$: caracteristic length $\zeta \sim q^{-1} \sim (g/a)^{1/2} \sim (T_c - T)^{-1/2}$

$$\langle |m(q)|^2 \rangle \sim k_B T/((q/\zeta)^2 + 1)$$

Caracteristic length diverges at T_c: critical fluctuations

Why a $\left(\vec{\nabla}M(r)\right)^2$ **contribution?**

If variations 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:

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

If $S_i = S(\cos\theta_i, \sin\theta_i, 0)$**, then** $\left(\vec{\nabla}M(r)\right)^2 = S^2\left(\frac{d\theta}{dr}\right)^2$

The $\left(\vec{\nabla}M(r)\right)^2$ **is justified if spatial fluctuations are small**

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

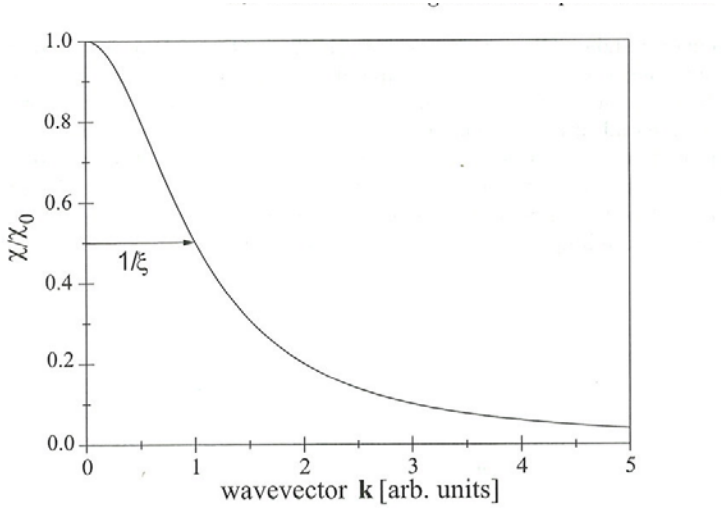
$$\left|\vec{\nabla}M(r)\right|^2 = \sum_{q,q'} qq'M(q)M^*(q')e^{i(q-q')r}$$

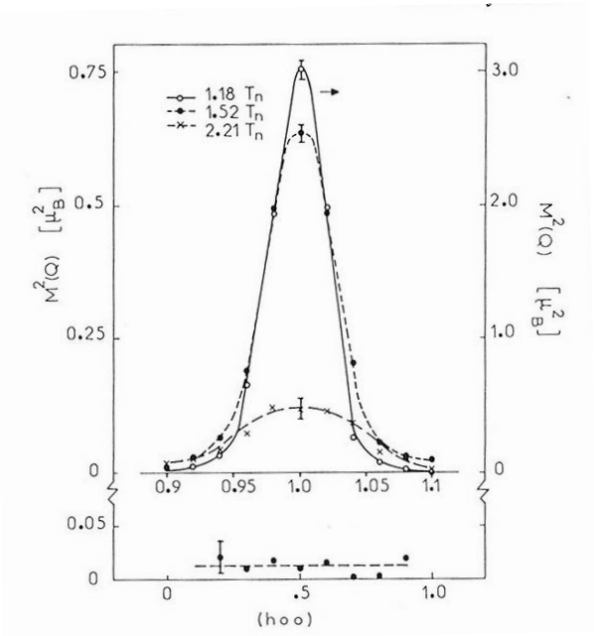
Integration over r: only q=q'

Correlation length can be observed with neutron scattering:

$\chi(q) \sim \langle|m(q)|^2\rangle/kT$ **through the fluctuation-dissipation theorem**

$$\langle|m(q)|^2\rangle \sim k_B T/((q/\zeta)^2 + 1)$$





Above T_c: width of $\chi(q)$ is $\approx \zeta^{-1}$ $\Rightarrow$ measure of the correlation length ζ : direct access to $\zeta(T)$

