Models in Magnetism

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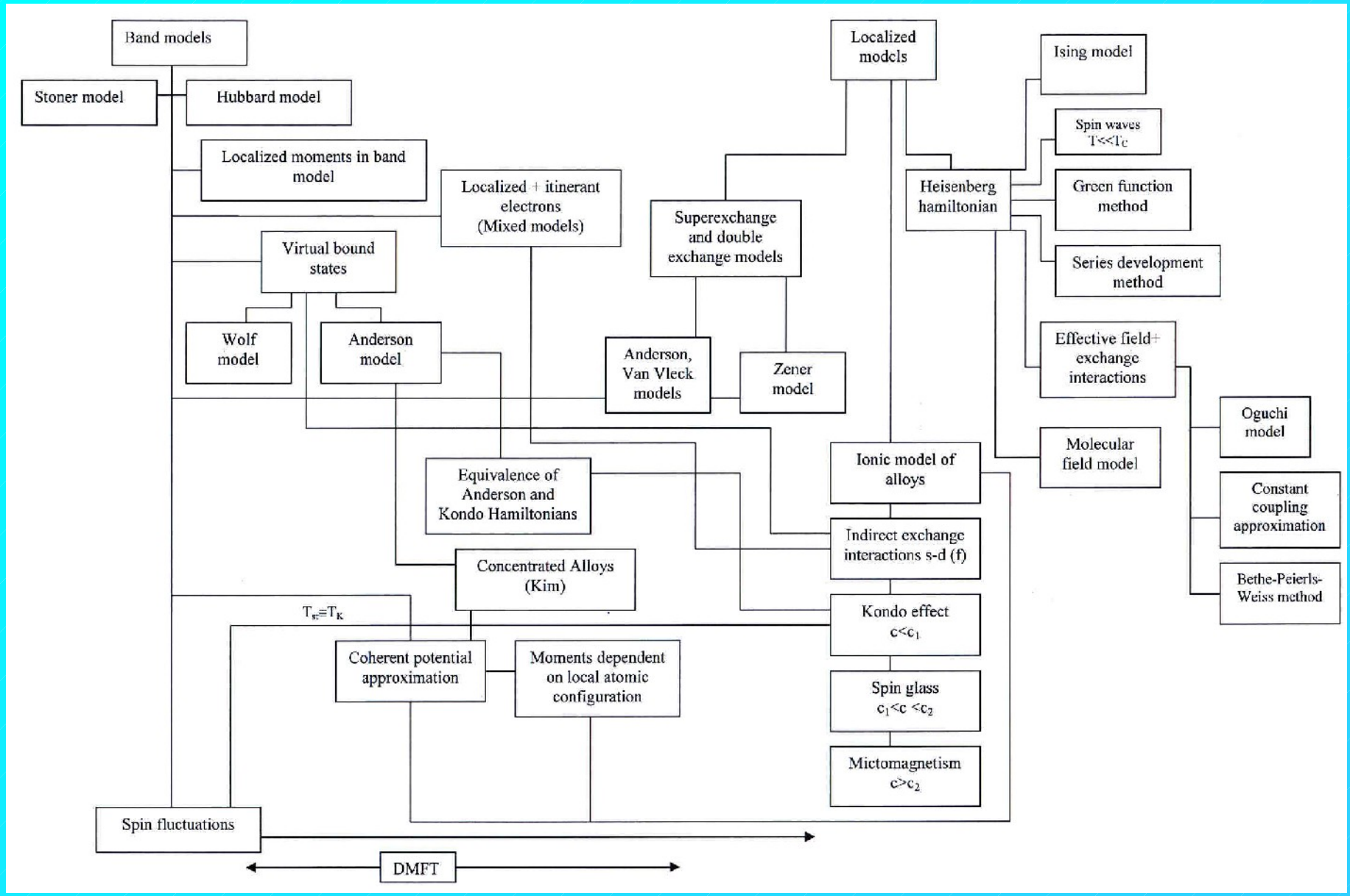
Short review:

- basic models describing the magnetic behaviour
- connections between models


Band models
Stoner model
Hubbard model
Localized moments in band model
Localized + itinerant electrons (Mixed models)
Virtual bound states
Wolf model
Anderson model
Equivalence of Anderson and Kondo Hamiltonians
Concentrated Alloys (Kim)
$T_{sf}=T_K$
Coherent potential approximation
Moments dependent on local atomic configuration
Spin fluctuations
DMFT
Localized models
Superexchange and double exchange models
Anderson, Van Vleck models
Zener model
Ionic model of alloys
Indirect exchange interactions s-d (f)
Kondo effect $c<c_1$
Spin glass $c_1<c<c_2$
Mictomagnetism $c>c_2$
Ising model
Spin waves $T<<T_C$
Heisenberg hamiltonian
Green function method
Series development method
Effective field+ exchange interactions
Molecular field model
Oguchi model
Constant coupling approximation
Bethe-Peierls-Weiss method

General problems

Dimensionality of the system, d;

Moments coupled:

all space directions d=3

in a plane d=2

one direction d=1

polymer chain d=0

Phase transition:

Existence of a boundary at d=4,

spatial dimensionality can be also continous, ε=

Number of magnetization components, n

Heisenberg model n=3

X-Y model n=2

Ising model n=1

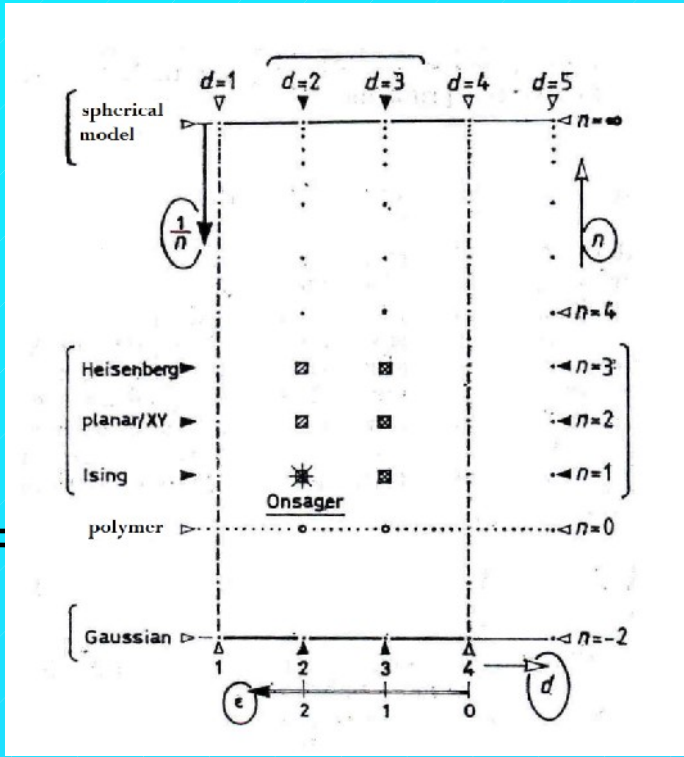
Phase transitions:

n→∞ spherical model (Stanley, 1968)

n=-2 Gaussian model

n can be generalized as continous

For d ≥ 4, for all n values, critical behaviour can be described by a model of molecular field approximation



