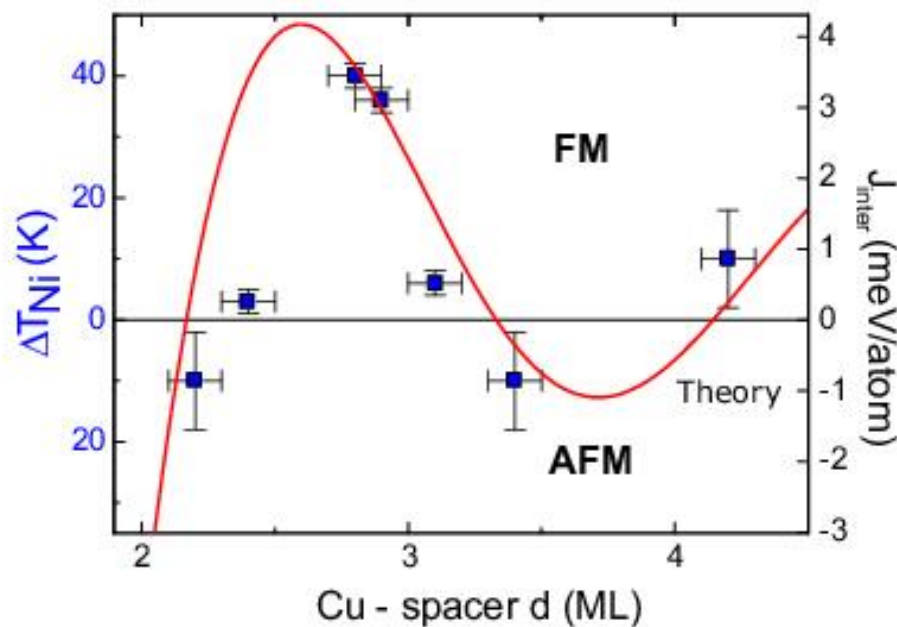
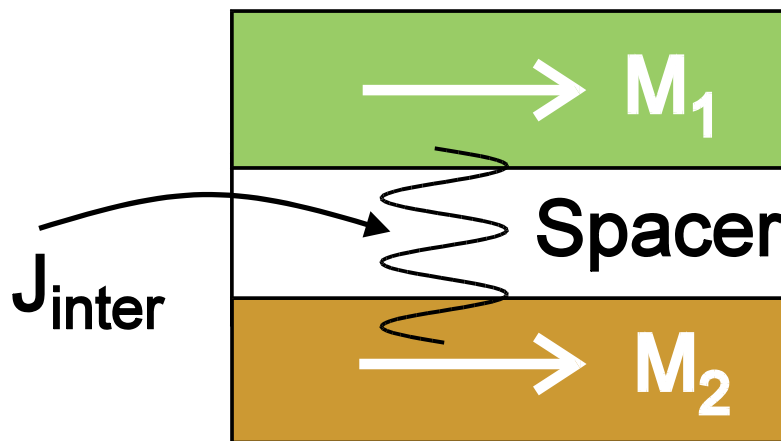


# Μαγνητικές Αλληλεπιδράσεις – Τάξη και Μαγνητικές δομές

P. Pouloupoulos, 18 June 2019, Patra



Η διάλεξη αυτή γίνεται διαδικτυακά στα πλαίσια των προβλημάτων του Covid-19. Οι διαφάνειες είναι μόνο για διευκόλυνση των φοιτητών για το εξ αποστάσεως μάθημα και δεν έχουν κανένα στόχο εμπορικής εκμετάλλευσης. Επίσης παρακαλώ τους φοιτητές να τις κρατήσουν μόνο για τους εαυτούς τους και τις εξετάσεις τους.

# Βιβλιογραφία

OXFORD MASTER SERIES IN CONDENSED MATTER PHYSICS

Magnetism in  
Condensed Matter

Stephen Blundell

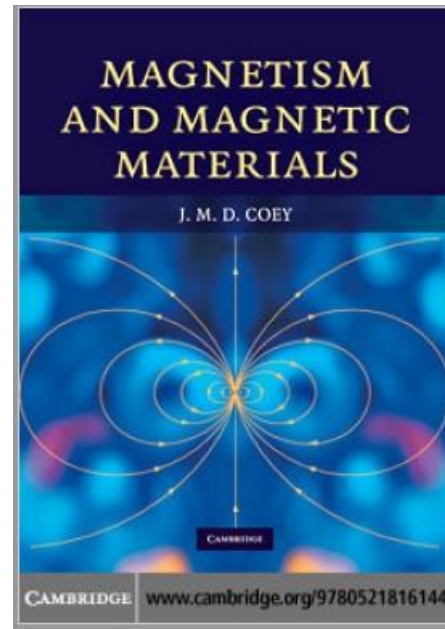
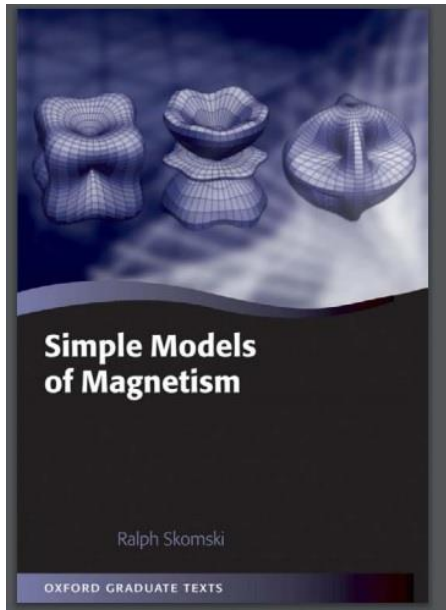


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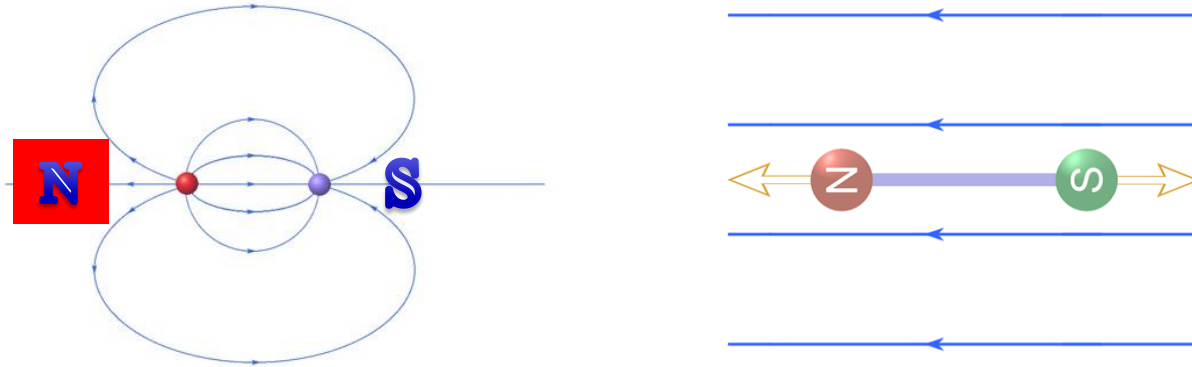
Introduction to  
**MAGNETISM**  
and  
**MAGNETIC  
MATERIALS**  
David Jiles



SPRINGER-SCIENCE+BUSINESS MEDIA, B.V.



# Magnetic Dipolar Interaction



$\mu = p \cdot l$ ,  $p$  strength,  $l$  is NS pole distance

Magnetic dipole in a magnetic field  $\mathbf{B}$  ( $\Phi/A$ ):

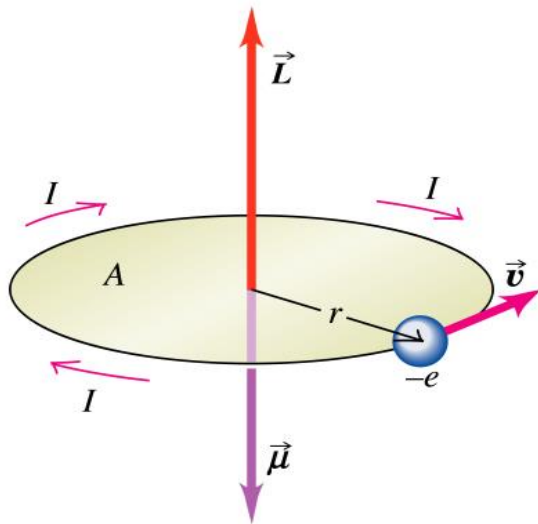
$$\text{Energy } E = - \boldsymbol{\mu} \cdot \mathbf{B}$$

Two magnetic dipoles  $\boldsymbol{\mu}_1$ ,  $\boldsymbol{\mu}_2$ , distance  $r$ :

$$E = (\mu_0/4\pi r^3)[\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2 - (3/r^2)(\boldsymbol{\mu}_1 \cdot \mathbf{r})(\boldsymbol{\mu}_2 \cdot \mathbf{r})]$$