Validity of Landau Ginzburg expansion

$$F = \int dr \frac{1}{2} a\, M(r)^2 + \frac{g}{2} \left(\vec{\nabla} M(r) \right)^2 - M(r).H_{ext}$$

The $\frac{1}{4} b\, M^4$ is neglected. This is valid as long as $\frac{1}{2} a\, M^2 \gg \frac{1}{4} b\, M^4$

If $\langle |m(q)|^2 \rangle \sim k_B T / (gq^2 + a + 3bM_0^2)$, $M^2 = \sum_q < |m(q)|^2 >$

This leads to the Landau- Ginzburg criterion fot the validity of Landau expansion: $\frac{b^2 (kT_C)^2}{2 a_0 g^3} \ll \frac{|T - T_C|}{T_C} \ll 1$

If T_c is small , Landau expansion is not valid. Quantum fluctuations become more important than thermal fluctuations

$\Rightarrow$ **Quantum critical point (QCP)**

Improving the mean field approximation

-**Phenomenological fit of Landau expansion**

-**Low T: spin waves**

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Mean field results can be tested with

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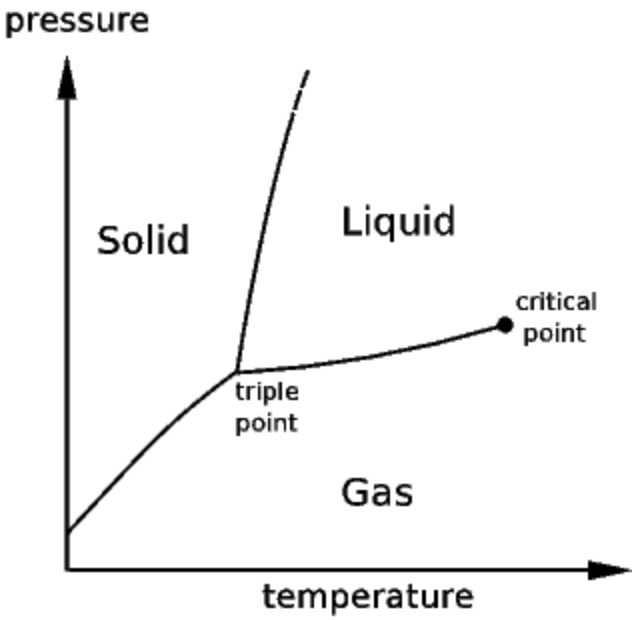
Some generalities on phase transitions and critical phenomena

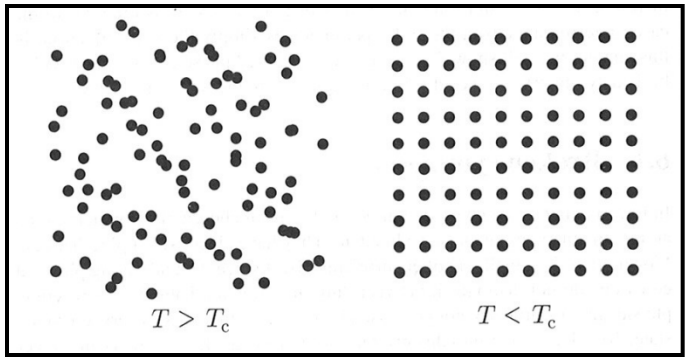


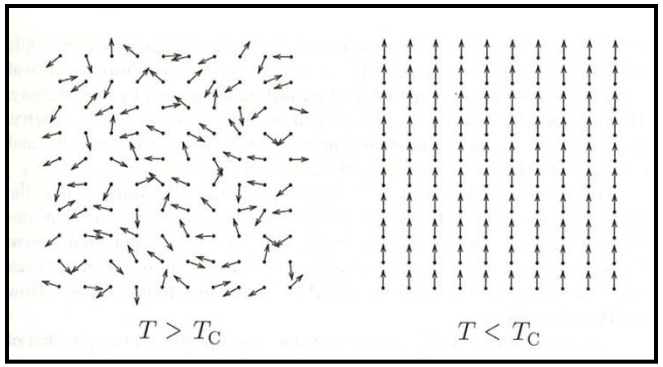
-**Liquid-solid transition: spontaneous symmetry breaking at T_c**

