Mean field theory of magnetic ordering

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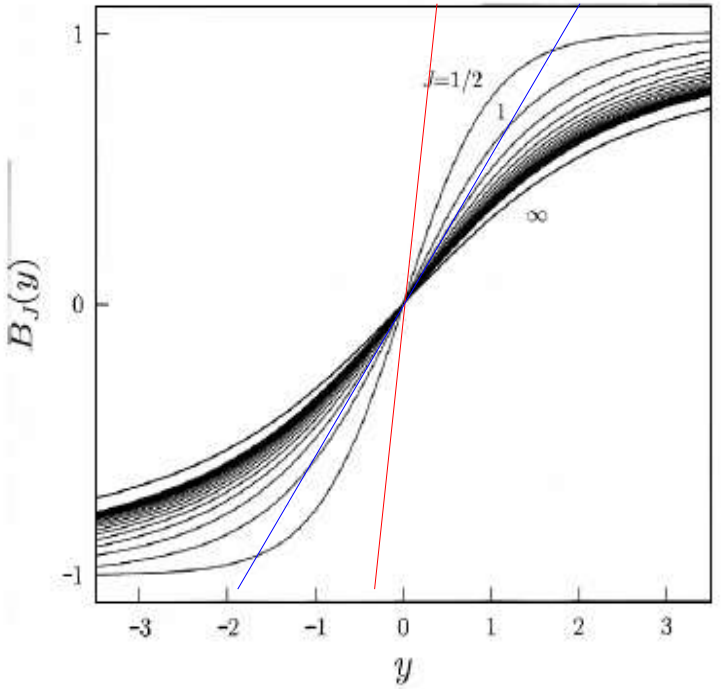


Literature

J.M.D. Coey, Magnetism and Magnetic Materials,
Cambride University Press, 628 pages (2010).
Very detailed

Stephen J. Blundell, Magnetism in Condensed Matter,
Oxford University Press, 256 pages (2001).
Easy to read, gives a condensed overview.

C. Kittel, Introduction to Solid State Physics,
John Whiley and Sons (2005)
Solid state aspects

Chapters of the two lectures

1. Classical approach
2. Interactions between magnetic moments
3. Magnetic phase transition in the mean field approximation
4. Thermodynamics and critical exponents
5. Magnetic orders
6. A sneak preview to quantum approach

Again size of Hilbert space

Atomic picture of quantum-mechanical moments is not feasible for even moderate numbers of atoms and even when we restrict ourself to the magnetic quantum numbers

Example: Already a cube of 3x3x3 Gd atoms, each with J=7/2, build a Hilbert space of $(2J+1)^{3*3*3}=8^{27} \approx 2.4 \times 10^{23}$ magnetic states

Again, we need to radically simplify the problem

Solution: **Describe the system as interacting classical magnetic moments**

$$-g_{JLS}\mu_B \frac{\hat{J}}{\hbar} \rightarrow -g_{JLS}\mu_B \frac{\vec{J}}{\hbar} = -\vec{\mu}$$

Q: Do we make a big mistake for ferromagnetic systems (magnetic moments aligned)? How about antiferromagnets (magnetic moments compensate)?

Dipole interaction

Each magnetic moment experiences the Zeeman energy caused by the magnetic field of each magnetic moment

$$E_D = \frac{\mu_0 g_{JLS}^2}{4\pi |r_{ij}|^3} \sum_{ij} \vec{J}_i \vec{J}_j - 3(\vec{J}_i \vec{r_{ij}})(\vec{J}_j \vec{r_{ij}})$$

Two atoms with 1 μ_B and 2Å distance results in 100μeV ~ 1K

Observed magnetic ordering temperatures of e.g. Fe of 1043K cannot be caused by dipolar interactions

We need a stronger interaction

Exchange interaction

Recall: exchange energy is the difference in Coulomb energy between symmetric and antisymmetric spatial wave functions and can be written as a product of spin operators

$$J = \frac{E_S - E_T}{2}, \; E_{ex} = -2\mathrm{J}\,\vec{S}_1\vec{S}_2$$

Coulomb potential at 2Å distance 7eV

J>0 : parallel spins are favoured (ferromagnetic coupling)
J<0: antiparallel spins are favoured (antiferromagnetic coupling)

Heisenberg model for N spins: $E = -\sum_{i,j=1}^{N} J_{ij}\vec{S}_i\vec{S}_j$

Electrons can be assumed as localized, as wave functions decay quickly and mainly nearest neighbors contribute to exchange (more details → Ingrid Mertig)

Nearest neighbor Heisenberg model: $E = -\sum_{i,j\ \mathrm{NN}} J\,\vec{S}_i\vec{S}_j$

Exchange interaction for delocalized electrons

In metals (e.g. Fe, Co, Ni) electrons are delocalized and form bands
Exchange interaction extends beyond nearest neighbors → Ingrid Mertig

Fe (bcc)			Co (fcc)			Ni (fcc)		
R_{0j}	N_s	J_{0j} (mRy)	R_{0j}	N_s	J_{0j} (mRy)	R_{0j}	N_s	J_{0j} (mRy)
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	8	1.432	$(\frac{1}{2}\frac{1}{2}0)$	12	1.085	$(\frac{1}{2}\frac{1}{2}0)$	12	0.206
(100)	6	0.815	(100)	6	0.110	(100)	6	0.006
(110)	12	−0.016	$(1\frac{1}{2}\frac{1}{2})$	24	0.116	$(1\frac{1}{2}\frac{1}{2})$	24	0.026
$(\frac{3}{2}\frac{1}{2}\frac{1}{2})$	24	−0.126	(110)	12	−0.090	(110)	12	0.012
(111)	8	−0.146	$(\frac{3}{2}\frac{1}{2}0)$	24	0.026	$(\frac{3}{2}\frac{1}{2}0)$	24	0.003
(200)	6	0.062	(111)	8	0.043	(111)	8	−0.003
$(\frac{3}{2}\frac{3}{2}\frac{1}{2})$	24	0.001	$(\frac{3}{2}1\frac{1}{2})$	48	−0.024	$(\frac{3}{2}1\frac{1}{2})$	48	0.007
(210)	24	0.015	(200)	6	0.012	(200)	6	−0.001
(211)	24	−0.032	$(\frac{3}{2}\frac{3}{2}0)$	12	0.026	$(\frac{3}{2}\frac{3}{2}0)$	12	−0.011
$(\frac{3}{2}\frac{3}{2}\frac{3}{2})$	8	0.187	$(2\frac{1}{2}\frac{1}{2})$	24	0.006	$(2\frac{1}{2}\frac{1}{2})$	24	0.001

Pajda et al. Phys. Rev. B 64, 17442 (2001)

Magnetic phase transition

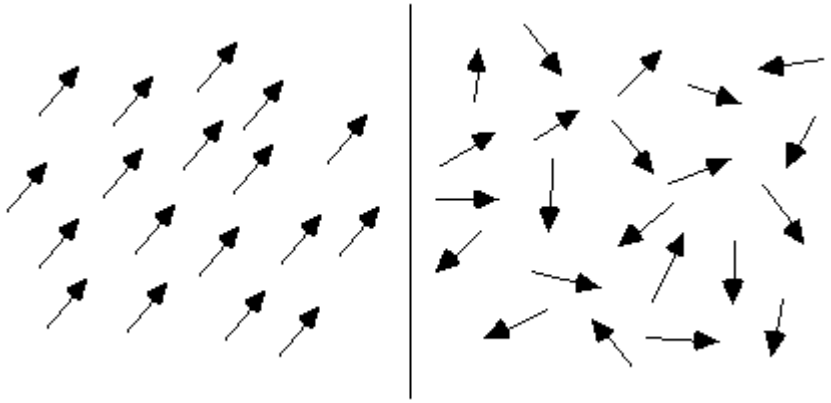
Phase transition between ordered (T<Tc) and disordered (T>Tc) phase

In ferromagnetic substances, moments progressively align in the ordered phase with lowering the temperature

A net magnetization or spontaneous magnetization is observed

Magnetic phase transition is of 2nd order, i.e. M continuously goes to zero when approaching Tc

Above Tc, the system is paramagnetic, and no spontaneous magnetization in present



$T<T_C$ $T>T_C$

Fe	1043K	EuS	16.5K
Co	1394K	GaMnAs	ca. 180K
Ni	631K		
Gd	289K		

Mean field approximation

Recall: magnetic moment in external magnetic field

Brillouin function gives average, i.e. mean value, of the projected magnetic moment along z