# The Bohr magneton

All magnetic phenomena result from forces between electric charges in motion



$$d\boldsymbol{\mu} = I d\mathbf{S}$$

This is equivalent to a **magnetic dipole**

In atoms

$$\mu_{Lz} = \pi r^2 I, \quad I = -e/T, \quad T = 2\pi r/v$$

$$L_z = m_e v r = h/2\pi$$

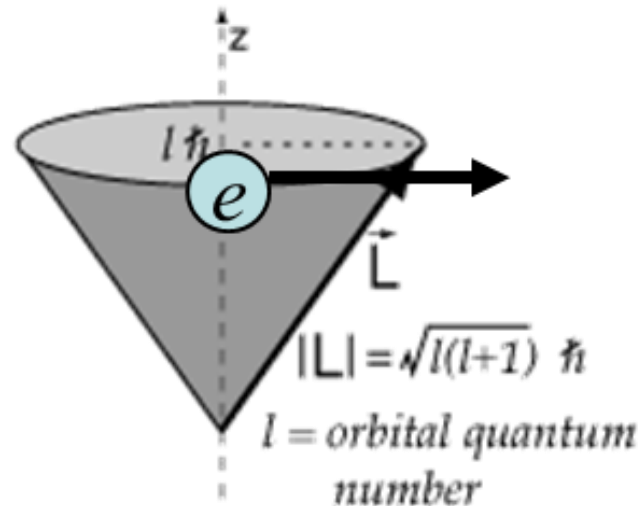
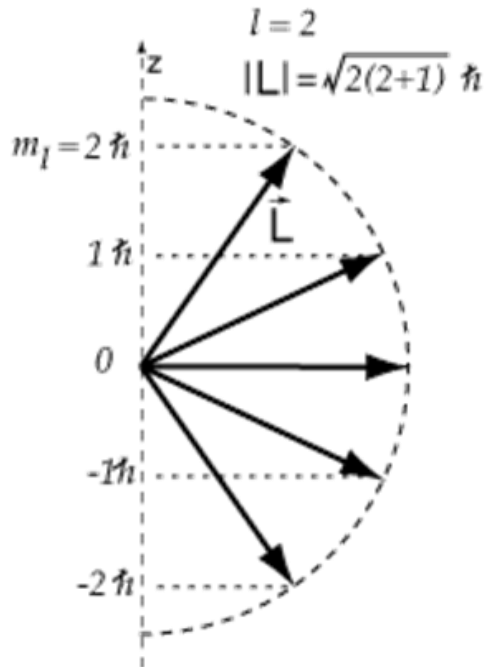
$$\mu_z = -\frac{e}{2m_e} L_z = -\frac{e\hbar}{2m_e} m_\ell = -\mu_B m_\ell$$

$$m_B = \mu_B = \frac{e\hbar}{4\pi m} = 9.27 \times 10^{-24} \text{ Am}^2$$

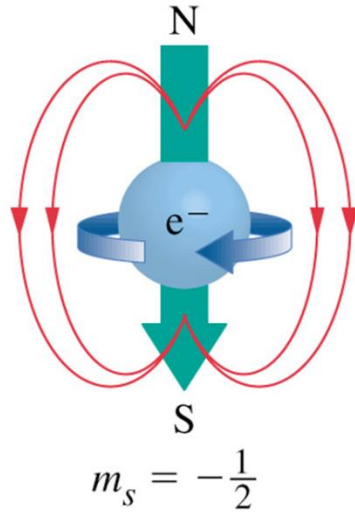
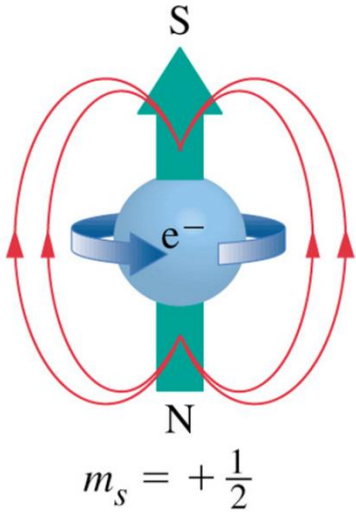
# Orbital Magnetic Moment in a H

The z component of angular momentum is quantized in units of  $\hbar/2\pi$ , so the magnetic dipole moment is quantized as well:

$$\mu_z = -\frac{e}{2m_e} L_z = -\frac{e\hbar}{2m_e} m_\ell = -\mu_B m_\ell$$

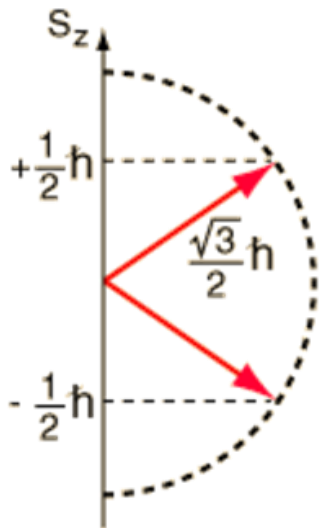


# Electron Spin Magnetic Moment



$$\vec{\mu}_s = -g \frac{e}{2m_e} \vec{S}$$

$$g = 2.002319304386$$



Electrons come in “spin up” and “spin down” states (Spintronics)

$$S_z = m_s \hbar \quad \text{where } m_s = \frac{1}{2} \text{ or } -\frac{1}{2}$$

The magnitude of the spin angular momentum is:

$$|\vec{S}| = \sqrt{s(s+1)} \hbar = \frac{\sqrt{3}}{2} \hbar$$

# Orbital and Spin Magnetic Moment

$$\boldsymbol{\mu}_{\text{tot}} = \boldsymbol{\mu}_o + \boldsymbol{\mu}_s$$

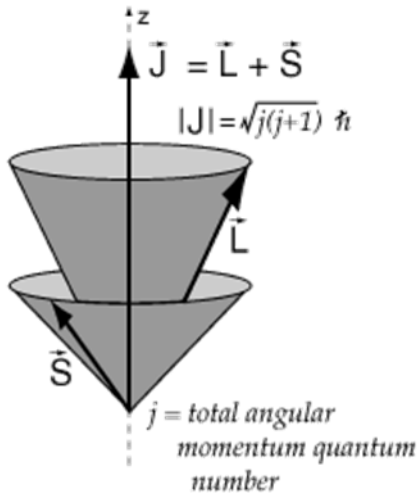
or

$$\bar{\boldsymbol{\mu}} = \bar{\boldsymbol{\mu}}_o + \bar{\boldsymbol{\mu}}_s = \frac{-e}{2m_e} \left\{ \bar{\mathbf{L}} + g\bar{\mathbf{S}} \right\}$$

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

**J** is the total angular momentum of the electron

# The vector model of the atom and the spin-orbit interaction



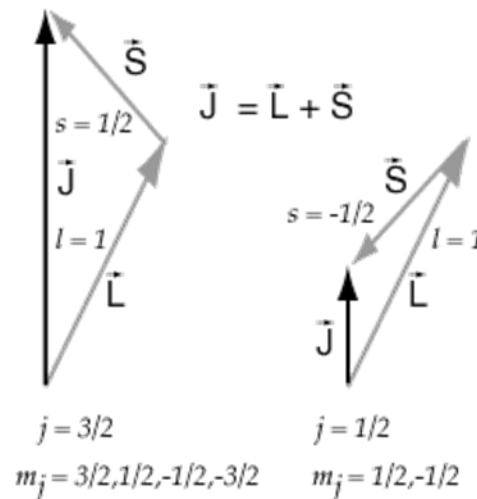
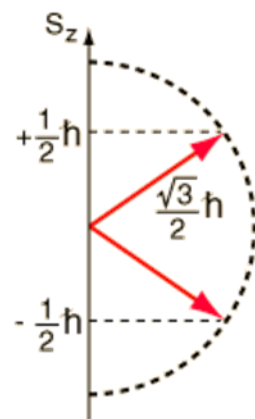
$$\vec{J} = \vec{L} + \vec{S}$$

$$|\vec{J}| = \sqrt{j(j+1)} \hbar$$

$$J_z = m_j \hbar \quad \text{with } m_j = j, j-1, \dots, -j$$

total angular momentum quantum number :

$$j = \ell + s, \quad \ell + s - 1, \dots, |\ell + s|$$





# Friederich Hund from Karlsruhe (1896-1997) and his three empirical rules for the ground state electronic configuration. In a series of decreasing importance:



- (1) *Minimize the Coulomb energy by arrange the electronic wave function so as to maximize  $S$ .*
- (2) *Similar: Maximize  $L$  so that the electrons avoid each other by moving in orbits rotating in the same direction.*
- (3) *Minimize the spin-orbit energy so  $J = |L-S|$  if the shell is less than half full or  $|L+S|$  if it is more than half full.*

Hund's rules predict the ground state of an incomplete shell  
But tell us nothing about excited states. They, therefore allow for an estimate of the magnetic moment of an ion assuming that only the ground state is populated.