-**Order parameter (spatial)**

-**A liquid has more symmetries as 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	$\lvert\psi\rvert e^{i\phi}$	–	superconductivity	flux lines

2nd order phase transitions:

- **Order parameter below T_c**
- **divergence of some thermodynamics quantities**

if $t = (T-T_c)/T_c$, and $h = \mu H/kT_c$

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

Critical exponents

they depend on

-the type of interactions (Heisenberg, X-Y, Ising…)

- the dimensionality of the system

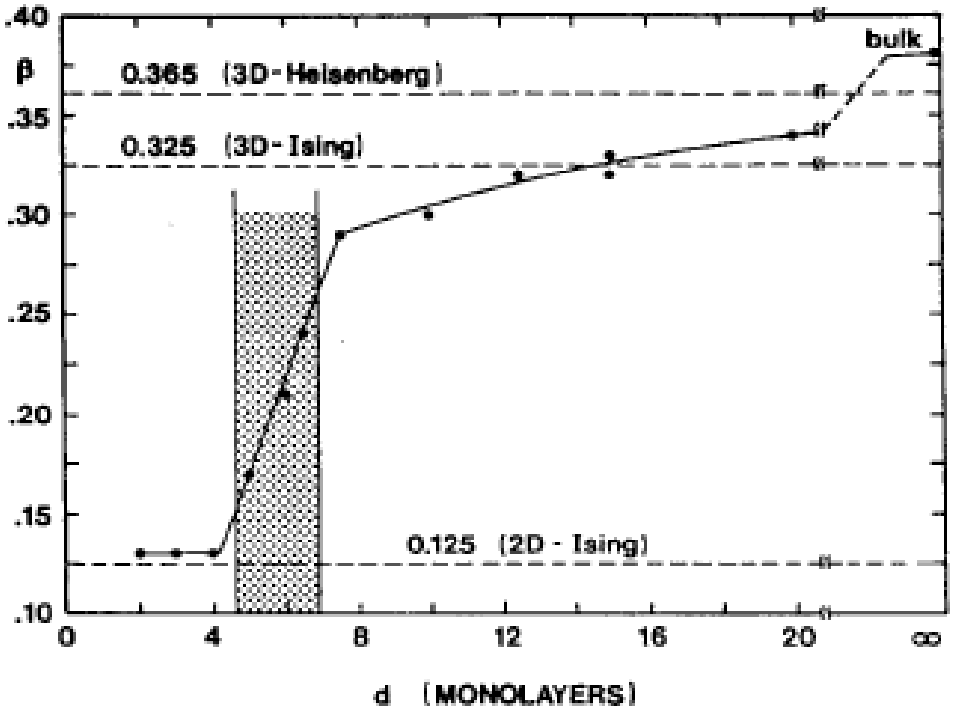
$$M(T) \propto (T_c - T)^{\beta} \quad , \quad \chi(T) \propto (T - T_c)^{-\gamma}$$

	D=1	D=2	D=3	Mean field
Heisenberg	No ordering		β = 036 γ = 1.39	
X-Y		γ = ∞ Kosterlitz- Thouless	β = 0.35 γ = 1.32	β = 1/2 γ = 1
Ising	Tc = 0 χ ~ exp(-2J/T)	β = 1/8 γ = 7/4	β = 0.32 γ = 1.24	

Several relations between the critical exponents:

$\alpha+2\beta+\gamma=2$, $\gamma = \beta(\delta - 1)$…..