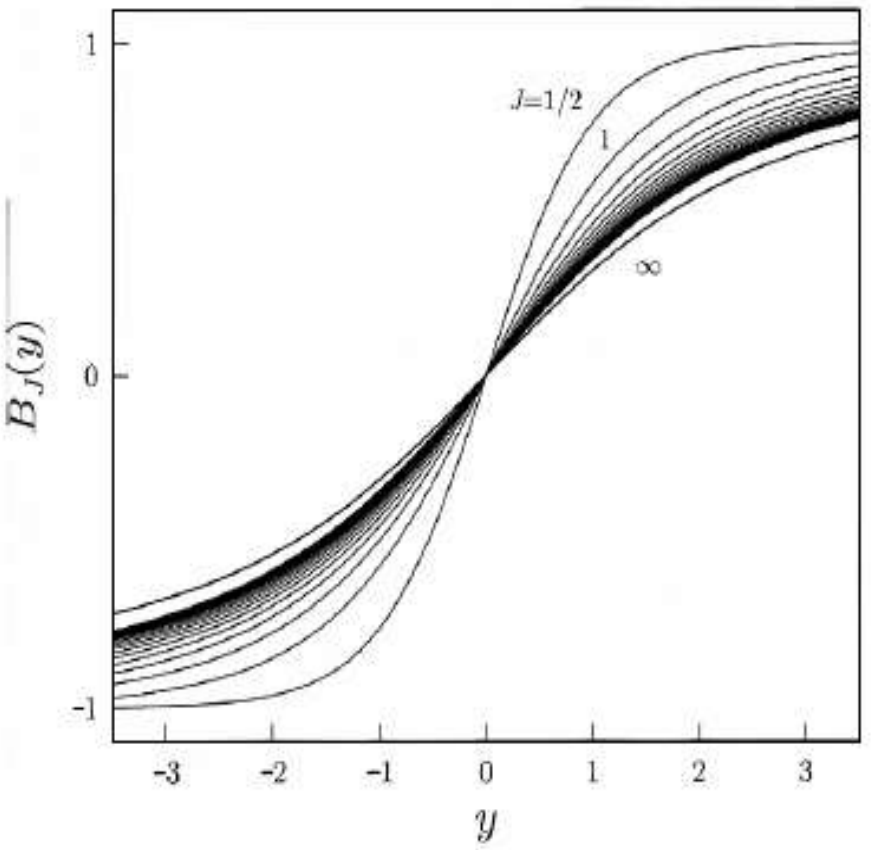
$$< \mu_z >= g\mu_B S B_S(y)$$

On average, a local magnetic moment feels the exchange interaction to its C nearest neighbours

This aligns the the local magnetic moment and can be thought of as an effective magnetic field B_e

$$< S_z >= S B_S(\frac{g\mu_B S(B + B_e)}{k_B T})$$

$$B_e = \frac{JC < S_z >}{g\mu_B}$$



$$y = \frac{g\mu_B SB}{k_B T}$$

Mean field approximation

$$< S_z >= SB_S(\frac{g\mu_B S(B + \frac{JC<S_z>}{g\mu_B})}{k_B T})$$

Result contains Brillouin function with argument of the result
Needs to be solved self consistently (graphically)

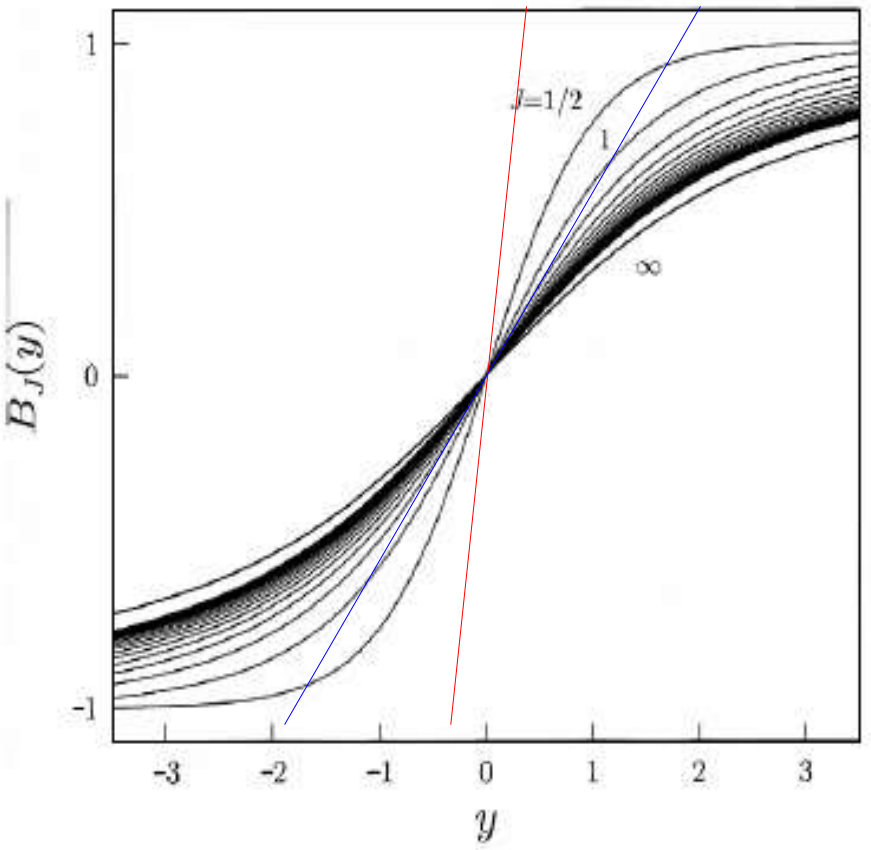
For high temperatures $\frac{B_e}{k_B T}$ is small, steep slope

Only one paramagnetic solution

For low temperature $\frac{B_e}{k_B T}$ is large, shallow slope

Spontaneous symmetry breaking with two solutions

Magnetization in ±z direction



$$y = \frac{g\mu_B SB}{k_B T}$$

Mean field approximation

For simplicity, we take S=1/2: $$< S_z >= \frac{1}{2}\tanh(\frac{\mu_B B + 2JC < S_z >}{k_B T})$$

With B=0 and $$x = \frac{2JC < S_z >}{k_B T}$$

we get: $$\frac{k_B T}{JC} x = \tanh x$$

The phase transition occurs when $$y = \frac{k_B T}{JC} x$$ is tangential to tanh x

$$\frac{k_B T_C}{JC} = 1, T_C = \frac{JC}{k_B}$$

$$\Rightarrow x = \frac{2JC}{k_B T} < S_z >= 2T_C/T < S_z >$$

Magnetization at low temperatures

At very low temperatures, we find: $T \to 0 \Rightarrow < S_z > \to \pm\frac{1}{2} \Rightarrow x \to \pm\infty$

$$\tanh x \approx \pm(1 - 2e^{-2x}), < S_z >= \pm\frac{1}{2}(1 - 2e^{-2T_c/T})$$

This looks like thermal activation, i.e. the reversal of individual spins in the saturated effective field (Boltzmann statistics)

Experiments deviate dramatically and find: $M(T) = M_0(1 - (T/T_C)^{3/2})$

There is no gap in the excitations spectrum

→ Michel Kenzmann

Magnetization at high temperatures

Near the Curie temperature, we find: $T \to T_C^- \Rightarrow < S_z > \to 0 \Rightarrow x \to 0$

$$\tanh x \approx x - x^3/3, < S_z > = (T_C/T) < S_z > + 4/3(T_C/T)^3 < S_z >^3$$

$$\Rightarrow < S_z > = (3/4(1 - T/Tc))^{\frac{1}{2}}$$

When approaching Tc, the magnetization vanishes with a critical exponent β=1/2

Agrees with Landau theory → Laurent Chapon

Specific heat

Inner energy for B=0: $E(T) = -\sum_{i,j=nn} 2J\vec{S}_i\vec{S}_j = -2NCJ < S_z >< S_z >= -2NCJ < S_z >^2$

Specific heat: $C_m = \frac{\partial E}{\partial T} = -4NCJ < S_z > \frac{\partial < S_z >}{\partial T}$

T>Tc (<Sz>=0): $C_m = 0$

When approaching Tc: $T \to T_C^-, E(T) = -\frac{3NJC}{2}(1 - T/T_C)$

$$\Rightarrow C_m = \frac{2NJC}{2T_C} = \frac{3}{2}Nk_B$$

Specific heat jumps at Tc, 2nd order phase transition

Entropy at Tc

$$S(T_C) = \int_0^{T_C} \frac{C_m(T)dT}{T} = -4NJC \int_0^1 \frac{< S_z > d < S_z >}{T}$$

$$= \frac{Nk_B}{2} \int_9^1 \ln \frac{1+x}{1-x} dx = Nk_B \ln 2$$

This, we could have had much easier

Susceptibility above Tc

Above Tc and at small fields, the magnetization is small

$$< S_z >= 1/2 \tanh(\frac{g\mu_B S(B + \frac{J<S_z>}{g\mu_B})}{k_B T} \approx \frac{\mu_B B + 2CJ < S_z >}{k_B T}$$

$$= \frac{\mu_B B}{k(t - T_C)}$$

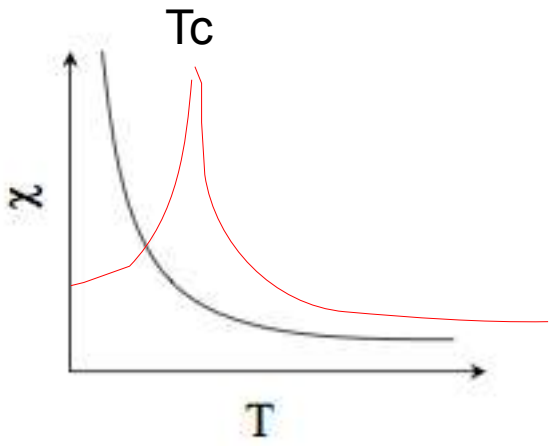
Susceptibility: $\chi = \frac{\partial M}{\partial B} \propto \frac{1}{T - T_C}$