*S. Blundell "Magnetism in Condensed Matter" Oxford Master Series in Condensed Matter, 2003*

# Exchange Interaction

## Wave function of a two-electron system:

$\Psi(r_1, r_2)$ ,  $r_{1,2}$  is the coordinate of the first (second) electron

We will use linear combinations of wave functions  $\psi(r_1)$ ,  $\psi(r_2)$ :

There are four possibilities:

$$\Psi(r_1, r_2) = \psi_\alpha(r_1)\psi_\beta(r_2) \quad (1),$$

$$\Psi(r_1, r_2) = \psi_\alpha(r_2)\psi_\beta(r_1) \quad (2),$$

$$\Psi(r_1, r_2) = \psi_\alpha(r_1)\psi_\beta(r_2) + \psi_\alpha(r_2)\psi_\beta(r_1) \quad (3),$$

$$\Psi(r_1, r_2) = \psi_\alpha(r_1)\psi_\beta(r_2) - \psi_\alpha(r_2)\psi_\beta(r_1) \quad (4)$$

Among all of them we need a solution which keeps the observed properties of the system unaltered when we exchange electrons, i.e. the  $\Psi^*\Psi$  stays the same while the electrons remain distinct (Pauli exclusion principle). We need an overall antisymmetric solution.

# Exchange Interaction

This means that the spin of the wave function must either be an antisymmetric singlet state  $\chi_S$  ( $S=0$ ) or a symmetric triplet state  $\chi_T$  ( $S=1$ )

$$\Psi_S = (1/\sqrt{2})[\psi_\alpha(r_1)\psi_\beta(r_2) + \psi_\alpha(r_2)\psi_\beta(r_1)]\chi_S$$

$$\Psi_T = (1/\sqrt{2})[\psi_\alpha(r_1)\psi_\beta(r_2) - \psi_\alpha(r_2)\psi_\beta(r_1)]\chi_T$$

$$E_{s(T)} = \int \Psi_{s(T)}^* \hat{H} \Psi_{s(T)} dr_1 dr_2$$

$$E_S - E_T = 2 \int \psi_\alpha^*(r_1)\psi_\beta^*(r_2)\hat{H}\psi_\alpha(r_2)\psi_\beta(r_1)dr_1dr_2$$

For a singlet state  $\mathbf{S}_1 \cdot \mathbf{S}_2 = -3/4$ , triplet =  $1/4$

$$\hat{H} = 1/4(E_S + 3E_T) - (E_S - E_T) \mathbf{S}_1 \cdot \mathbf{S}_2$$

# Exchange Interaction

If the exchange integral is

$$J = (E_S - E_T)/2 = \int \psi_\alpha^*(r_1) \psi_\beta^*(r_2) \hat{H} \psi_\alpha(r_2) \psi_\beta(r_1) dr_1 dr_2 \text{ then}$$

**In a simple Heisenberg Picture:**

$$\hat{H} = -2 \sum J_{ij} \mathbf{S}_i \mathbf{S}_j, i > j$$

$J_{ij}$  is the exchange coupling constant

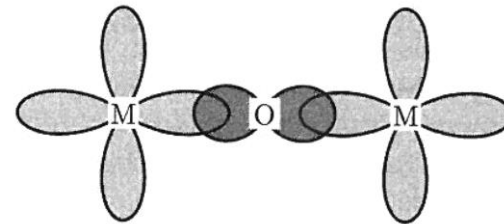
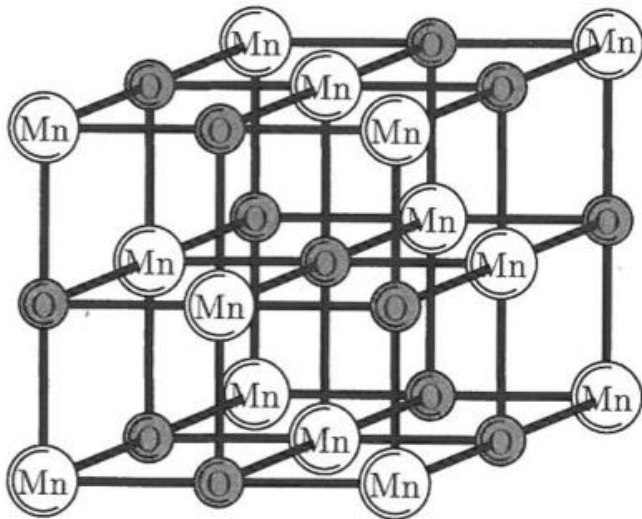
$J_{ij} > 0$  ferromagnetism

$J_{ij} < 0$  antiferromagnetism

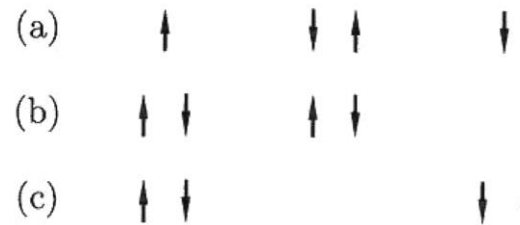
This exchange is direct because there is no need for intermediate atoms

# Indirect Exchange Interactions

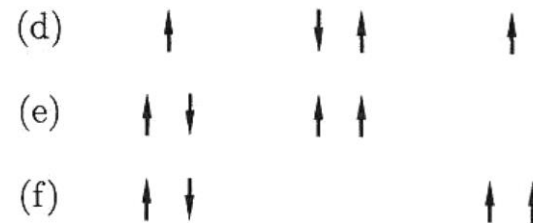
## Ionic solids: superexchange interaction



antiferromagnetic



ferromagnetic



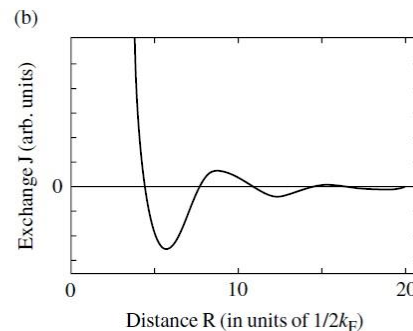
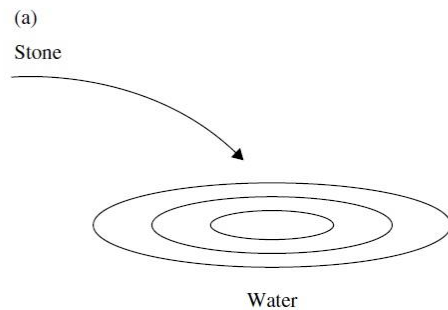
# Indirect Exchange Interactions

## Metals: RKKY interaction

In metals, the exchange interaction between magnetic ions can be mediated by the conduction electrons

**A localized magnetic moment spin polarizes the conduction electrons**

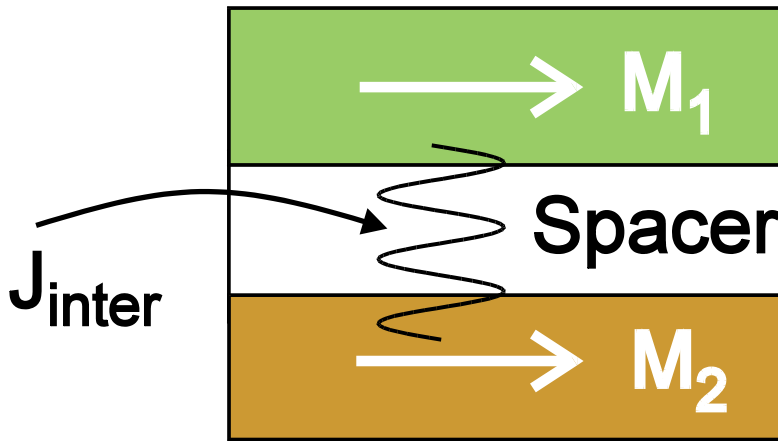
**This polarization, in turn, couples to a neighbouring localized magnetic moment a distance away**



$$J_{\text{RKKY}} \propto \frac{\cos(2k_F r)}{r^3}$$

Fig. 2.16 RKKY interactions: (a) mechanical analogy and (b) distance dependence. In nonmagnetic metals, the oscillations are known as Friedel oscillations.