Comparison with experimental data

magnetization versus temperature M=f(T)

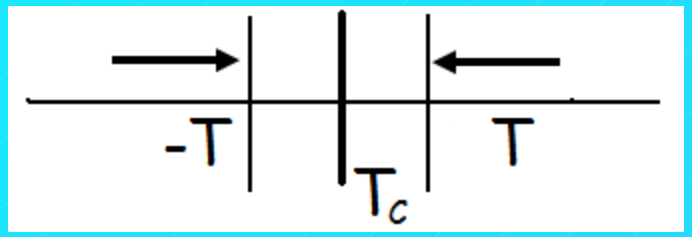
magnetic susceptibility χ=f(T)

behaviour in critical region

$$\frac{M(T)}{M(O)} \propto t^{\beta}$$

$$\chi \propto t^{-\gamma}$$

$$cp \propto t^{-\alpha}$$



$$t = \frac{|T_C - T|}{T_C} \leq 10^{-1} - 10^{-2}$$

Transition metals: 3d Fe,Co,Ni

Fe g= 2.05-2.09

Co g=2.18-2.23

Ni g=2.17-2.22

Moments due mainly to spin contribution

For 3d metals and alloys

Moments at saturation $\mu = gS0$,

Effective magnetic moments $\mu_{eff} = g\sqrt{S_p(S_p+1)}$

generally r=Sp/So>1

Rare-earths: 4f shell presence of spin and orbital contribution

Magnetic insulators: localized moments

Localized moments:

Heisenberg type Hamiltonian: exchange interactions

$$\mathcal{H} = \sum_{i,j} J_{ij} \mathbf{S}_i \mathbf{S}_j$$

Jij exchange integral direct n=3 system

Difficulty in exact computation of magnetic properties: many body problem

Approximations

Ising model (Ising 1925)

Exact results in unidemensional and some bidimensional lattices

$$\mathcal{H} = -2J \sum_{i,j} S_{iz} S_{jz}$$

- **Unidimensional**

neglect the spin components $\perp$ **H**

strong uniaxial anisotropy

- **Linear Ising lattice** : not ferrromagnetic

$$\chi \cong \frac{1}{T} \exp(2J/k_B T)$$

- **Square bidimensional** lattice, J1,J2

M=[1-(sh2k1sh2k2)-2]1/2 Onsager (1948)

$k_1 = \frac{J_1}{k_B T}$, $k_2 = \frac{J_2}{k_B T}$ Yang (1952)

- **Tridimensional** lattice: series development method
- **Spherical Ising model** (Berlin-Kac, 1951)

arbitrary values for spins but $\sum_i S_i^2 = ct$

can be solved exactly in the presence of an external field

d≥4; critical exponents are independent of d and of the geometry of the system

Molecular field models :

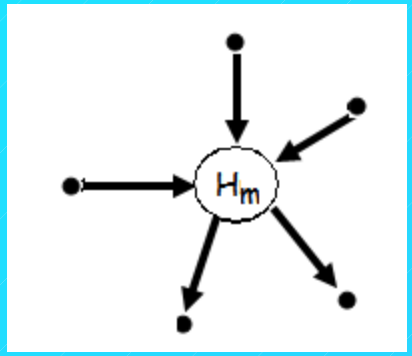
Methods which analyse exactly the interactions in a small part of crystal, and the interactions with remaining part are described by an effective field, Hm , self consistently determined:

small portion $\rightarrow$atom (molecular field approach Weiss (1907)

- Magnetic domains
- Molecular field: aligned magnetic moments

in the domains

Hm=NiiM



Total field HT=H+Hm; M=χ0H$\rightarrow$M=χ0(H+NiiM)$_{\chi} = \frac{\chi_0 H}{1 - N_{ii}\chi_0}$

Self consistency:

$$M = \chi_0 H + N_{ii}\chi_0 M = \chi_0 H + N_{ii}\chi_0(\chi_0 H + N_{ii}\chi_0 M) =$$

$$= \chi_0 H(1 + N_{ii}\chi_0) + (N_{ii}^2 \chi_0^2) M =$$

$$= \chi_0 H[1 + (N_{ii}\chi_0) + (N_{ii}\chi_0)^2 + (N_{ii}\chi_0)^3 + \ldots =$$

$$= \frac{\chi_0 H}{1 - N_{ii}\chi_0} = \chi H$$

Reverse reaction: corrections are time distributed: n correction after n-1 one

Molecular field:

act at the level of each particle

$$\mathcal{H}_m = -2J_{ij}\mathbf{S}_i\sum_{j=1}^{z}\mathbf{S}_j$$

$$\mathcal{H}_m = -g\mu_0\mu_B\mathbf{S}_i\mathbf{H}_m$$

$$N_{ii} = \frac{2zJ_{ij}}{Ng^2\mu_B^2\mu_0}$$

$S \rightarrow J$

$M(T) = M(0)B_J(x) \qquad x = \dfrac{\mu_0\mu_B g J H_T}{k_B T}$

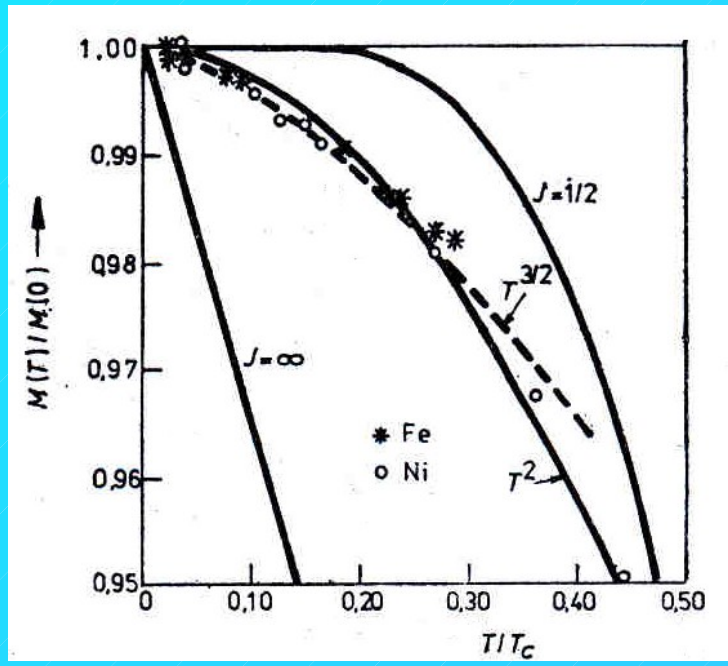
Low temperatures $\dfrac{M(T)}{M(0)} = 1 - \dfrac{1}{J}\exp\left(\dfrac{-3\ T_C}{J+1\ T}\right) + \cdots$

experimental $\dfrac{M(T)}{M(0)} \propto T^{3/2}$

$T < T_C$, close to T_C

$\dfrac{M(T)}{M(0)} \propto t^{\beta}$ $\qquad \beta = 1/2$

$\beta = 1/3$ exp.