Critical exponents depend on the dimensionality



(K. Baberschke)

critical exponenent β in thin Ni films on W: at 6 monolayers

transition from 2- to 3- dimensional behavior

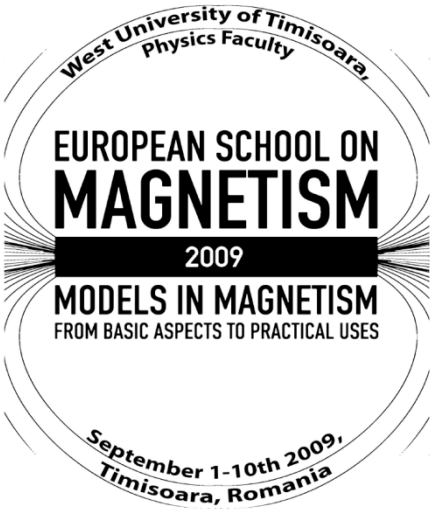
Magnetism at finite temperature: molecular field, phase transitions

-The Heisenberg model in molecular field approximation: ferro, antiferromagnetism. Ordering temperature; thermodynamics

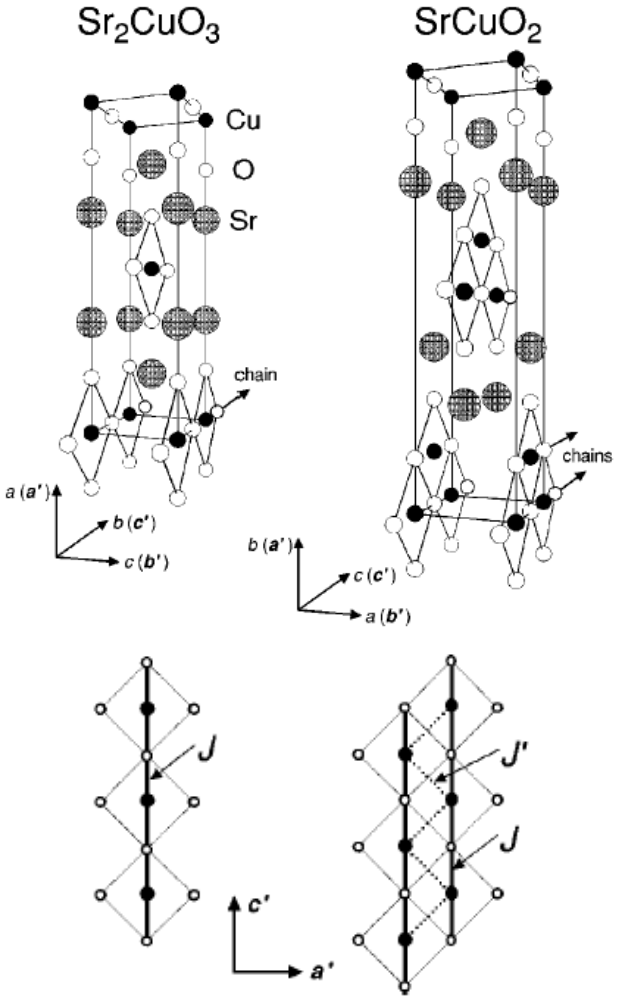
- Mean field for itinerant systems

- Landau theory of phase transitions

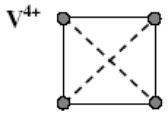
- Beyond mean field:
critical exponents
spin waves
Dimensionality effects: absence of phase transition in 1D and 2D models