# Coupled Layers – Interlayer Exchange Coupling

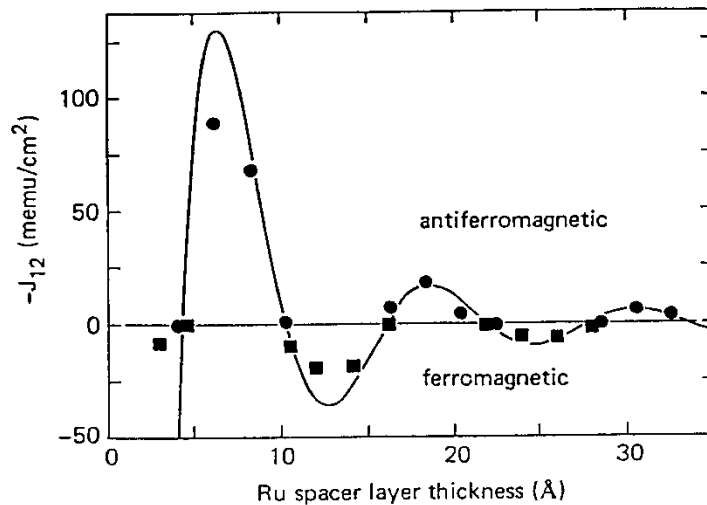


$$E_{12} = -J_{inter} \cos(\theta_1 - \theta_2):$$

$$J_{inter} > 0 \uparrow \uparrow$$

$$J_{inter} < 0 \uparrow \downarrow$$

**Oscillation of  $J_{inter}$  with the spacer thickness  $d$**



*S.S.P. Parkin et al.,  
APL 68, 686 (1991)*

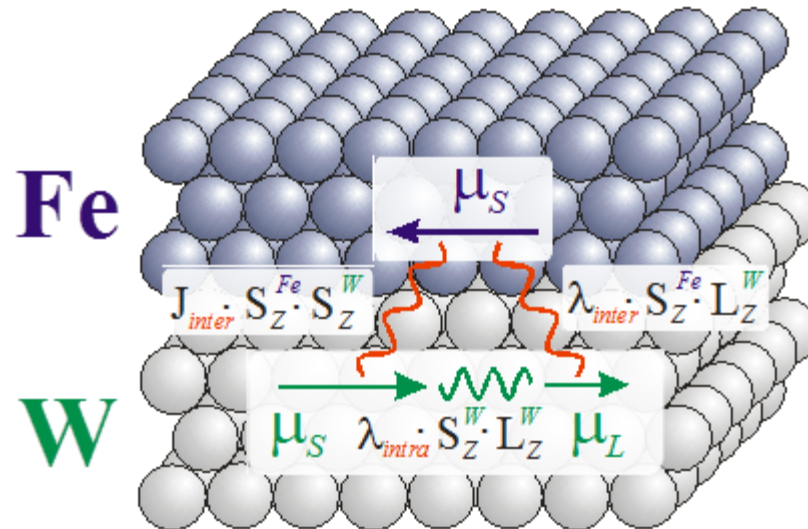
# Anisotropic Exchange Interaction

## Dzyaloshinsky-Moriya interaction

The spin-orbit interaction plays a role similar to the electrons of O in superexchange

Spin-orbit interaction and the violation of third Hund's rule

*F. Wilhelm et al, PRL 87, 207202 (2001)*



$$J_{inter} \cdot S_Z^{Fe} \cdot S_Z^W > \lambda_{inter} \cdot S_Z^{Fe} \cdot L_Z^W > \lambda_{intra} \cdot S_Z^W \cdot L_Z^W$$



# Τάξη και Μαγνητικές δομές Σιδηρομαγνητισμός

## Το μοριακό πεδίο του Weiss

In ferromagnetic materials there are large areas of the material called Weiss domains (magnetic domains) where all the spins are parallel due to the exchange interactions. As early as 1907 Weiss without the knowledge of Heisenberg exchange postulated that: A molecular field exists within the ferromagnet which orders the moments against the thermal motion. It is so large that the ferromagnet can be saturated even without an external magnetic field.

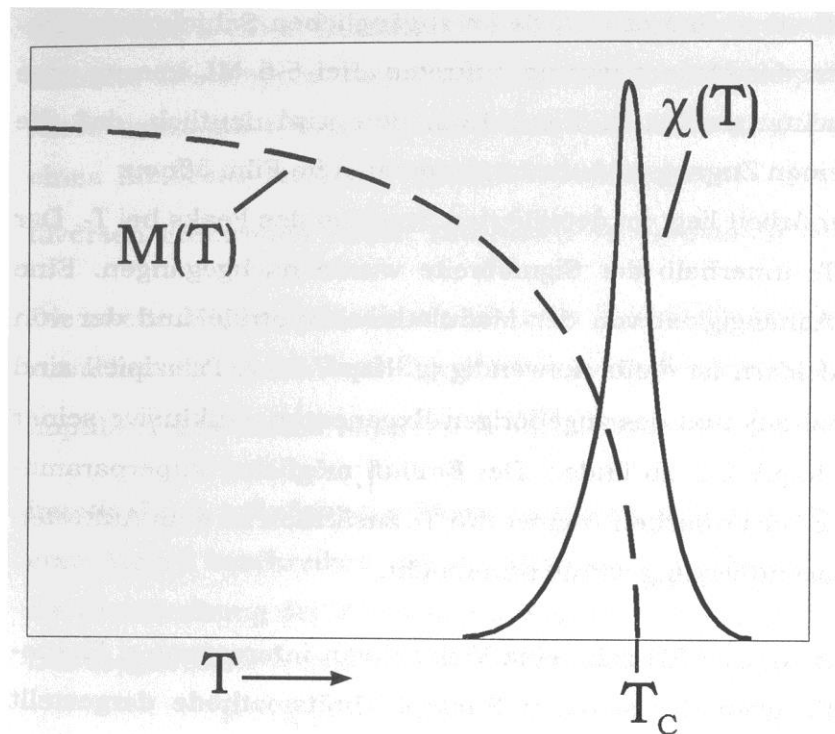
$$B_{MF} = \lambda M, \text{ M is the Magnetization (spin-sum/V)}$$

# Second Order Phase Transition

– the order parameter is  $M$

$\chi = dM/dH$ ,  $T_c = \text{Curie Temperature}$

If  $z$  is the nearest neighbor number and  $J$  the exchange then  $k_B T_c \sim zJ$ ,  $T_c$  is of the order of 1000 K, compared to 1K for dipolar interactions



*H. Stanley, 'Introduction to Phase Transitions and Critical Phenomena', Clarendon, Oxford (1971)*

# Theory of Paramagnetism

The probability of finding a dipole  $\mu$  in a field  $\mathbf{B}$  (including in our case the MF) at an angle  $\theta$  with respect to  $\mathbf{B}$ , considering thermal motion is (Boltzmann statistics):

$$f(\theta) = e^{-\frac{V}{kT}} = e^{\frac{\mu B \cos \theta}{kT}}$$

The average value of  $\mu$  along the field axis  $z$  is

$$\bar{\mu}_z = \frac{\int \mu_z f(\theta) d\Omega}{\int f(\theta) d\Omega}$$

$\Omega$  is solid angle

For  $\mu_z = \mu \cos\theta$ ,  $d\Omega = 2\pi \sin\theta d\theta$ ,  $\cos\theta = x$  and  $\alpha = \mu B/kT$ :

$$\bar{\mu}_z = \frac{\mu \int_{-1}^1 x e^{\alpha x} dx}{\int_{-1}^1 e^{\alpha x} dx}$$

$$\Rightarrow \bar{\mu}_z = \mu \left[ \frac{e^a + e^{-a}}{e^a - e^{-a}} - \frac{1}{a} \right]$$

$= \mu(\coth\alpha - 1/\alpha) = L(\alpha)$   
L is the Langevin function

$$L(a) = \frac{a}{3} - \frac{a^3}{45} + \frac{2a^5}{945} - \dots$$

For small  $\alpha = \mu B/kT$ ,  
 $M_s = N\mu$

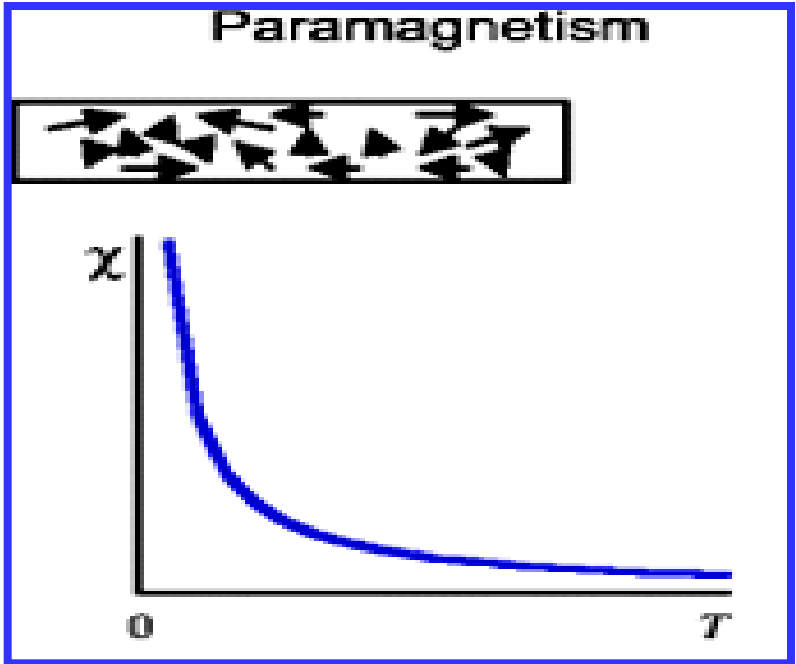
$$L(a) \approx \frac{a}{3}$$

$$M = N\bar{\mu}_z = \frac{N\mu^2 B}{3kT}$$

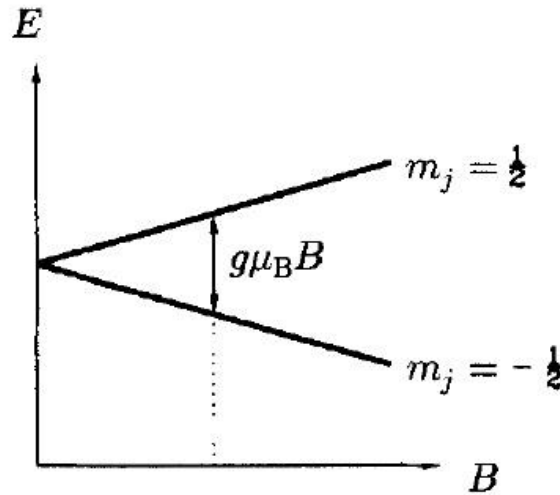
$$\Rightarrow \frac{M}{H} = \chi = \frac{N\mu_0\mu^2}{3kT}$$

$$\chi = \frac{C}{T}$$

**Curie law of paramagnetism**



# Paramagnetism for $L = 0$ and $J=S=1/2$



**Fig. 2.6** The energy of a spin- $\frac{1}{2}$  magnetic moment as a function of magnetic field.

$$m_J = \pm \frac{1}{2}, \text{ and for } g=2, \mu = \mu_B \text{ or } -\mu_B$$

Similar to the classic picture,  $M/M_s = \tanh \alpha$ ,  
 $\chi$  has the same value as in Curie law