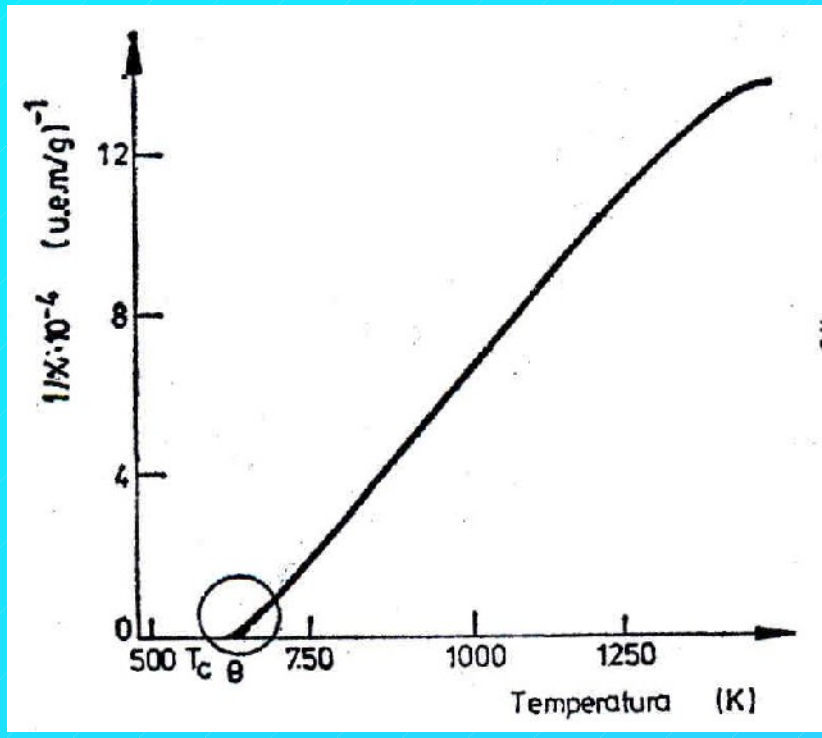


T>TC $$\chi = \frac{C}{T - \theta}$$

MF: $\chi^{-1} \propto T$ in all temperature range

experimental around TC:

$\chi \propto t^{-\gamma}$ $\gamma = 4/3$



MF: $\theta = TC$

experimental for Fe,Co,Ni

$$\frac{\theta - T_C}{T_C} \cong (2.4 - 4.8)\%$$

Interactions between a finite number of spins +molecular field

Oguchi method(1955); Constant coupling approximation (Kastelijn-Kranendonk, 1956); Bethe-Peierls-Weiss method (Weiss 1948)

Oguchi:

pair of spins

$\mathcal{H}_0 = -2J_{ij}S_iS_j - g\mu_0\mu_B(S_{iz} + S_{jz})H_T$ HT $\rightarrow$ molecular field for z-1 neighbours

TC$\neq\theta$ θ/TC=1.05 (cubic lattice)

χ-1 nonlinear variation around TC

Spin Waves

Slater (1954): exact solution for Heisenberg Hamiltonian: all spins (except one) are paralelly aligned

$$\mathbf{S}_t = \sum \mathbf{S}_i; \qquad S_t = NS, \qquad S_t' = NS - 1$$

$N \rightarrow$ number of atoms

$$\mathcal{H} = -g\mu_B B \sum_i S_{iz} - 2J \sum_{neigh.} S_j S_l$$

Many spin deviations: additivity law $\Delta E(n) \cong n\Delta E(1)$

(non rigorous, corrections)

repulsion of spin deviations: atoms with S, no more 2S deviations

attraction: total exchange energy is lower when two spin deviations are localized on neighbouring atoms

- Semiclassical description of spin wave: Bloch (1930) (Heller-Kramers 1934, Herring-Kittel 1951, Van Kranendonk-Van Vleck, 1958)
- Holstein-Primakoff folmalism (1940)

$$M=M(0)(1-AT3/2) \quad T/TC\leq 0.3$$

- Renormalization of spin waves (M.Bloch, 1962)

Keffer-London: effective field proportional with mean magnetization of atoms in the first coordination sphere (1961)

replaced by an effective spin at T, proportional with the angle between two neighbouring spins

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The system is equivalent, at a given temperature, with a system of independent spin wave, having excitation energy (renormalized energy) equal with the energy of spin wave in harmonical approximation, multiplied by a self consistent term which depends on temperature

The model describe the temperature dependence of the magnetization in higher T range

Series development method (Opechowski, 1938, Brown, 1956)

The magnetic properties of the system described by Heisenberg hamiltonian, can be analysed around TC, by series development method in T-1

T>TC

$\chi \propto (T-TC)^{-\gamma}$ $\gamma=4/3$; For S=1/2 kBTC/J=1.8-1.9 (z=6)

=2.70 (z=8)

Green function method (Bogolyubov-Tyablikov, 1959)

Bitemporal Green function for a ferromagnet (S=1/2). Temperature dependence of magnetization obtained by decoupling Green function equation. The analysis has been made in lowest decoupling order (random phase approximation)

$M=M(0)(aT^{3/2}+bT^{5/2}+cT^{7/2})$

$\beta=1/2$; $\gamma=2$

Analysis in the second order of Green function decoupling (Callen, 1963)

kBTC/J values only little higher than those obtained by series development method.

Antisymmetric exchange interactions:

(Dzialoshinski 1958)

General form of bilinear spin-spin interaction

$$\mathcal{H} = \sum_{\alpha,\beta} J_{\alpha\beta} S_{i\alpha} S_{j\beta} \quad \alpha,\beta = x,y,z$$

$J\alpha\beta$

$J^S_{\alpha\beta} \quad J^S_{\alpha\beta} = J^S_{\beta\alpha}$

$J^A_{\alpha\beta} \quad J^A_{\alpha\beta} = -J^A_{\beta\alpha}$

$$\mathcal{H}^a_{ij} = d_{ij}(S_i \times S_j) \quad d_{ij} = -d_{ji}$$

$$\mathcal{H}^s_{ij} = J_{ij}\mathbf{S}_i\mathbf{S}_j$$

Explain weak ferromagnetism in α-Fe2O3

MFe MFe

Indirect excahnge interactions through conduction electrons (RKKY) (Ruderman-Kittel, Kasuya, Yoshida (1954-1956))