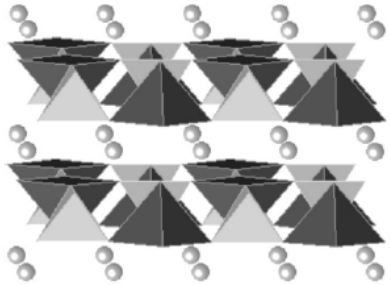


Phase transitions and low dimensionality

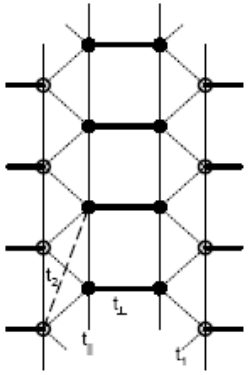


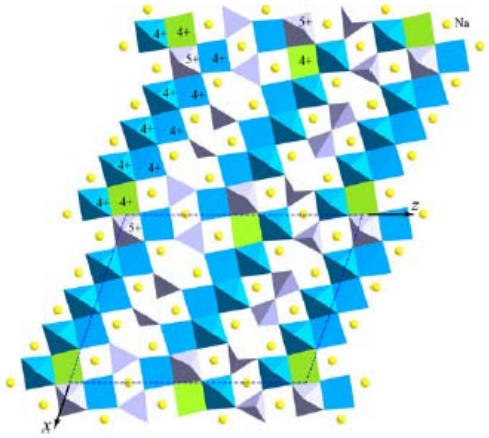
$Li_2VO(Si,Ge)O_4$





NaV_2O_5





Magnetic properties of 1-dimensional and 2-dimensional spin systems (⇒ workshop Tuesday 8th)

-Models calculations

-Heisenberg spins: no magnetic order in 1D and 2D and T > 0 (Mermin-Wagner theorem)

Spin waves argument:

Magnetization at T≠0: $M(T) = M(0) - N_{SW}$, with N_{SW} = number of excited spin waves

$$N_{SW} \propto \int \frac{k^{d-1}}{\exp(\varepsilon / T) - 1} dk$$

If $\varepsilon(k) = ck^2$: integral is divergent for d=1 and d=2 (for d=3: $T^{3/2}$)

No long range magnetic ordering for Heisenberg spins with short range interactions in 1-D and 2-D at T>0

Qualitative argument for the absence of ordering in 1D and 2D

Fluctuations in Landau theory:

$$M(r)^2 = (M_0 + m(r))^2$$

$$\Rightarrow < M(r)^2 > = M_0{}^2 + < m(r)^2 >$$

$$= -\frac{a(T)}{b} + \sum_q < |m(q)|^2 >$$

$$= \frac{a(T)}{b} + A\sum_q \frac{kT}{\Gamma q^2 + a(T) + 3bM_0{}^2}$$

In 1D and 2D the integral is divergent near T_C: fluctuations become larger than M_0. No long range magnetic ordering at $T \neq 0$

(Mermin-Wagner theorem)

Heisenberg spins with anisotropy

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

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

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
→ surfaces and thin films

Examples of 2D systems:

- Compounds with in-plane interactions >> interplane interactions

examples: La_2CuO_4….