# Paramagnetism for any J

Here,  $M/M_s = B_J(\alpha)$ , Brillouin function, for  $\alpha: \mu = g_J \mu_B J$

$$B_J(\alpha) = \left[ \frac{2J+1}{2J} \coth\left[\frac{\alpha(2J+1)}{2J}\right] - \frac{1}{2J} \coth\left(\frac{\alpha}{2J}\right) \right]$$

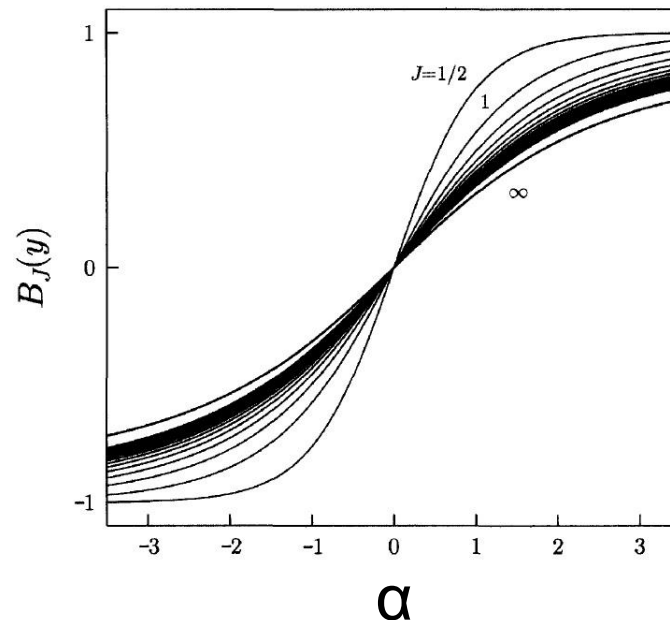
limits

$$B_\infty(\alpha) = L(\alpha)$$

$$B_{1/2}(\alpha) = \tanh(\alpha)$$

For low fields:  $\chi = N\mu_0 \mu_{\text{eff}}^2 / 3k_B T$ ,  $\mu_{\text{eff}} = g_J \mu_B \sqrt{J(J+1)}$

Lande value  $g_J = 3/2 + [S(S+1) - L(L+1)] / [2J(J+1)]$



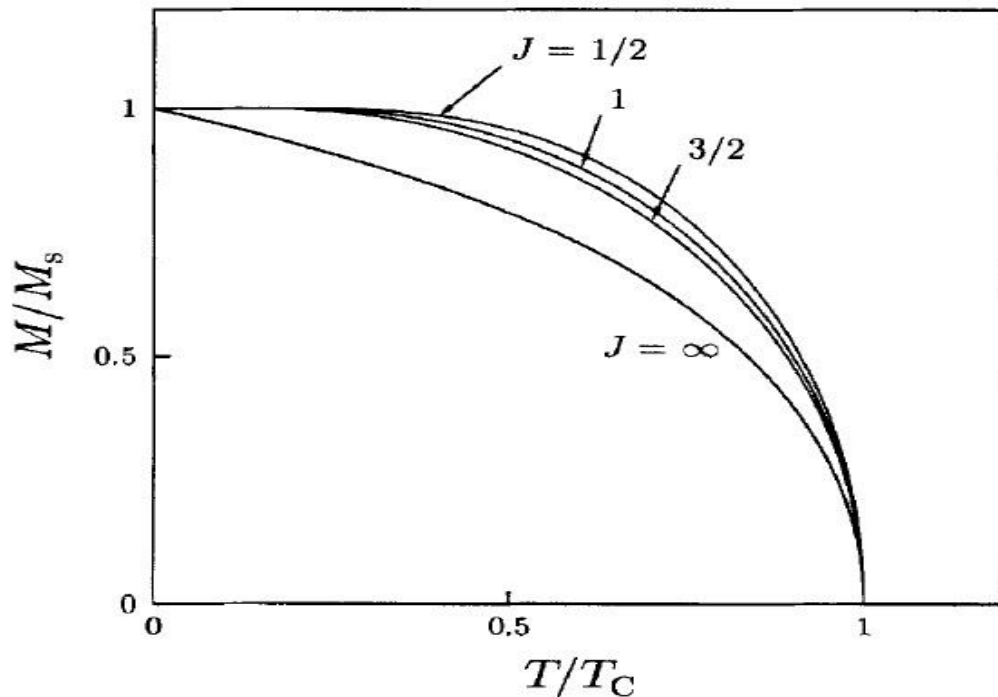
# Coming back to Molecular Field

Here,  $M/M_s = B_J(\alpha)$ , Brillouin function

$$B_J(\alpha) = [(2J+1)/2J] \coth[\alpha(2J+1)/2J] - (1/2J) \coth(\alpha/2J)$$

$$\alpha = g_J \mu_B J (B + \lambda M) / k_B T$$

For  $B = 0$

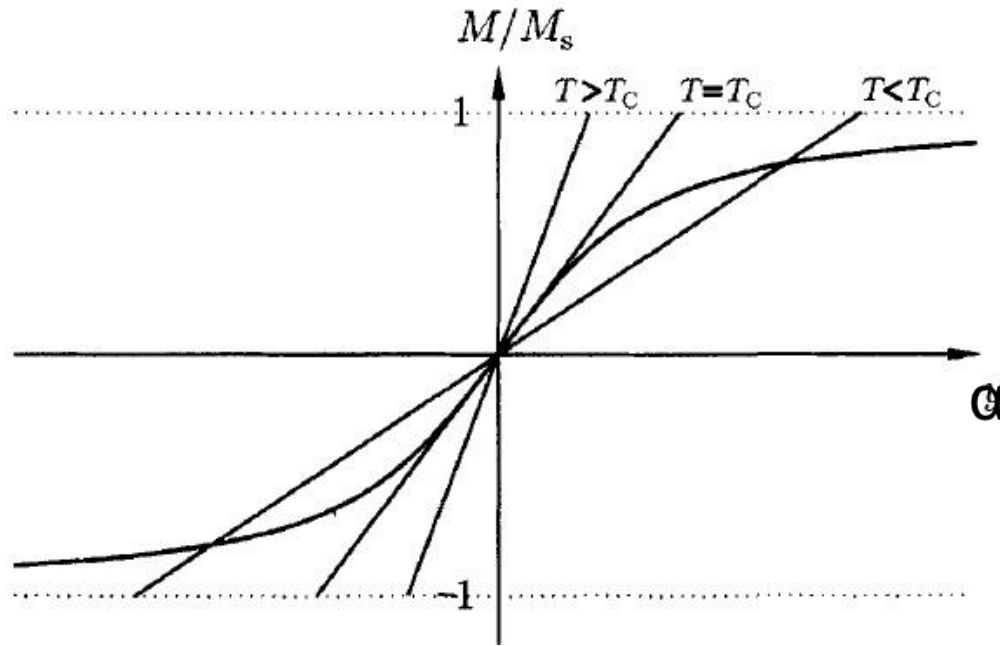


$$T_c = g_J \mu_B (J+1) \lambda M_s / 3k_B = N \lambda \mu_{\text{eff}}^2 / 3k_B,$$

for  $J=1/2$ ,  $T_c=1000$  K, BMF = 1500 T



# Magnetic Susceptibility (slope) for $B = 0$



$$X = \lim_{B \rightarrow 0} (\mu_0 M/B) \propto 1/(T - T_c) \text{ Curie-Weiss law}$$

# Dimensionality Aspects

$$\mathcal{H} = -2 \sum_{i < j} J_{ij} \left\{ a \cdot (\mathbf{S}_i^x \mathbf{S}_j^x + \mathbf{S}_i^y \mathbf{S}_j^y) + b \cdot \mathbf{S}_i^z \mathbf{S}_j^z \right\}$$

Universalitätsklasse	Wechselwirkung	Modell
$n = 1$	$a = 0, b = 1$	$2D$ -Ising
$D = 2$ $n = 2$	$a = 1, b = 0$	$2D$ -XY
$n = 3$	$a = b = 1$	$2D$ -Heisenberg
$n = 1$	$a = 0, b = 1$	$3D$ -Ising
$D = 3$ $n = 2$	$a = 1, b = 0$	$3D$ -XY
$n = 3$	$a = b = 1$	$3D$ -Heisenberg