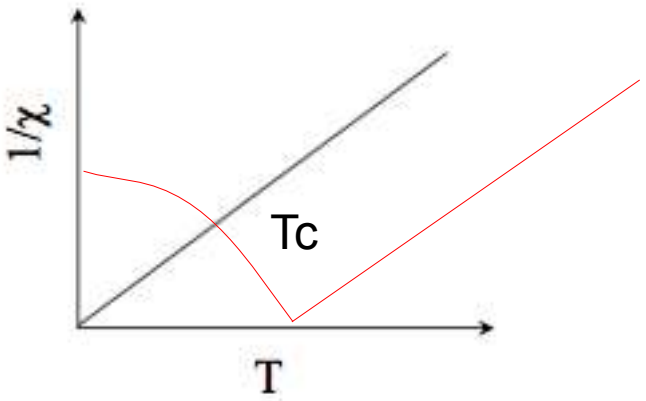
Above the Curie temperature, the system behaves as a paramagnet with susceptibility shifted to T+Tc

Below the Curie temperature, the mean field approximation does not give a meaningful answer

Susceptibility above Tc

Curie - Weiss





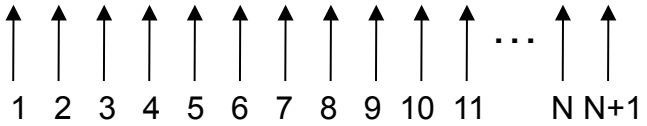
Critical exponents

$$M_S \propto |T_C - T|^{\beta} \qquad M_{T=T_C} \propto \pm |H|^{1/\delta}$$
$$\chi \propto |T - T_C|^{-\gamma} \qquad \xi \propto |T_C - T|^{-\nu}$$

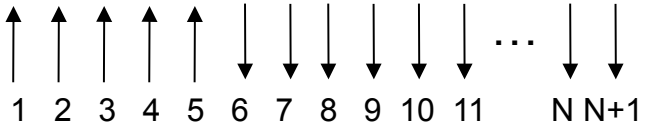
Exponent	β	γ	δ	ν
Landau-Theory	0,5	1	3	0,5
2d-Ising	0,125	1,75	15	1
2d-XY	0,23	2,2	10,6	1,33
3d-Ising	0,325	1,240	4,816	0,630
3d-XY	0,345	1,316	4,810	0,669
3d-Heisenberg	0,365	1,387	4,803	0,705

Ising : spin can only point along ±z direction
XY : spin lies in the xy-plane
Heisenberg : spin can point in any direction in space
Landau : classical theory

The 1D-Ising chain



One domain wall



Energy cost: $\Delta E = \frac{J}{2}$

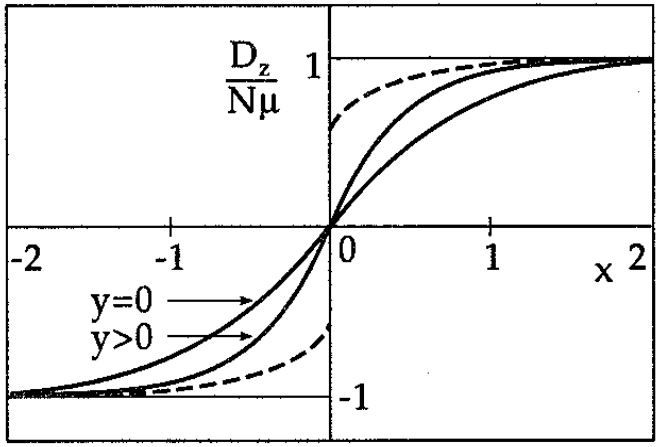
Entropy gain: $\Delta S = k_B \ln(N)$

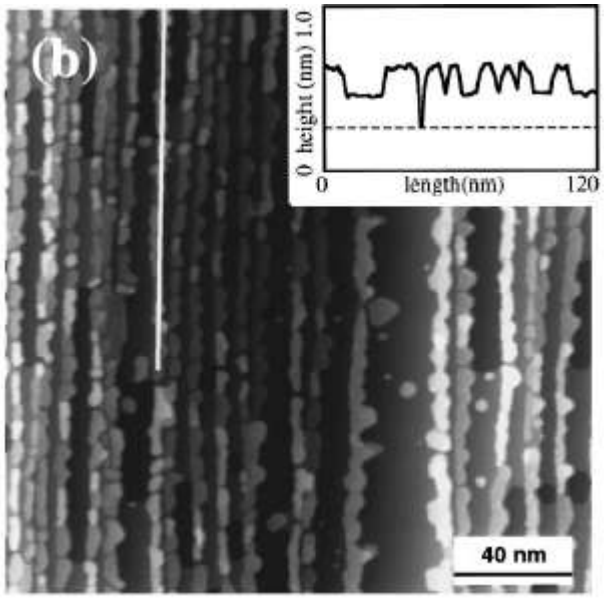
long Ising chain: $N \to \infty \Rightarrow \Delta S \to \infty$

$$F = (U + \Delta E) - T \underbrace{(S + \Delta S)}_{\to \infty} \to -\infty$$

Entropy always wins and no ordering occurs

1D Ising chain



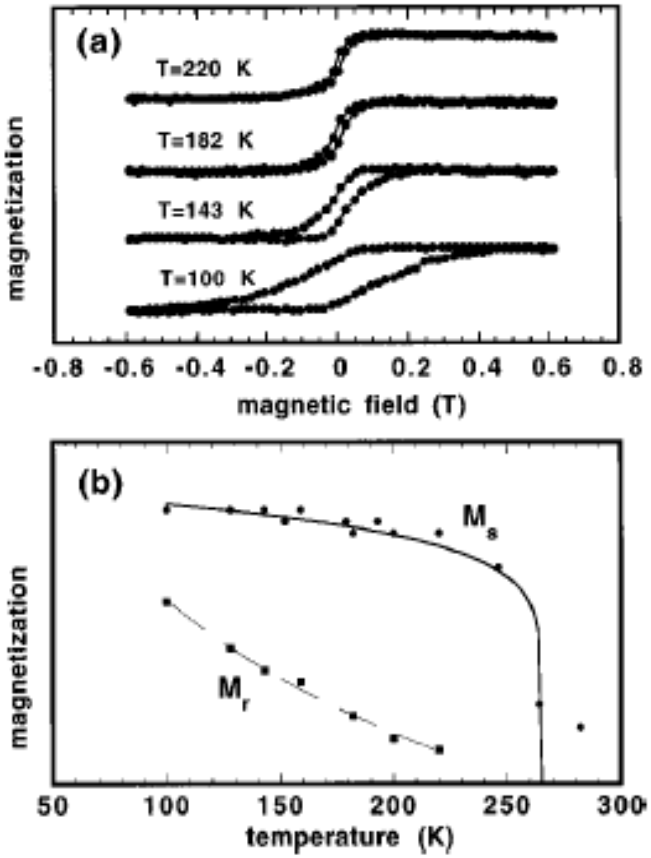


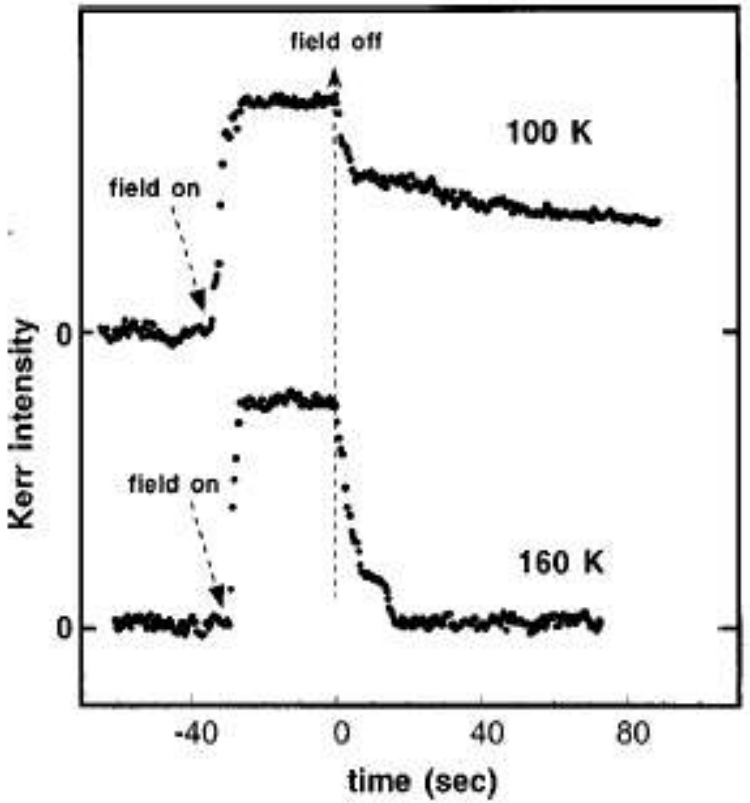
M=0 for H=0 independent of temperature.

Experimental realisation by step edge decoration of Cu(111) steps with Co.

Co shows magnetization perpendicular to the plane due to surface anisotropy.