4f shell: small spatial extension

La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu

4fo 4f7 4f14

3d dilute alloys in nonmagnetic host

$\mathcal{H}$s-d(f)=J**sS**

$\mathcal{H}$= $\mathcal{H}$s-d+$\mathcal{H}$cond.el+$\mathcal{H}$zz

First order perturbation theory

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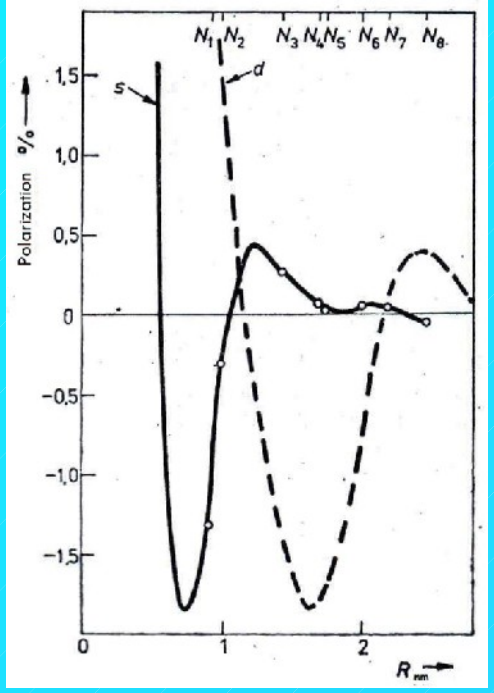
Second order

$$J(Rnm) \propto J2F(x)$$

$$F(x) = \frac{x\cos x - \sin x}{x^4}; \qquad x = 2k_F R_{nm}$$

Oscillatory polarization: decrease as R_{nm}^{-3}

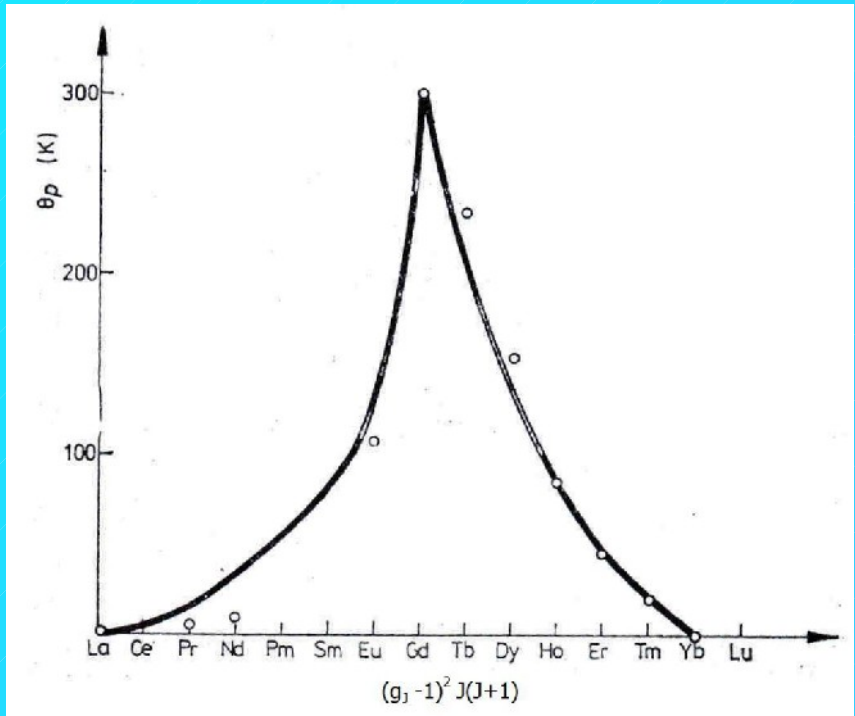
Example: Stearns 1972: Polarization of s and d itinerant 3d electrons: iron T>TC



$\Theta = GF(x)$

$G = (gJ-1)2J(J+1)$ De Gennes factor

Rare earths F(x) are similar



Exchange interactions 4f-5d-3d:

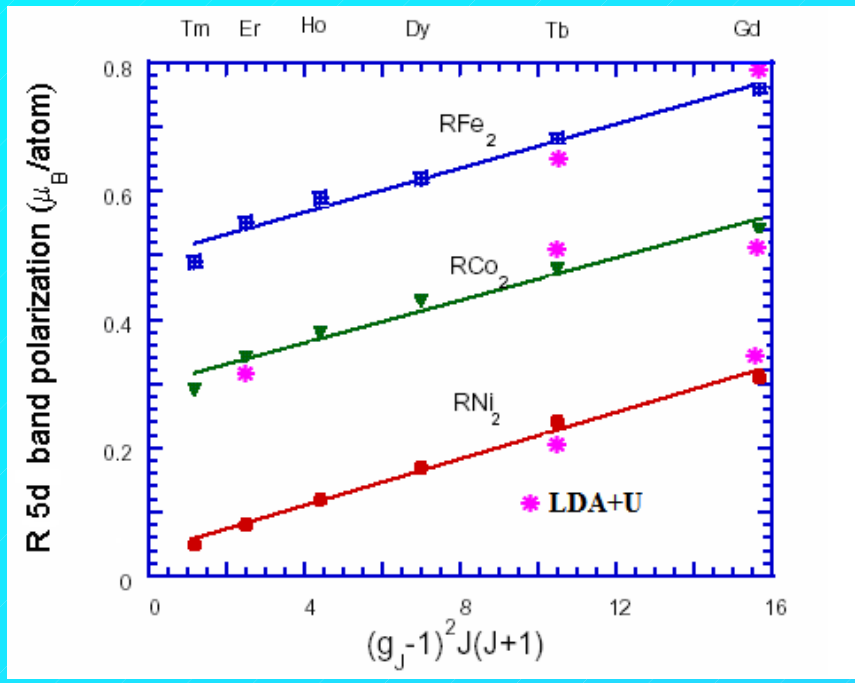
R-M compounds

R=rare-earth

M=3d metal

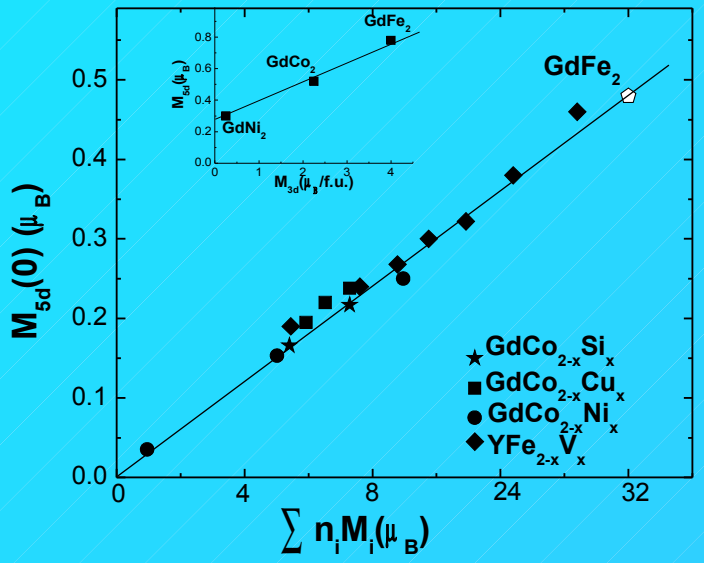
$M5d = M5d(0) + \alpha G$

$G = (gJ-1)2J(J+1)$



$$M_{5d}(0) \propto \sum n_i M_i$$

ni number of 3d atoms in the first coordination shell, having Mi moment



Band models

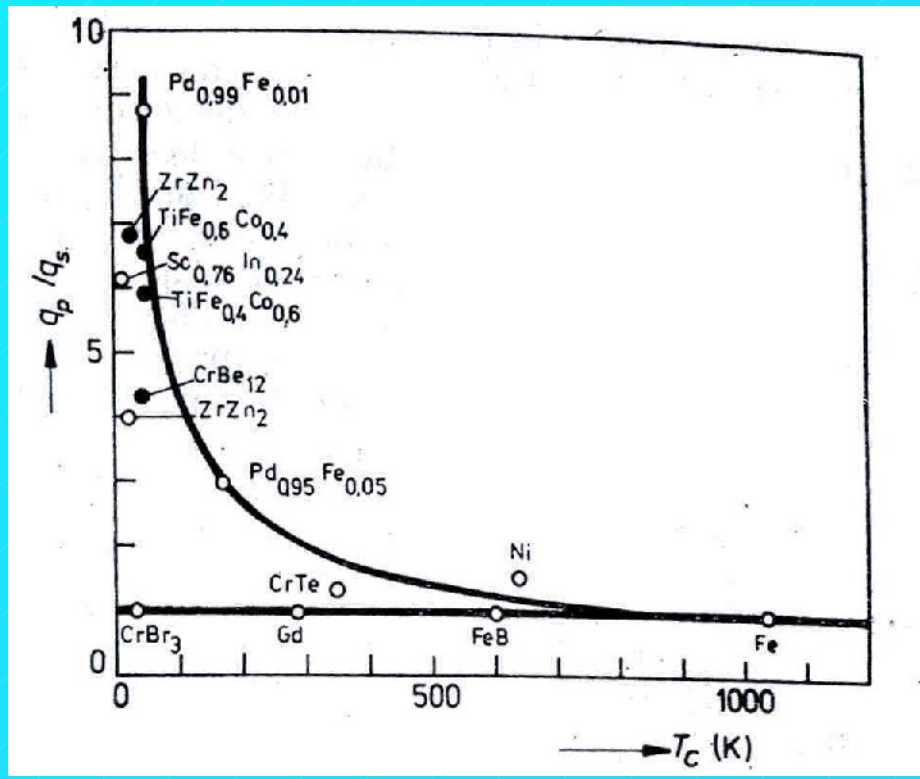
- non integer number of μB MFe=2.21 μB

  MCo=1.73 μB

  MNi=0.61 μB

- presence of 3d bands: widths of ≅1 eV

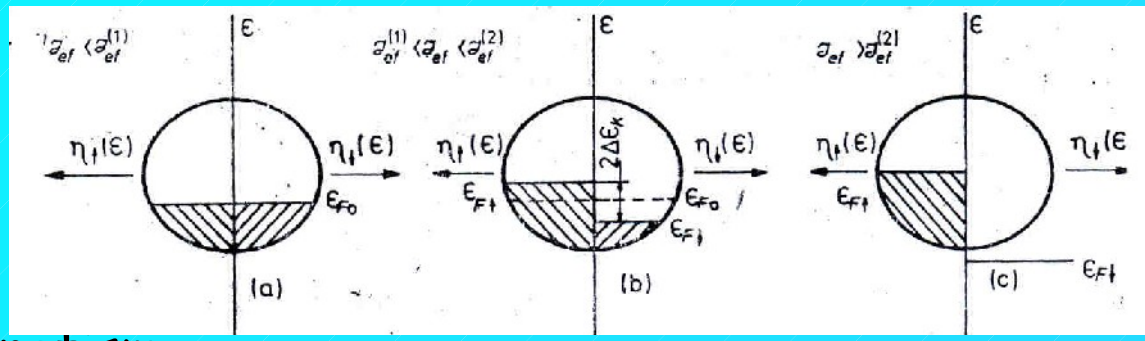
- difference between the number of spins determined from saturation magnetization and Curie constant



Stoner model

s,d electrons in band description

$\Delta E = \Delta E_{ex} + \Delta E_{kin}$



Spontaneous splitting 3d band

$J_{eff}\eta(E_F) \geq 1$

Stoner criterion for ferromagnetism

Sc,Ti,V, 3d band large, strongly hybridized with (4s,4p) band→ small density of sates at EF; Jeff close to that of free electron gas

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no magnetic moments and magnetic order

Cr,Mn,Fe,Co,Ni: 3d band narrow (high density of states around EF)

Jeff, more close to values in isolated atom

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magnetic moments and magnetic ordering

Many models based on the band concept were developed

ZrZn2 $M(T)=M(0)[1-T^2/T_C^2]$

Hubbard model (Hubbard, 1963, 1964)

Hamiltonian: a kinetic term allowing for tunneling ("hopping") of particles between sites of the lattice and a potential term consisting of on site interaction

Particles: fermions (Hubbard original work)

bosons (boson Hubbard model)

Good approximation: particles in periodic potential at low T (particles are in the lowest Bloch band), as long range interactions can be neglected.

Extended Hubbard model: interactions between particles on different sites are included.

Based: tight binding approximation, electrons occupy the standard orbitals of atoms and hopping between atoms.

$$\mathcal{H} = \sum_{i,f} \sum_{\sigma} T_{if} a_{i\sigma}^{+} a_{f\sigma} + \frac{J}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$

$J \to \infty$, exact fundamental state

$J=0$, band description

$\frac{T_{ij}}{J}$ localized moments

ratio ⇕ intermediate state

delocalized moments

Models considering both band and localized features

- Friedel (1962), Lederer-Blandin (1966)

Starting from band model+features of Heisenberg model

Local polarization ($Jef\eta(EF)\geq 1$)+ oscillatory exchange interactions

- Zener modified model (Herring) lattice of atoms having x and x+1 d electrons, respectively

The additional electron (Zener) is itinerant "hopping" from a lattice site to another

- Stearns model

Indirect coupling of localized d electrons through d itinerant electrons. 95 % d electrons are in narrow band (localized) and 5 % of d electrons are itinerant (Fe).

Approximation based on ionic configurations

coexistence of different ionic configurations 3d9, 3d8, 3d7

there is a possibility for impurity to have another fundamental state of an excited configuration by virtual transition.

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an effective coupling between impurity and conduction electrons

In zones situated between stable configurations there are regions characterized by fluctuations between configurations

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both localized and itinerant magnetic behaviour

Spin fluctuations:

Stoner model: itinerant electrons treated as a free electron gas; even the molecular field concept was introduced do not describe the properties of 3d metals at finite temperature

Spin fluctuations: abandoned the concept of single particle excitation; introduced thermally induced collective excitations