**Tabelle 2.1:** Klassifikation verschiedener theoretischer Modellsysteme.

# Critical Exponents

Exponent		Bedingung
$\alpha$	$c_H \propto  t ^{-\alpha}$	$T \rightarrow T_C, H = 0$
$\beta$	$M \propto (-t)^\beta$	$T \rightarrow T_C^-, H = 0$
$\gamma$	$\chi \propto  t ^{-\gamma}$	$T \rightarrow T_C, H = 0$
$\delta$	$M \propto  H ^{1/\delta}$	$T = T_C, H \rightarrow 0$
$\nu$	$\xi \propto  t ^{-\nu}$	$T \rightarrow T_C, H = 0$
$\eta$	$G^{(2)}(r) \propto 1/r^{d-2+\eta}$	$T = T_C, H = 0$

$$\begin{array}{l}
 M_S \propto |T_C - T|^\beta \\
 \chi \propto |T - T_C|^{-\gamma}
 \end{array}
 \quad \left| \quad
 \begin{array}{l}
 M_{T=T_C} \propto \pm |H|^{1/\delta} \\
 \zeta \propto |T_C - T|^{-\nu}
 \end{array}
 \right.$$

Landau : mean field approach

Ising : spin only in the z direction

XY : spin in the xy plane

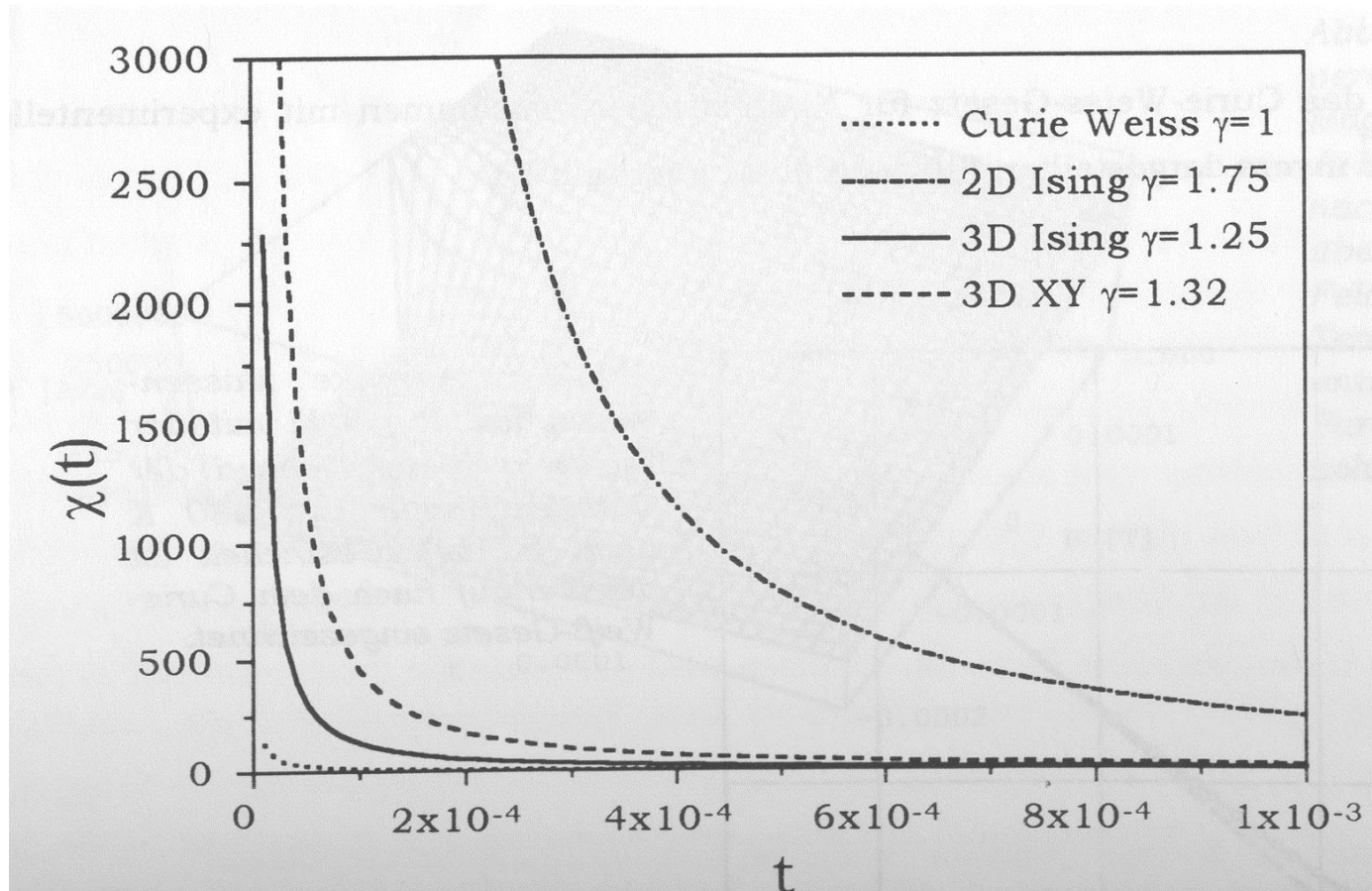
Heisenberg : spin in any direction in space

Exponent	$\beta$	$\gamma$	$\delta$	$\nu$
Landau-Theory	0,5	1	3	0,5
2d-Ising	0,125	1,75	15	1
2d-XY	0,23	2,2	10,6	1,33
3d-Ising	0,325	1,240	4,816	0,630
3d-XY	0,345	1,316	4,810	0,669
3d-Heisenberg	0,365	1,387	4,803	0,705

$t = (T - T_C)/T_C$  is the reduced temperature



# Dimensionality and Susceptibility



# Dimensional Crossovers

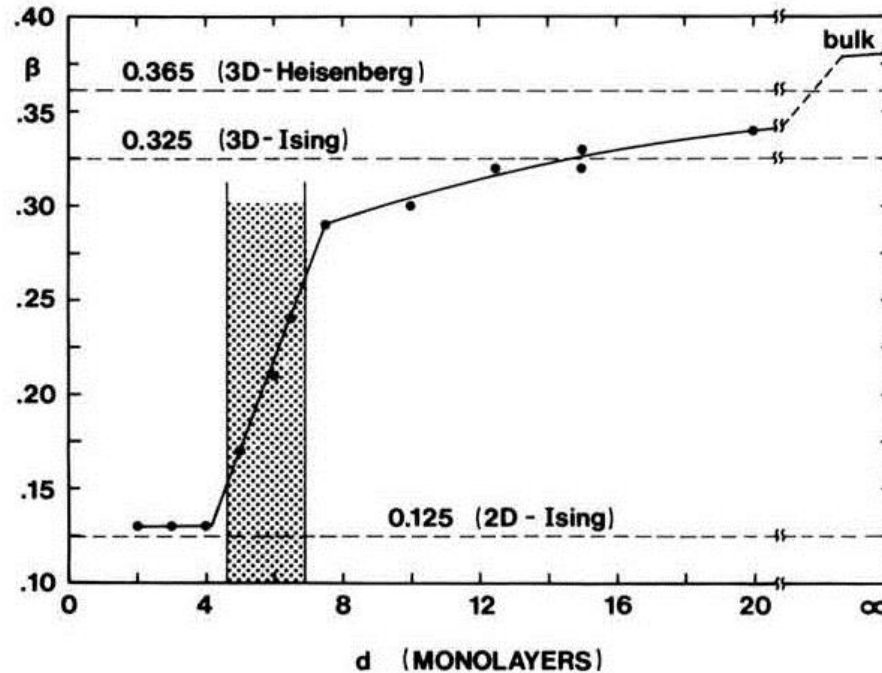
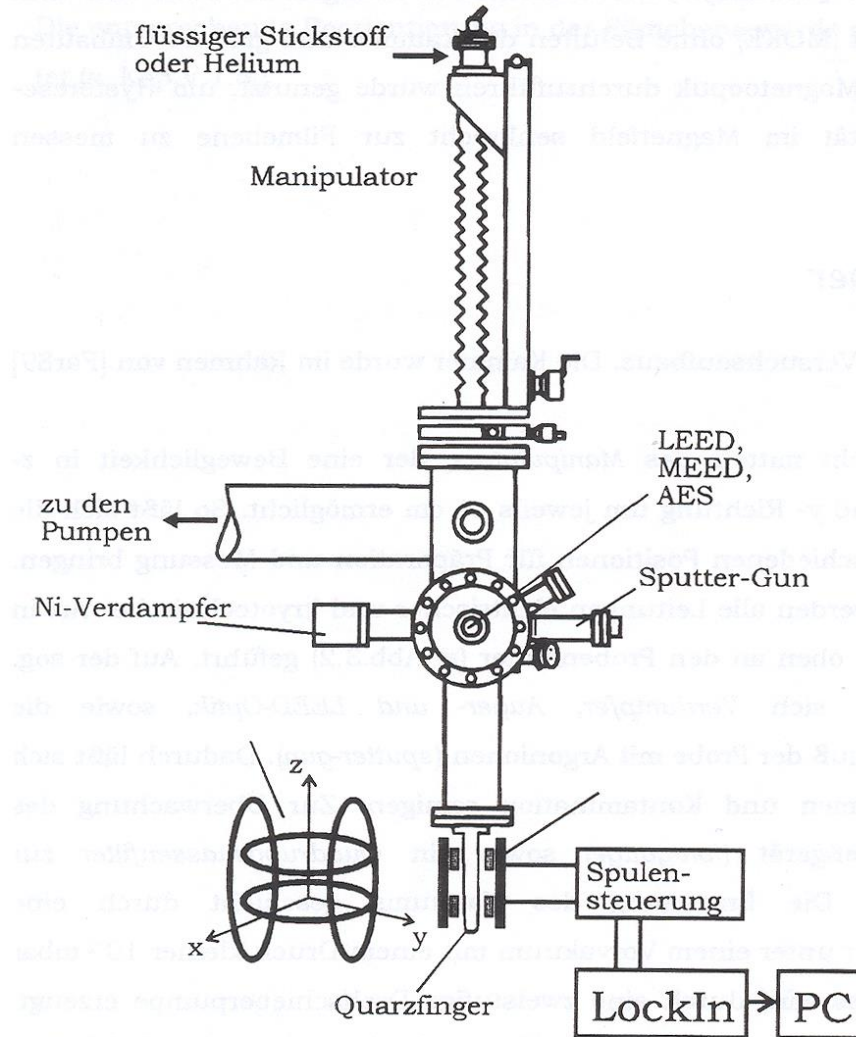