Glauber dynamic



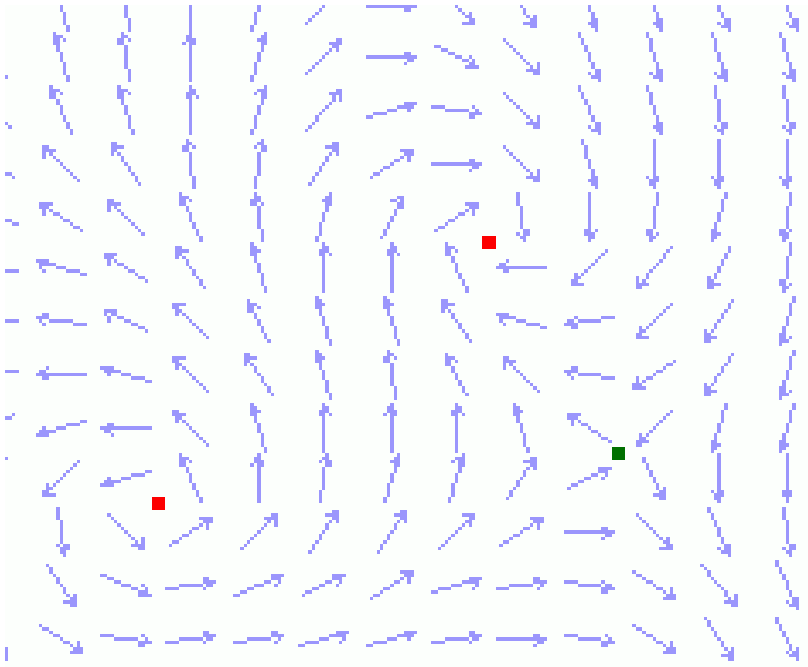


Experiment shows remanence in the MOKE loop.
Magnetization is only metastable.

J.Shen Phys. Rev. B (1997)

The Mermin-Wagner theorem

Similar to the Ising model, the Mermin-Wagner theorem predicts Tc=0K for three dimensional spins in two dimensions that interact via the exchange interaction



A Kosterlitz-Thouless phase transition (self similar vortex state) is predicted for T=0

2D Heisenberg - model

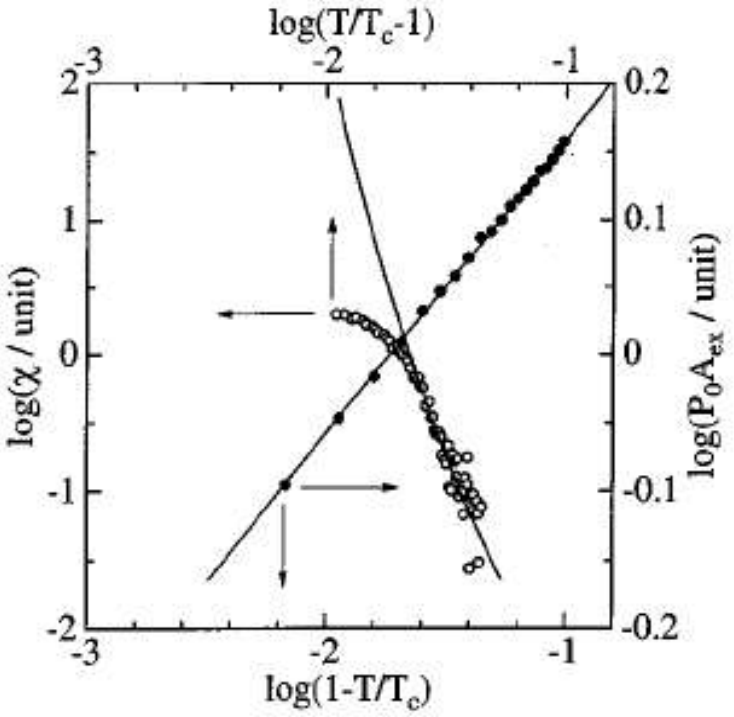


FIG. 3. Double logarithmic plot of susceptibility χ(○) and spontaneous magnetization M(●) vs reduced temperatures (data from Fig. 2). The full lines represent fits to the power law and to the exponential law, respectively

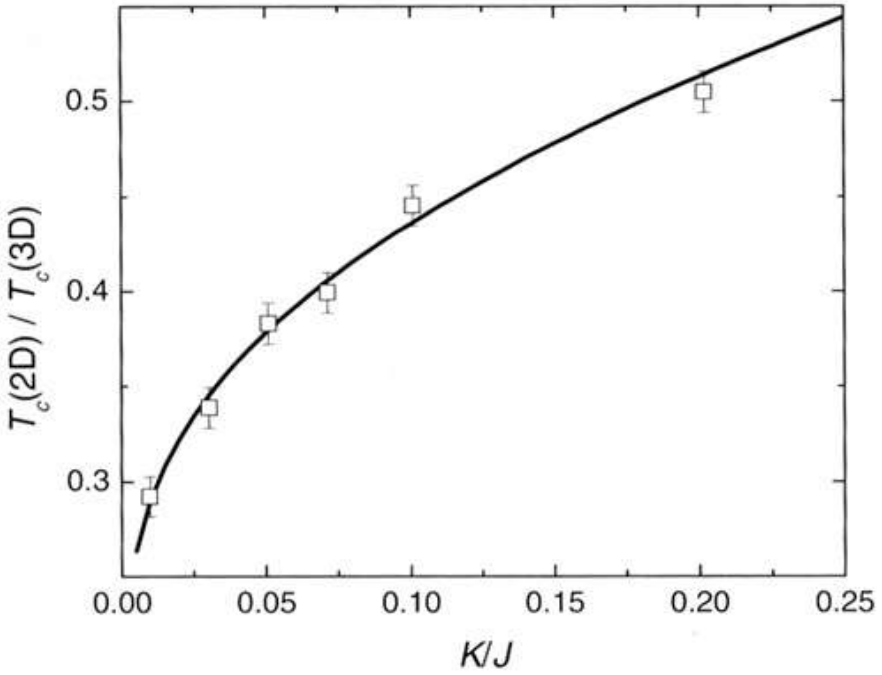
2 atomic layers of Fe/W(100)

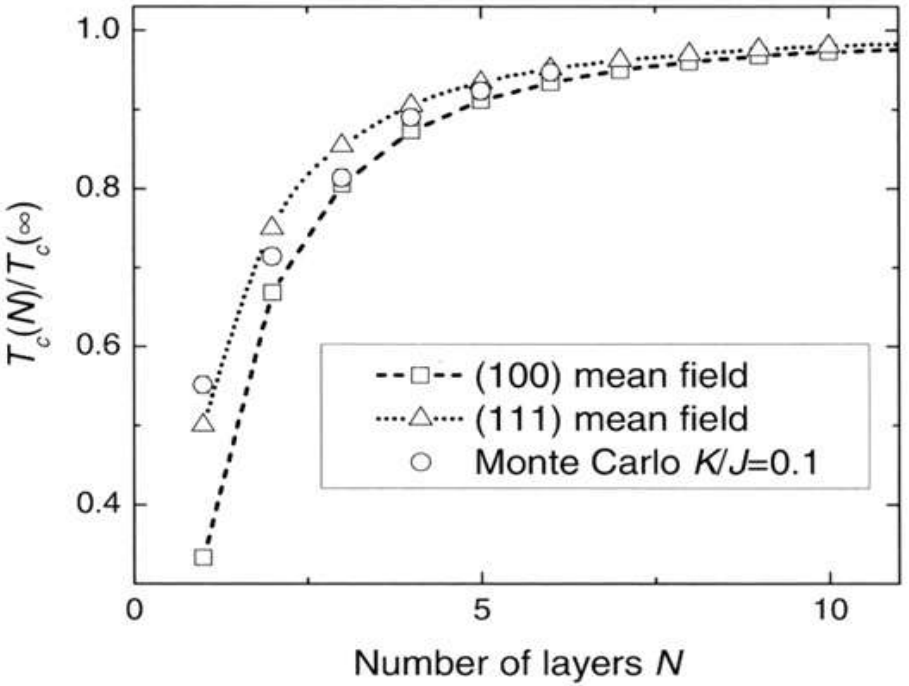
Two easy direction in the film plane, hard axis normal to the plane

Expected ordering temperature 0K, observed 207K

HJ Elmers, J. Appl. Phys. (1996)