deviations (fluctuation) from their average

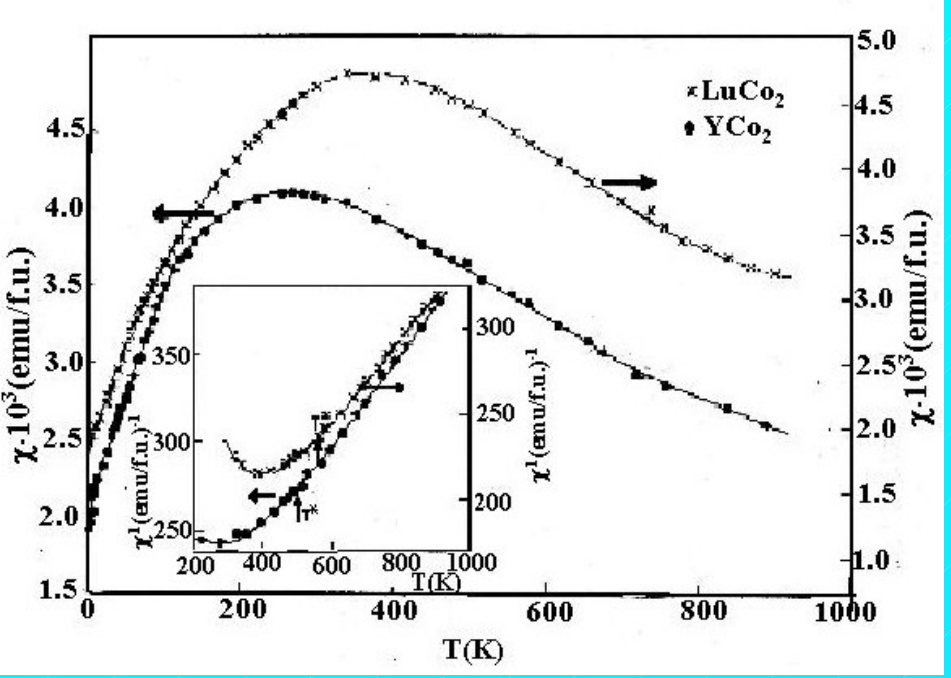
probability distribution of these fluctuations

$$\chi_k = \frac{\chi_k^0}{1 - \chi_k^0 \frac{J_{ef}}{\mu_0 \mu_B^2}} = \frac{\chi_k^0}{1 - J_{ef}\eta_k(E_F)}$$

The system is paramagnetic $\chi_k > 0$

For some k value $J\eta(EF)=1 \rightarrow$ magnetic moments having a life time τ

$$\tau \propto \frac{n_d(E_F)}{1 - Jn_d(E_F)}$$

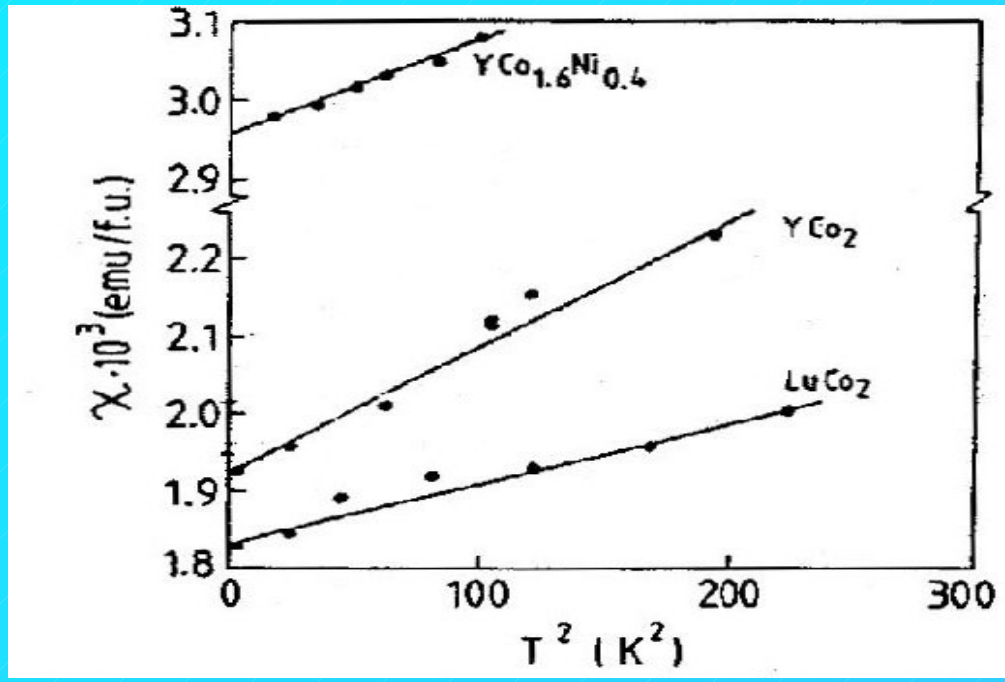


Exchange enhanced paramagnet

$s=[1-Jn(EF)]-1$

s-Stoner exchange enhancement factor

$s \cong 10$



Self consistent theory of spin fluctuations

Wave number dependent susceptibility, χq, for a nearly ferromagnetic alloy has a large enhancement for small q values

$$\chi_q = \frac{\overline{\chi}_q}{1 - J\overline{\chi}_q(\mu_0\mu_B^2)}$$

Frequency of longitudinal spin fluctuations $\omega^* \propto \frac{1}{\tau}$

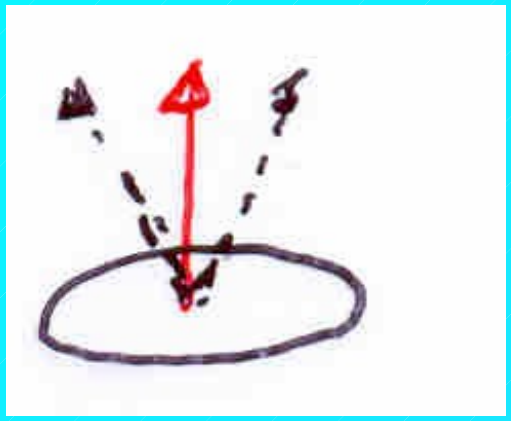
τ-lifetime of LSF

Low temperature

(thermal fluctuations-transversal slow)

$$\omega^* > \frac{k_B T}{\hbar}$$

$$\chi = s\chi_p\left[1 + \frac{\pi^2}{6}\left(2\frac{\eta''}{\eta} - 1.2\frac{\eta'^2}{\eta^2}\right)_{E_F} s^2T^2\right]$$



Approximation for nonmagnetic state

$\chi \propto T2$

$\chi(T)$ as T ↗

$\eta'' > 0$ (necessary condition, not sufficient)

High temperature

Average mean amplitude of LSF is temperature dependent

$$\left\langle S_{loc}^2 \right\rangle = 3k_B T \sum_q \chi_q$$

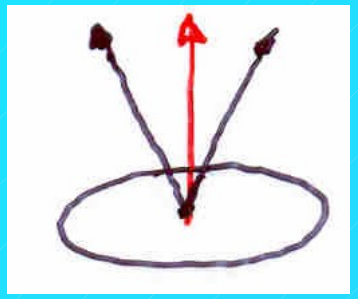
Sloc as T up to T* $\left(S_{loc}\right)$