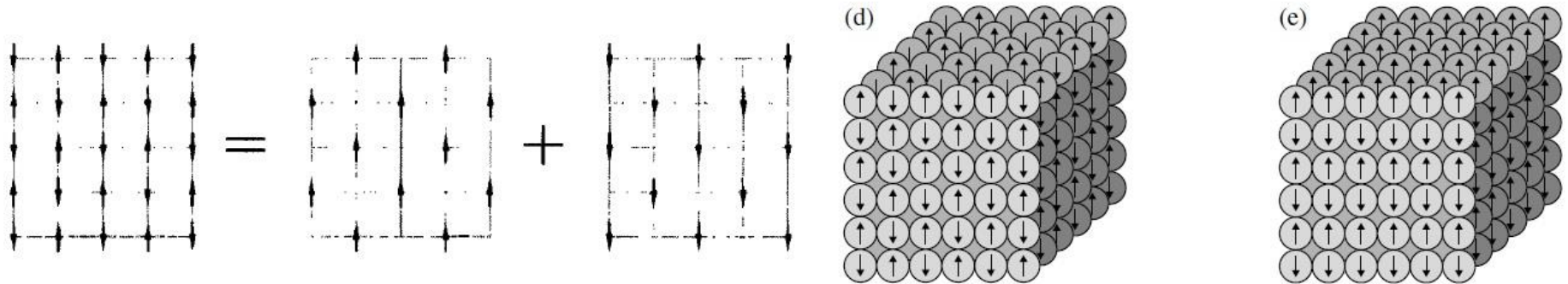
FIG. 2. Critical exponent  $\beta$  as a function of film thickness (error bars are given in Table I). The dashed lines show the theoretical values for a 3D Heisenberg, 3D Ising, and 2D Ising system. The shaded regime marks the crossover from 3D to 2D.

*Ni(111)/W(110), Y. Li and K. Baberschke  
Phys. Rev. Lett. 68, 1208-1211 (1992)*

# Experimental Setup



# Antiferromagnetism ( $J < 0$ )



Two interpenetrating sublattices, with same  $M$

$$\lambda < 0, B_+ = -|\lambda|M_- \text{ and } B_- = -|\lambda|M_+$$

$$M = MsB_J(g_J\mu_B J|\lambda|M/k_B T)$$

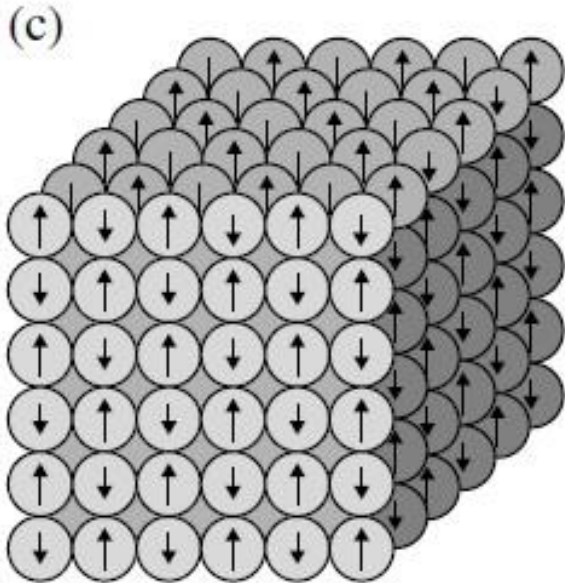
$$T_N = g_J\mu_B(J+1)|\lambda|Ms/3k_B$$

$X = \lim_{B \rightarrow 0} (\mu_0 M/B) \propto 1/(T+T_N)$  Curie-Weiss law

$X \propto 1/(T-\theta)$ ,  $\theta$  is the Weiss temperature

$\theta = 0$  (παρα-),  $< 0$  (αντισιδηρο-),  $> 0$  (σιδηρο)μαγνήτης

# Ferrimagnetism



Two interpenetrating sublattices, with different M

Classic example



The molecular field in each sublattice has different strength. Consequently we have two spontaneous magnetizations with different temperature dependence. The total M can change sign at the compensation point. Curie-Weiss law does not hold.



# Helical Order (Non-collinear Magnet)

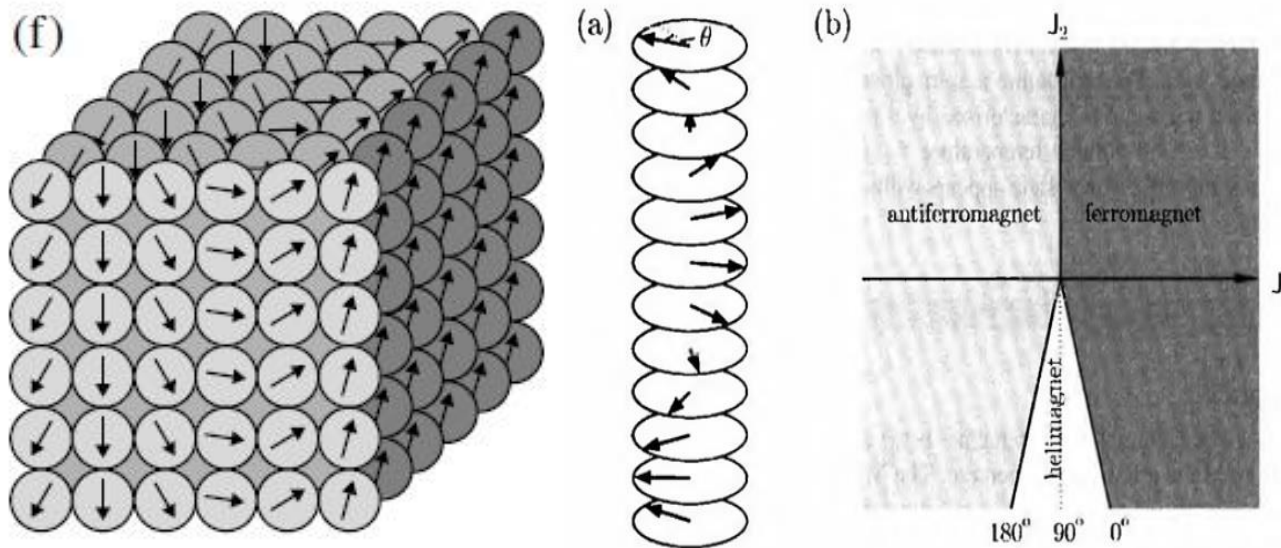


Fig. 5.15 (a) Helimagnetic ordering. (b) The phase diagram for the model of planes coupled by a nearest-neighbour exchange constant  $J_1$  and a next-nearest-neighbour exchange constant  $J_2$ .