Limits of the Mermin-Wagner theorem

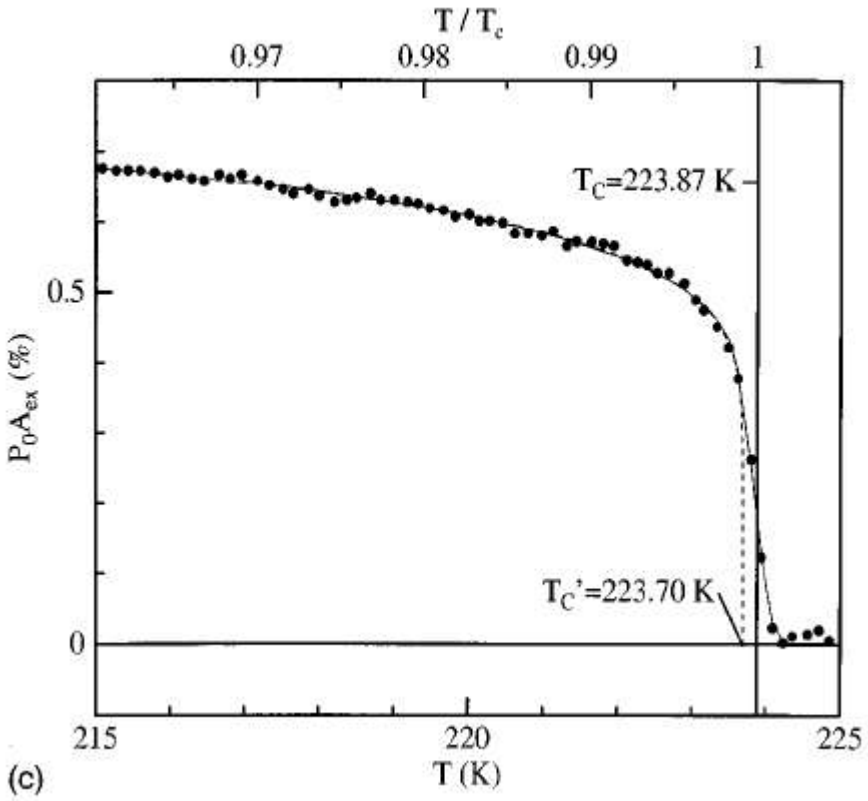




Even slightest anisotropies lead to break down of Mermin-Wagner theorem. A magnetization for T>0 results.

When film thickness increases, the ordering temperature of the 2D-system Quickly approaches that of the 3D system.

1 ML Fe/W(110): 2D-Ising



Uniaxial magnetic anisotropy in the film plane results in 2D Ising model

Critical exponent: β=0.133 (0.125)

HJ Elmers, Phys. Rev. B (1996)

The fluctuation-dissipation theorem

For T>0, any system is thermally fluctuating $S_z = S_z(t)$

The autocorrelation function describes the spectrum of the fluctuations

$$S_z(\omega) = \int_{-\infty}^{+\infty} S_z(t) e^{i\omega t} dt, P(\omega) = |S_z(\omega)|^2$$

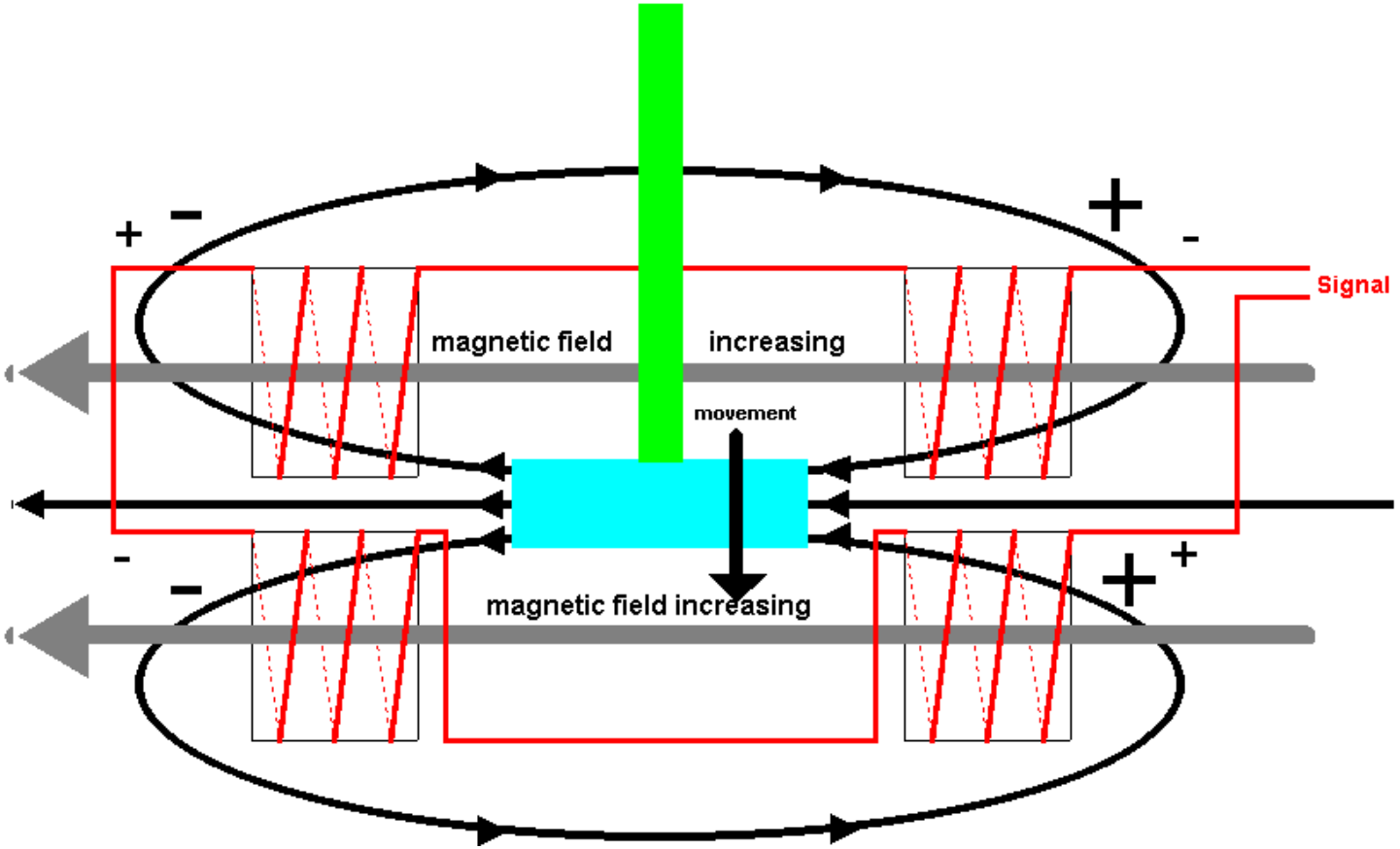
Fluctuations are small deviations from the equilibrium

Also external stimulus can lead to small deviations (linear response)

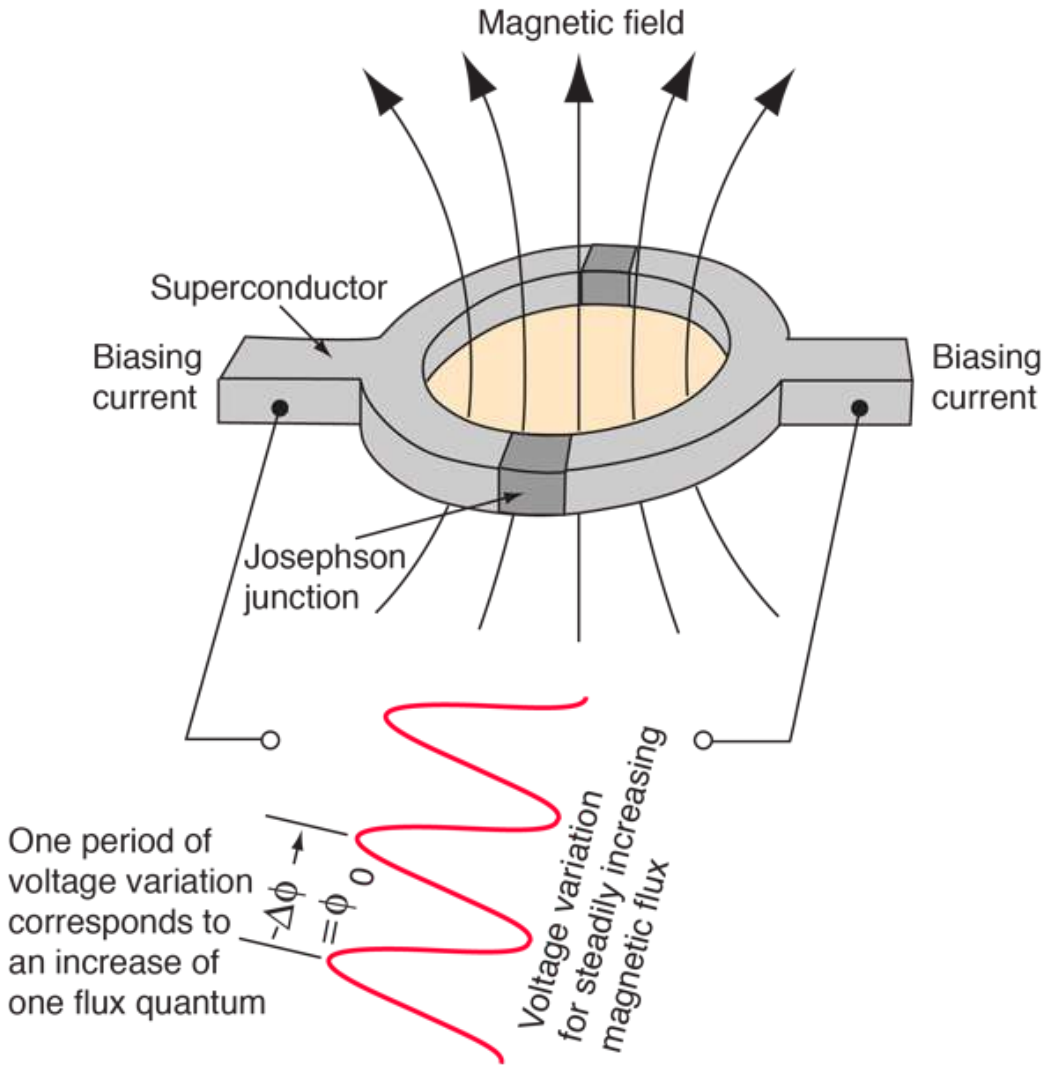
The two scenarios are linked: $P(\omega) = \frac{2K_B T}{\omega} \mathrm{Im}\chi(\omega)$