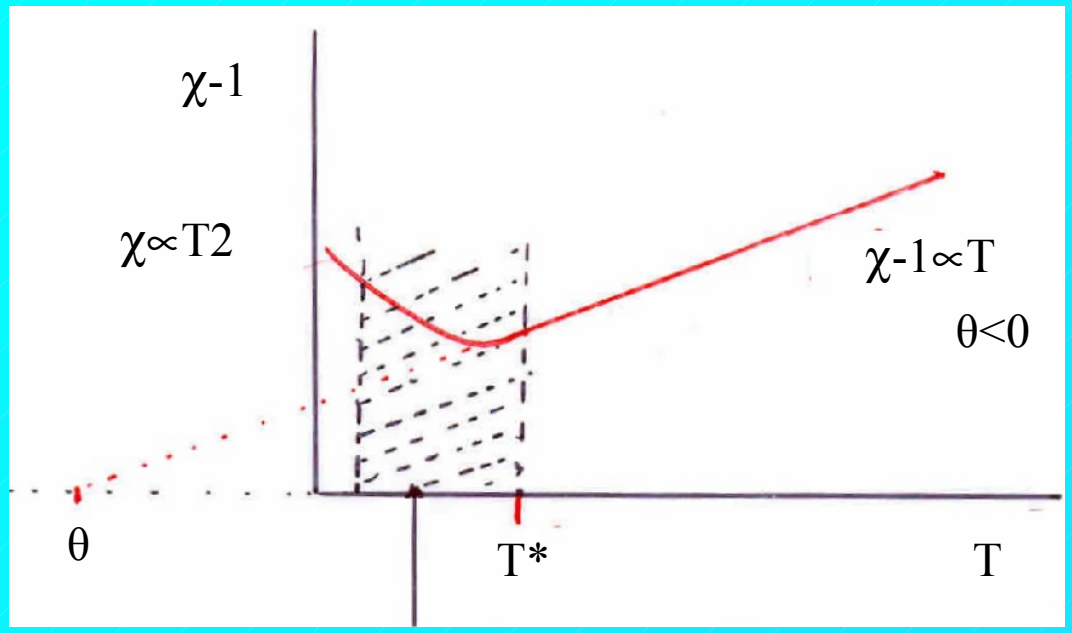
S_{loc} determined by charge neutrality condition

The system behaves as having local moments for temperatures T > T* where the frequency of spin fluctuations

$$\omega^* < \frac{k_B T}{\hbar}$$

S_{loc}





C-W type

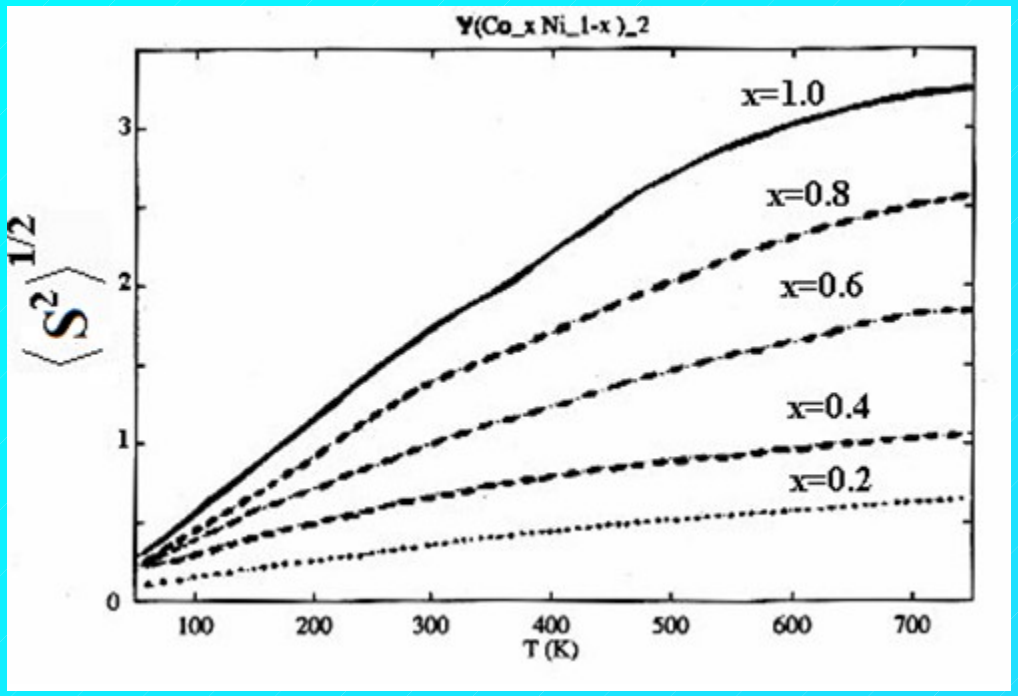
Crossover between low T regime governed by spin fluctuations and high T classical regime

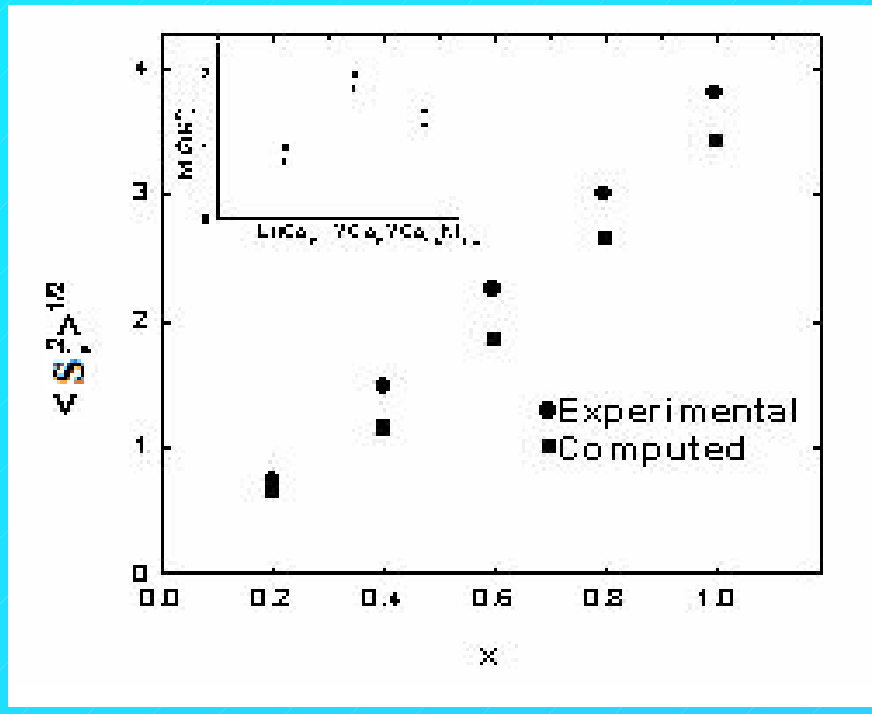
Gaussian distribution of spin fluctuations (Yamada)

$$\chi_s^{-1} = a_1 - \alpha + \frac{5}{3}a_3 S^2 + \frac{35}{9}a_5 S^4 + \frac{35}{3}a_7 S^6 + \ldots$$