This case is common for Rare Earths, e.g. Dy

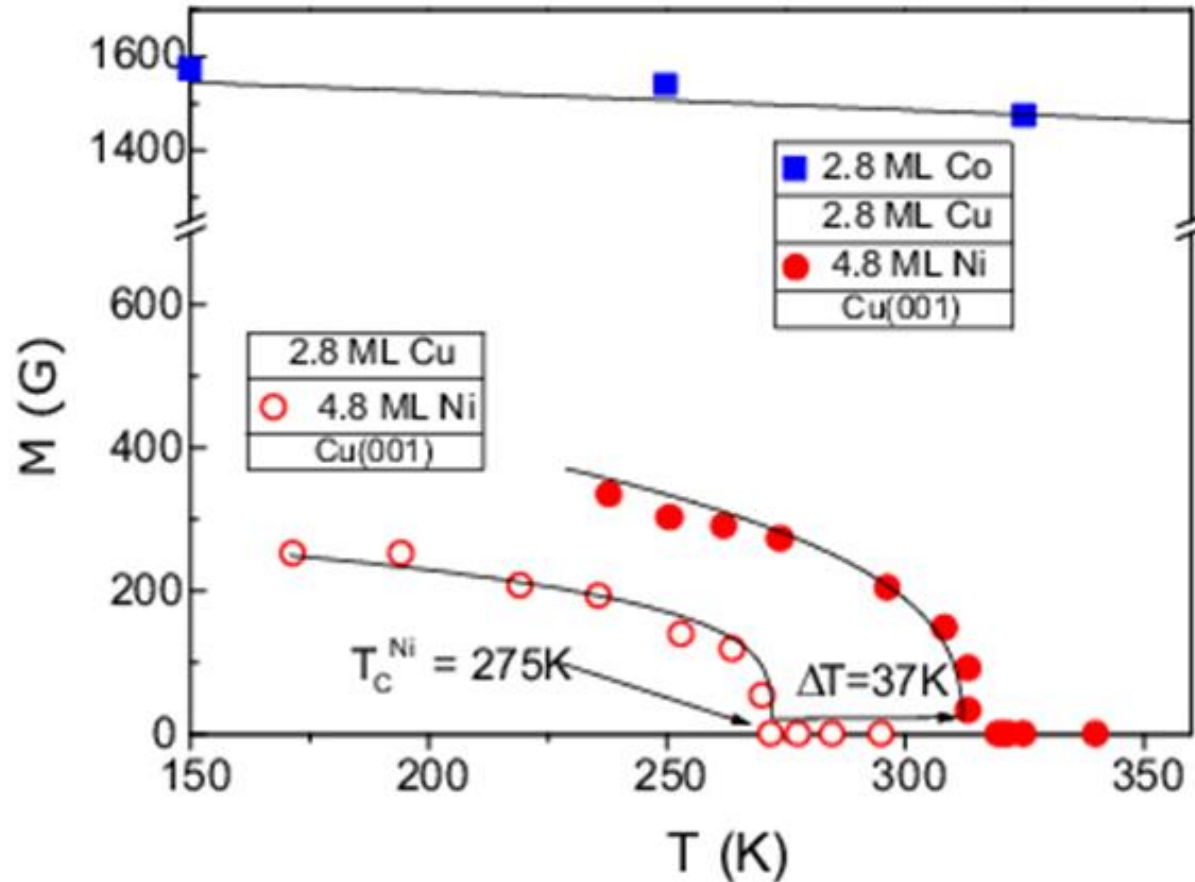
$$E = -2NS^2(J_1 \cos\theta + J_2 \cos 2\theta)$$

$$\partial E / \partial \theta = 0 \Rightarrow$$

$$(J_1 + 4J_2 \cos\theta) \sin\theta = 0 \text{ or}$$

$$\cos\theta = -J_1 / 4J_2$$

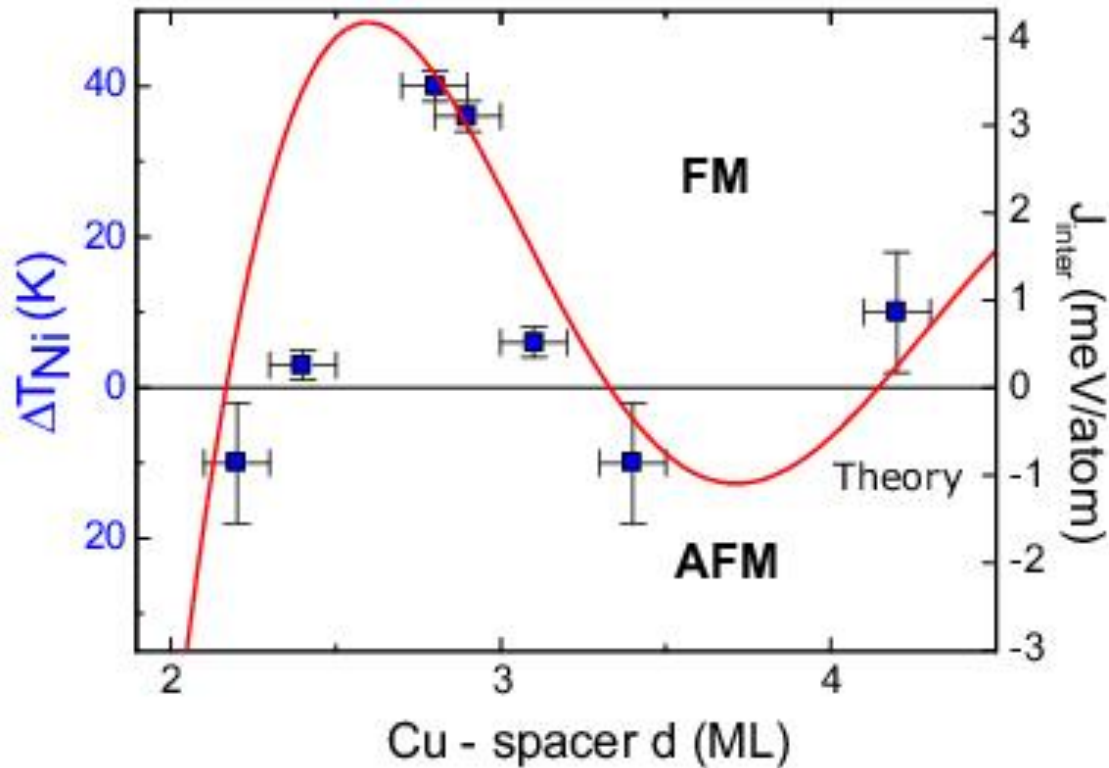
# Question: Influence of $J_{\text{inter}}$ on the $T_C$



*U. Bovensiepen et al., PRL 81, 2368 (1998)*

*Also P. Pouloupoulos and K. Baberschke, Wandlitz 2000.*

# Oscillations of $T_C$ with $J_{\text{inter}}$

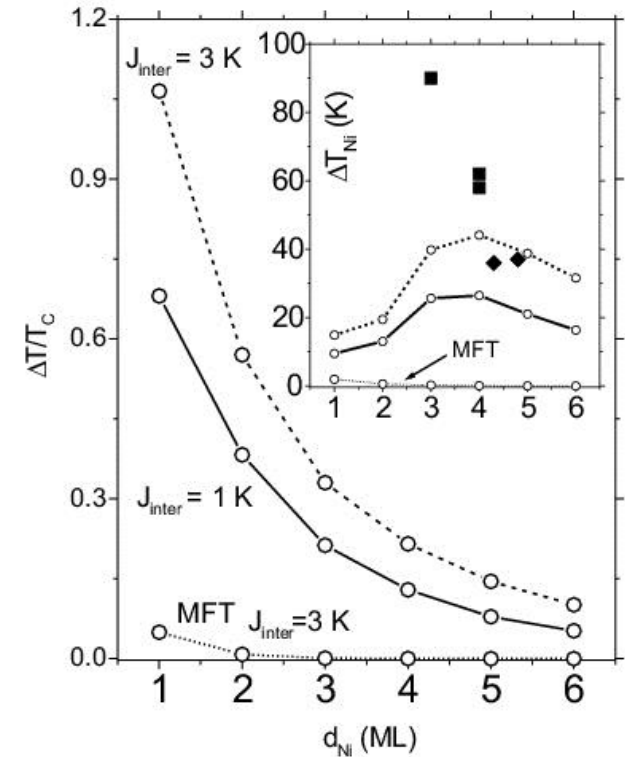
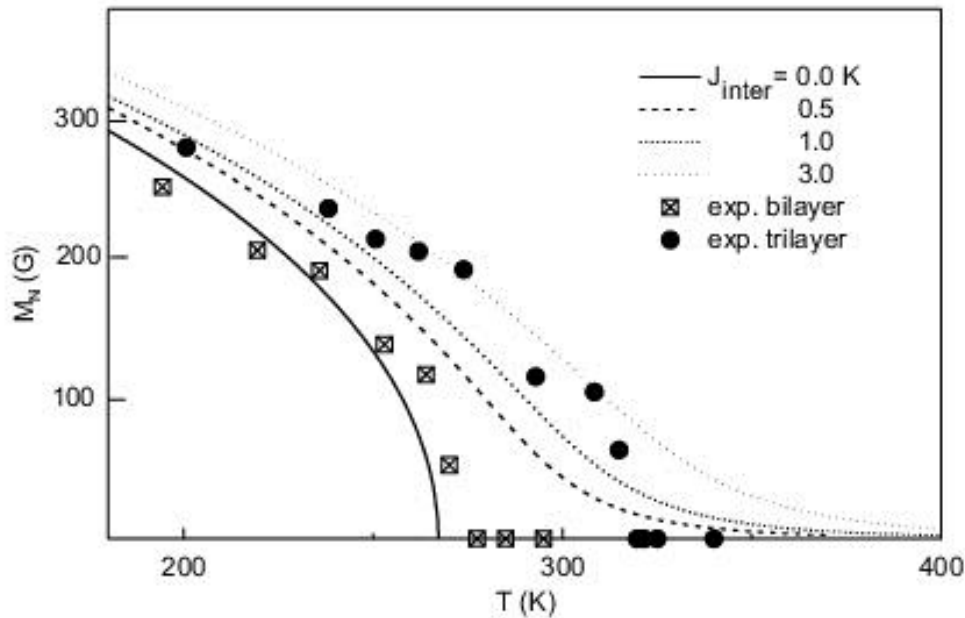


The calculation is based on the molecular field theory

*A. Ney et al., PRB59, R3938 (1999)*

*P. Pouloupoulos & K. Baberschke, J. Phys.: Cond. Matt. 11, 9495 (1999)*

# Reasonable explanation based on 2D-effects



*P. Jensen et al., PRB 60, 14994 (1999)*

*P. Jensen et al., JAP 87, 6692 (2000)*