Fluctuations are linked to dissipation in the system

Vibrating sample magnetometer

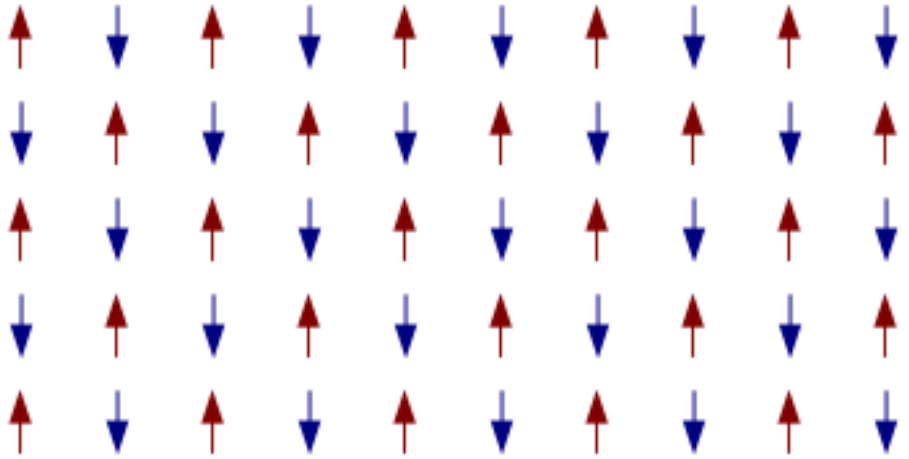


SQUID



Antiferromagnets

J<0
Spins align antiparallel below T_N



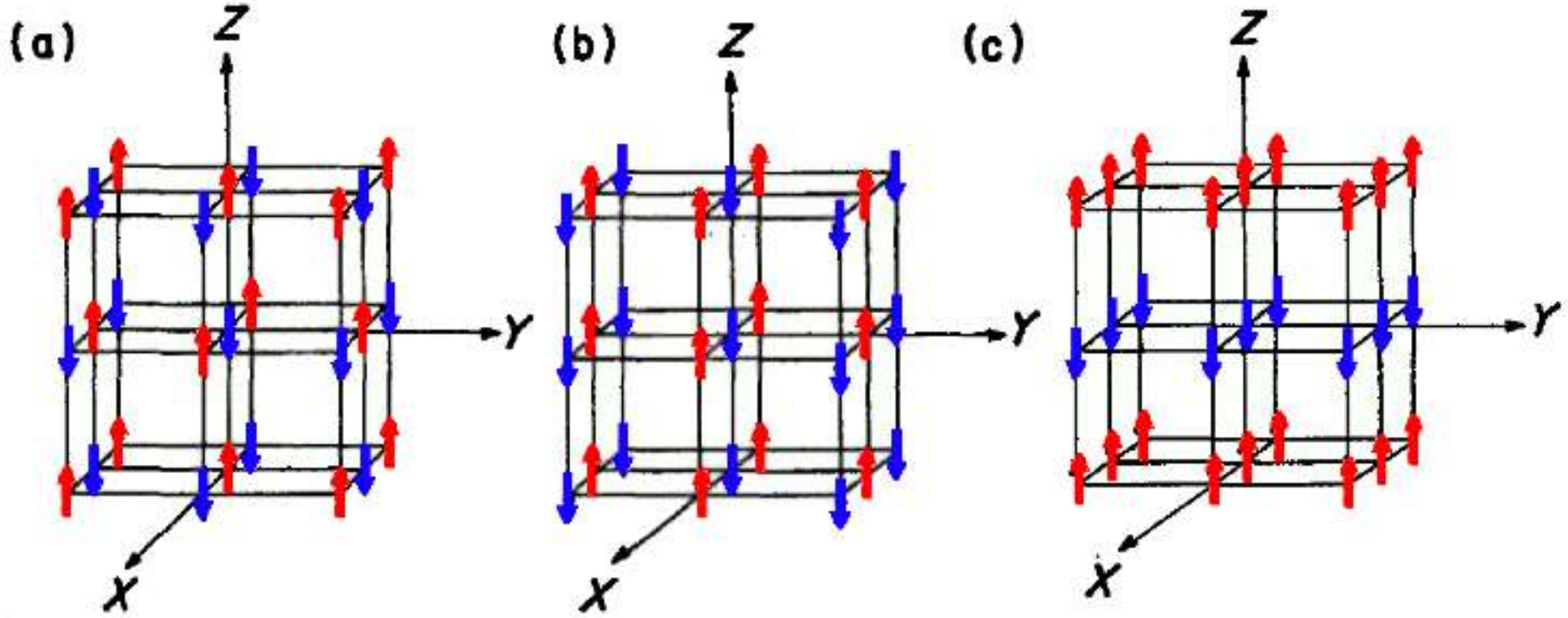
Elements : Mn, Cr …
Oxides : FeO, NiO …
Semiconductors : URu_2Si_2 …
Salts : MnF_2 ...

Above Néel temperature T_N, they become paramagnetic

Cr	297K
FeO	198K
NiO	525K

Can be described by two or more ferromagnetically ordered sub-latices
Moments in magnetic unit cell compensate

Antiferromagnets



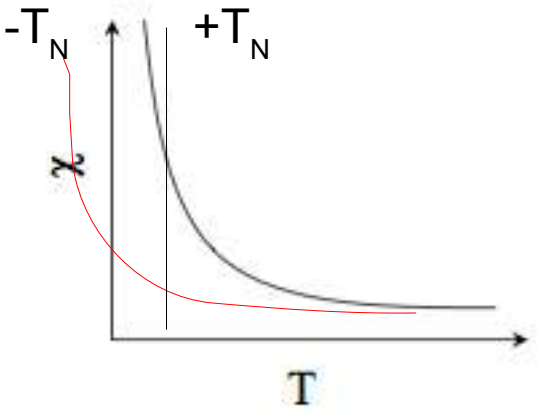
Depending on the crystal structure, many different antiferromagnetic configurations may exist

Antiferromagnets

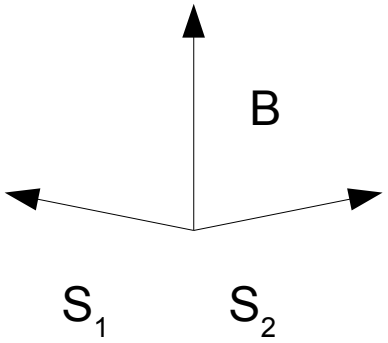
Susceptibility above T_N:

$$\chi = \frac{\partial M}{\partial B} \propto \frac{1}{T + T_N}$$

Maximum at T_N but no singularity



Susceptibility below T_N:



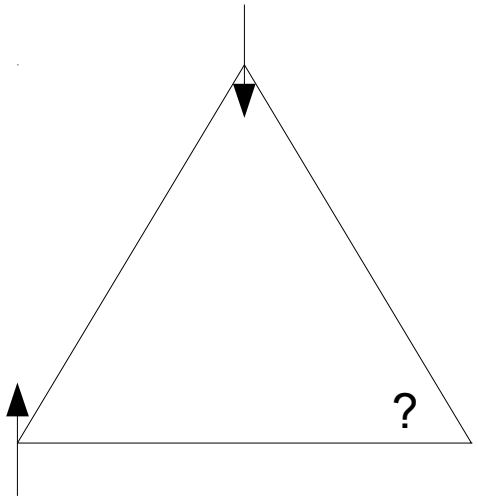
If the field is applied normal to the direction of the spins the Zeeman energy rotates the spins versus the exchange