- Ultrathin films : 2d character if

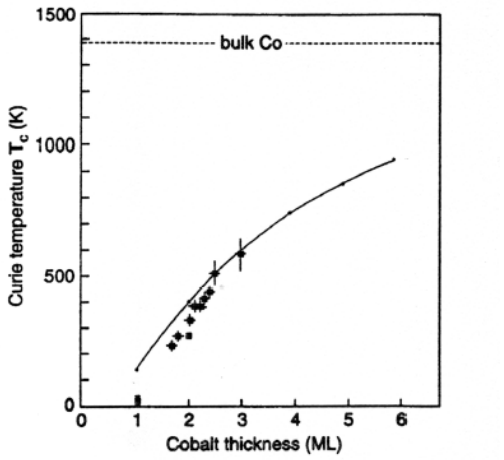
- d< $2\pi/k_F$ 0.2 -2 nm

- d<exchange length: depends on the nature of exchange: 0.2 – 10 nm

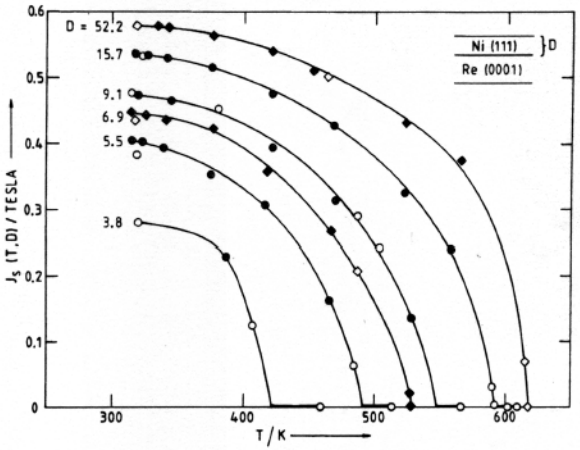
- Surfaces of bulk materials

- Superlattices F/NM: interlayer interactions

Reduction of Curie temperature



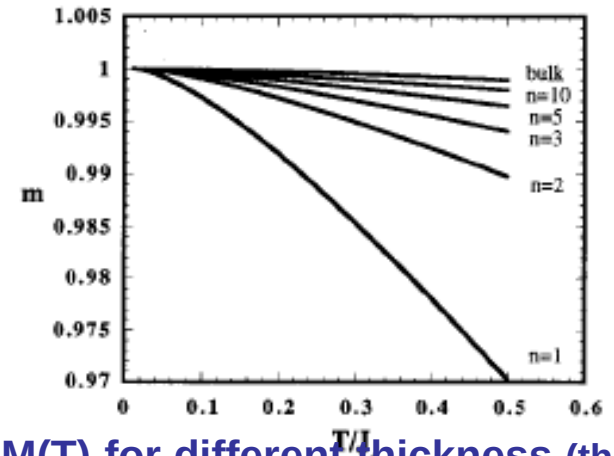
T_c for Co thin films



Magnetization of Ni films

In 2D: - no order if no anisotropy (spin waves divergence)

- with anisotropy: reduced T_c (reduction of nb of nearest neighbors T_c α zJS(S+1) + spin wave effects)



M(T) for different thickness (theory)

From 3D to 2D behavior:

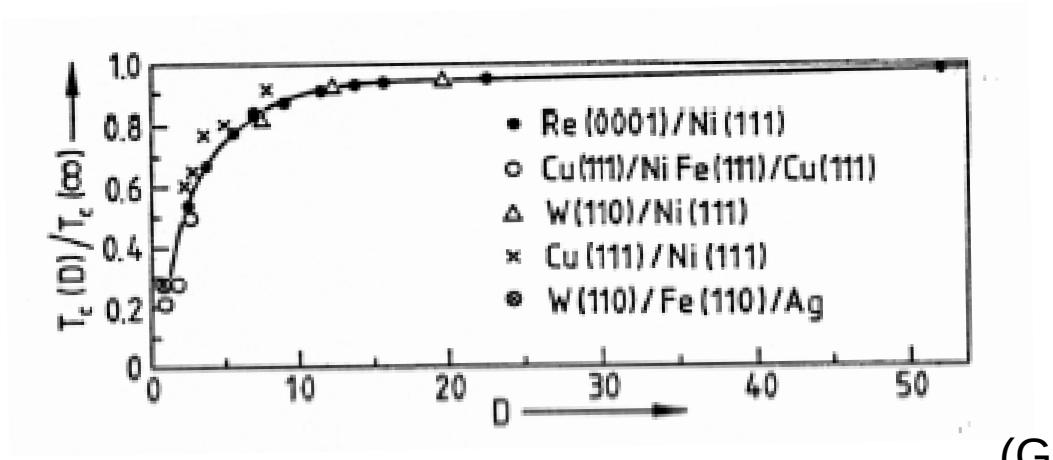
- In 3D systems correlation length diverges at Tc: $\xi = \xi_0 \left| \frac{T - T_C}{T_C} \right|^{-\nu}$

- 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

- Problems for low dimension systems