Exchange is not temperature depended and thus χ is constant

Antiferromagnets

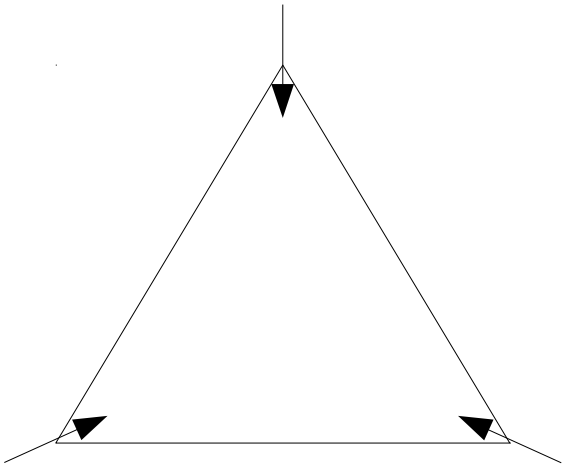
Frustrated systems

$$E_{ex} = 2\mathrm{J}\,\vec{S}_1\vec{S}_2 + 2\mathrm{J}\,\vec{S}_2\vec{S}_3 + 2\mathrm{J}\,\vec{S}_3\vec{S}_1$$



$$E_{ex} = 2\,J\,S^2$$

Interactions cannot be satisfied



$$E_{ex} = 2\times 3\,J\cos(120\,°)\,S^2 = 3\,J\,S^2$$

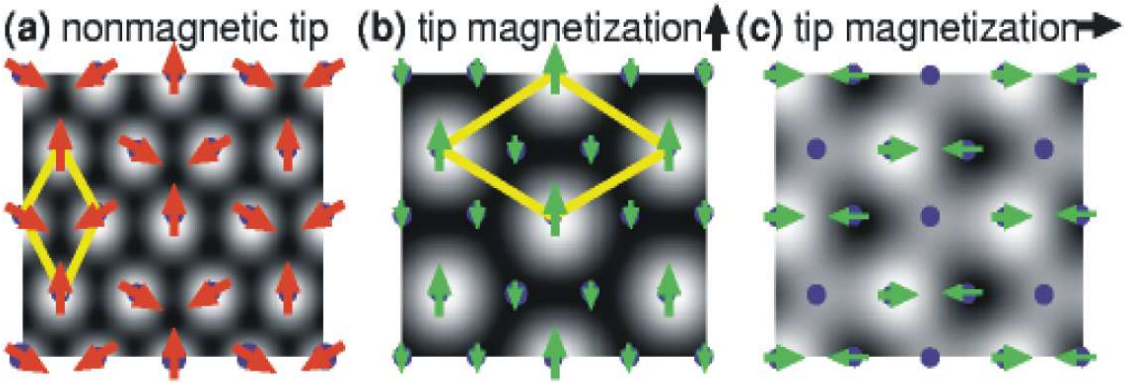
Energetic compromise with 120° angles (Néel state)

Also happens in 3D in fcc crystals (triple q structure)

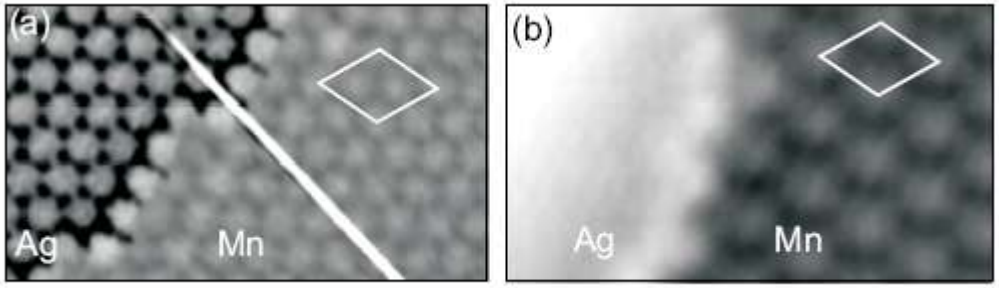
Antiferromagnets

Sp-STM: Mn/Ag(111)

Theory:



Experiment:



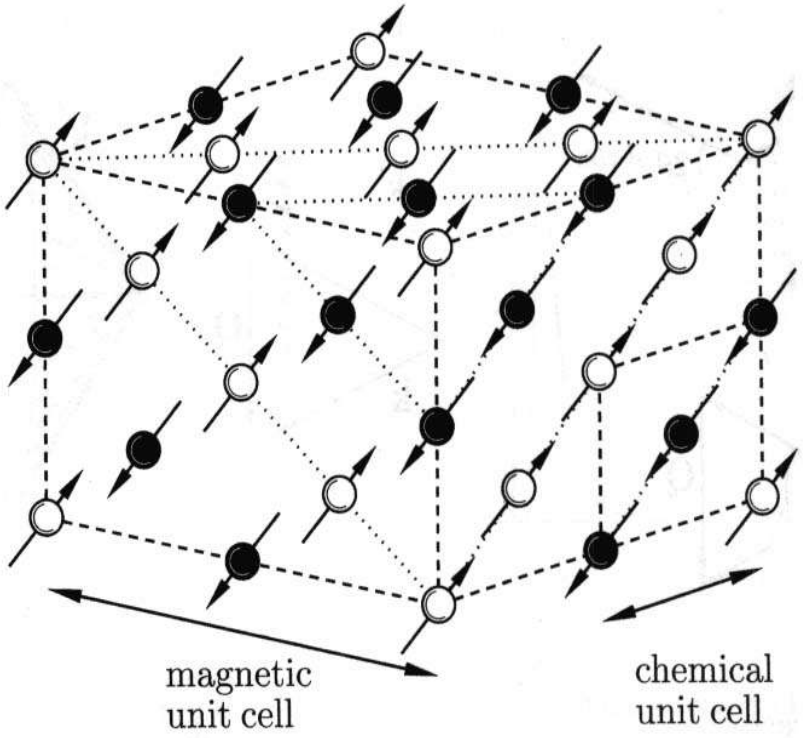
Gao, Wulfhekel, Kirschner, Phys. Rev. Lett. (2008)

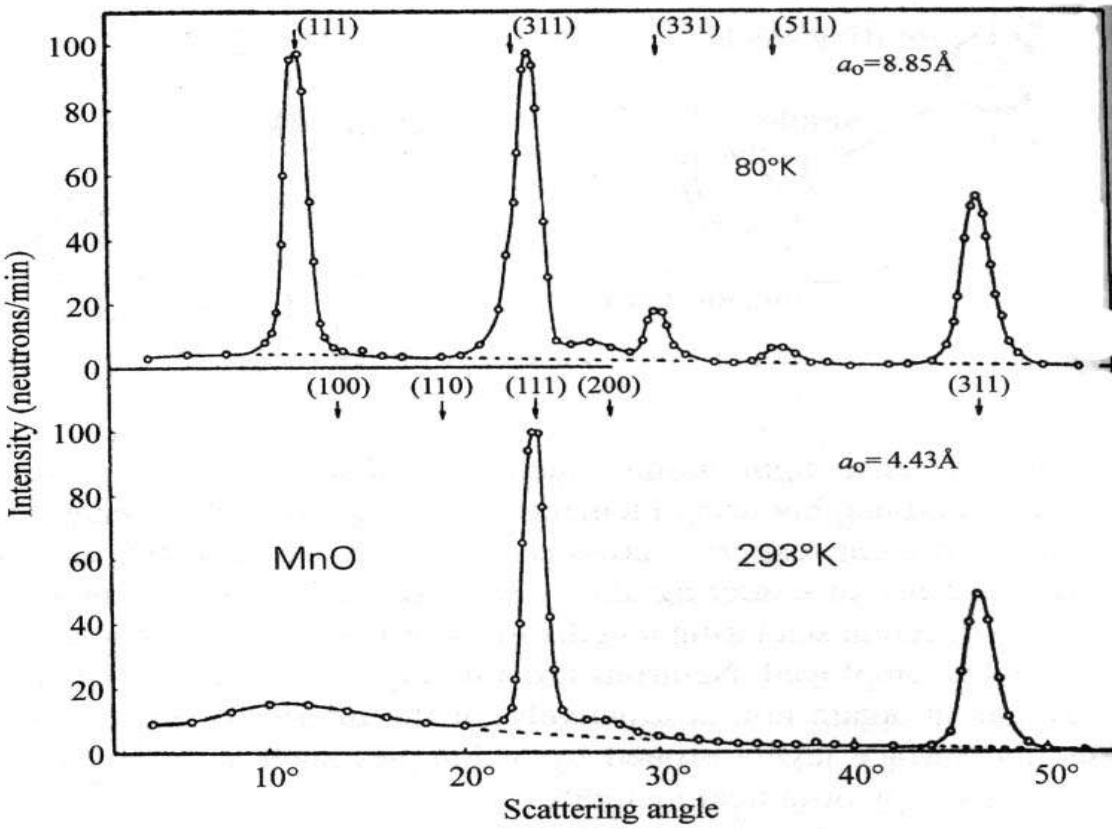
Neutron scattering

MnO

T_N(MnO)=121K

Neutron diffraction pattern

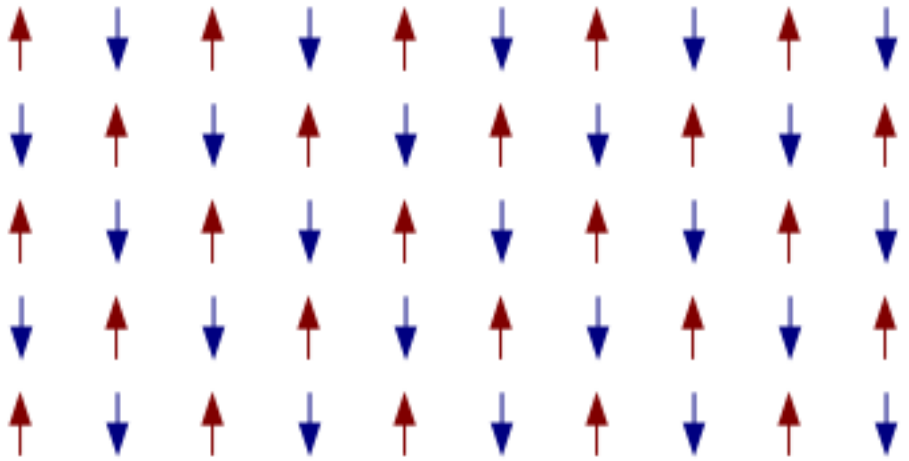




Mechanism: magnetic moment of neutron interacts with magnetic moment of sample resulting in scattering depending on the local magnetic moment

Ferrimagnets

J<0
Spins align antiparallel below T_C



Atoms of the different sublattices have different magnetic moment

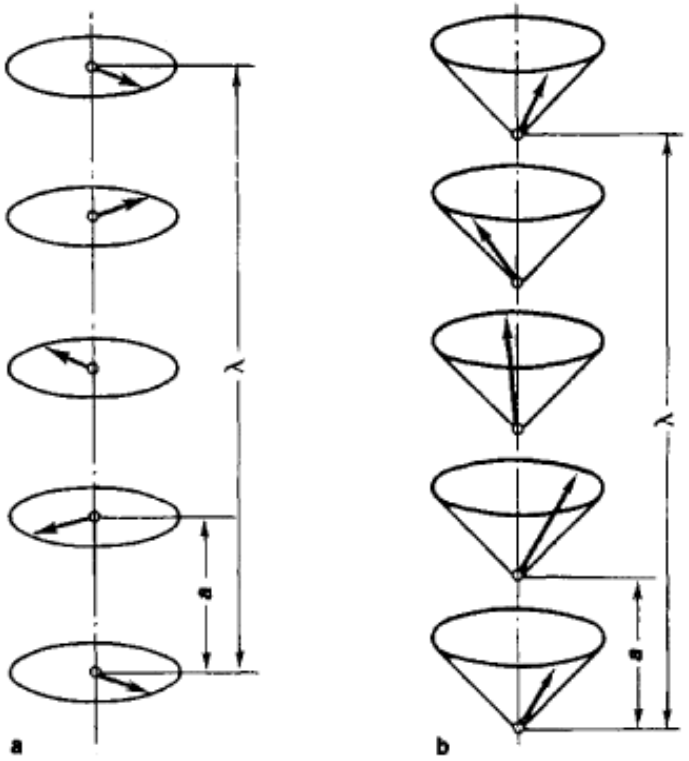
Total magnetization does not vanish

Examples: ferrites and manganites (e.g. Fe_2O_3)

Helimagnets

Nearest neighbor interaction ferromagnetic

Due to antiferromagnetic next-nearest neighbor interaction or Dzyaloshinkii-Moriya interaction a slight tilt between neighbors is induced and a spiral is formed



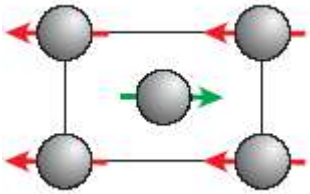
Examples:

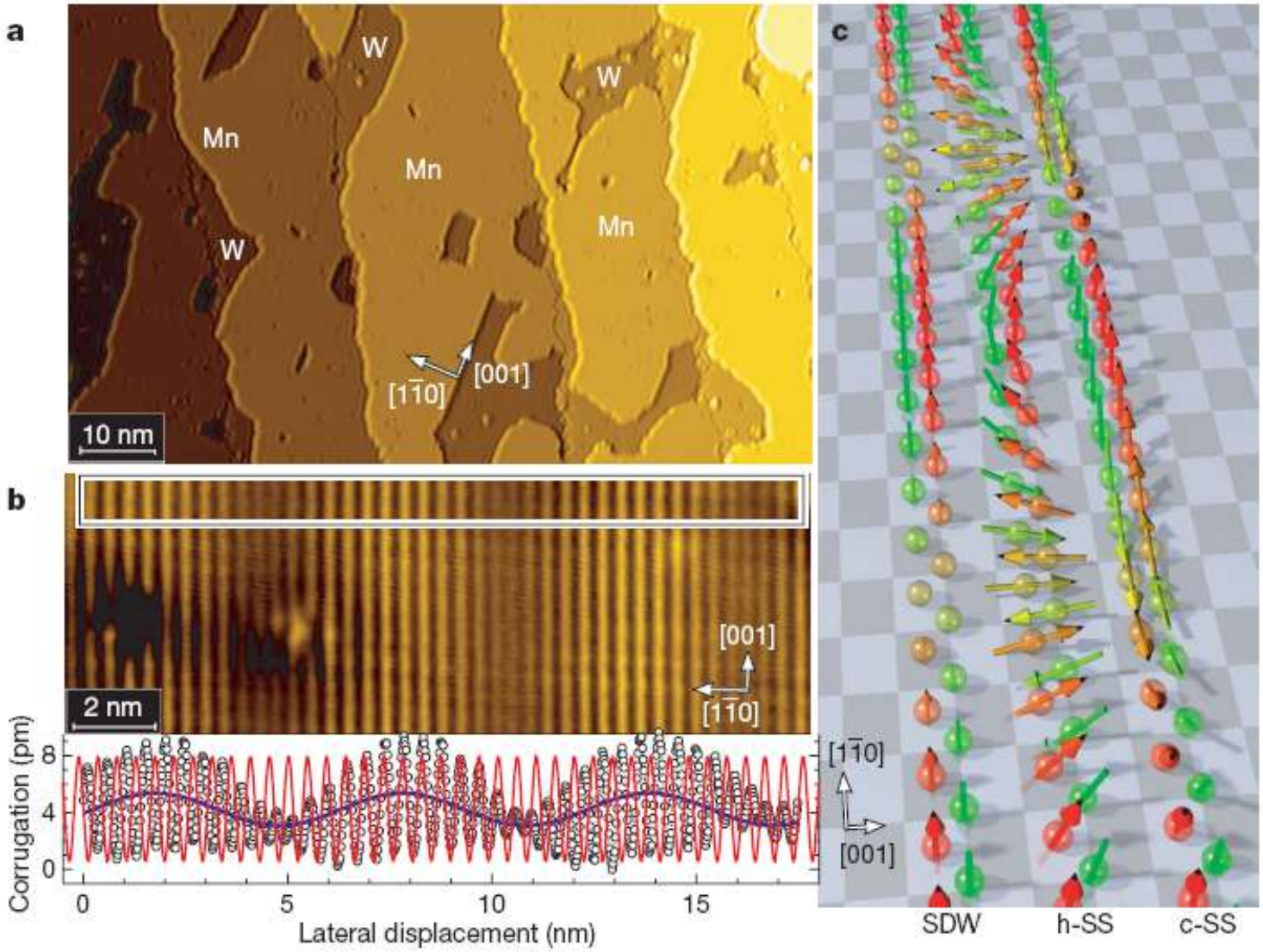
Rare earth magnets

Non-centrosymmetic crystals (MnSi)

Dzyaloshinsky-Moria Interaction observed with STM

1 ML Mn auf W(110)





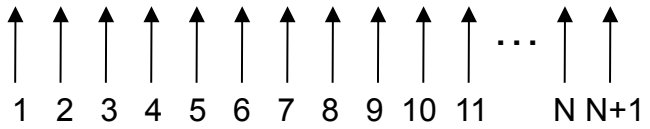
M.Bode et al., Nature (2007)

Ferromagnets

Classical solution (all moments parallel) and quantum solution (all S_z components e.g. maximal) both describe states of maximal total spin momentum, which is very large

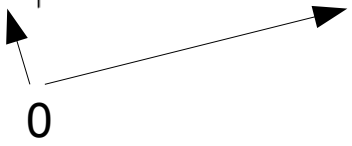
Correspondence principle holds

Quantum-mechanical eigenstate: symmetric spin states with Sz=+S

$\psi =$ 

This state is an eigenstate:

$$\hat{H}^{ii+1} = -2J\hat{S}_z^i\hat{S}_z^{i+1} - J\hat{S}_+^i\hat{S}_-^{i+1} - J\hat{S}_-^i\hat{S}_+^{i+1}$$

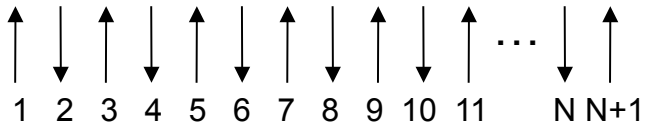


Antiferromagnets

Classical solution (moments antiparallel) has a vanishing total spin momentum

Correspondence principle will not hold

Quantum-mechanical eigenstate is unknown →



This state is not an eigenstate:

$$\hat{H}^{ii+1} = -2J\hat{S}_z^i\hat{S}_z^{i+1} - J\hat{S}_+^i\hat{S}_-^{i+1} - J\hat{S}_-^i\hat{S}_+^{i+1}$$

One of these is 0, the other flips both spins

→Michel Kenzelmann

Spin of an antiferromagnet

For a state of 3 antiferromagnetically coupled spins of spin 5/2, we find:

Ground state wave function is doublet with

$$\hat{S} = \hat{S}_1 + \hat{S}_2 + \hat{S}_3 \qquad < \hat{S}_z >= \pm\frac{1}{2}$$

Even large antiferromagnets may have a small net moment