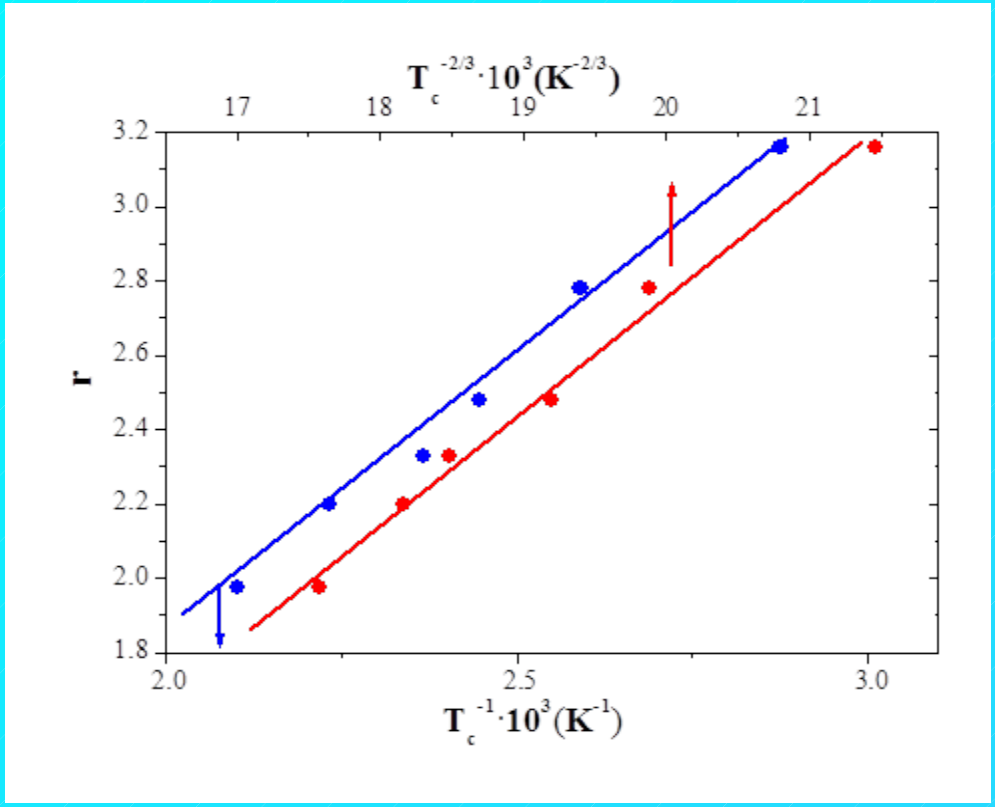
where the mean square value of the fluctuating magnetization, S^2, is given by:

$$\langle S^2 \rangle = \frac{3}{2\pi^2} k_B T q_m A^{-1} \left(1 - \frac{tg^{-1}\left(q_m \sqrt{A\chi}\right)}{q_m \sqrt{A\chi}} \right)$$





A system can be magnetic or nonmagnetic depending on the temperature (Schrieffer 1967)



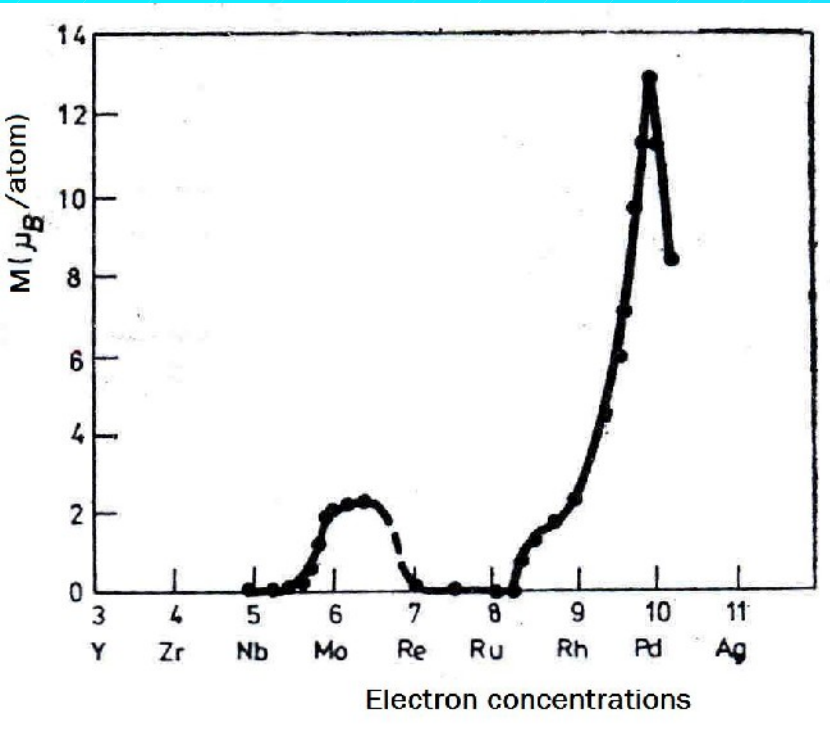
GdxY1-xCo4Si

Model: weak ferromagnetic behavior

Dilute magnetic alloys

Small number of magnetic atoms (3d) in nonmagnetic metallic matrix

3d moments as Fe, dependent on metallic matrix (Clogston 1962)



Friedel model: virtual bound state (level)

Resonance phenomena between d states

and k states of conduction electrons

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Package of waves centered on impurity atom (virtual bound level)

prediction concerning the appearance of magnetic moment on impurity and experimental data

	ε_F(eV) ($\times 1{,}6 \cdot 10^{-19}$ Joule)	4,2	5,5	5,5	7	7,5	9,5	13
		PdH	Au	Ag	Cu	Mg	Zn	Al
2	Sc							
3	Ti							–
4	V							–
5	Cr	+	+	+	+		+	–
4	Mn	+	+	+	+	+	+	–
3	Fe	+	+		+	+	–	–
2	Co	+	+		–			–
1	Ni	–	–		–		–	–

Wolff model:

Considers scattering of conduction electrons by the potential of impurity atom.

The virtual level can be evidenced by a maximum in scattering section of the conduction electron.

When the virtual level is rather narrow and close to EF, the impurity develops an exchange potential which polarizes the electrons in their neighbor

Anderson model:

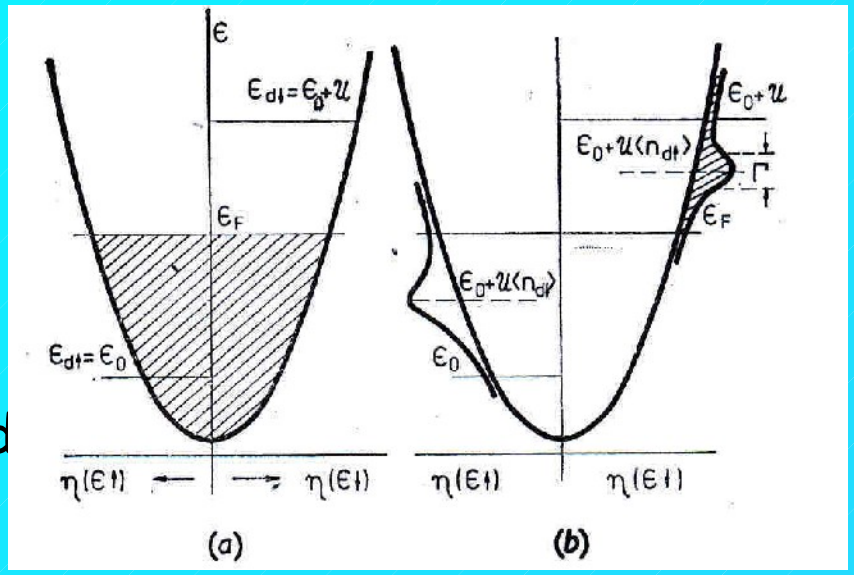
Magnetic impurity,

Bands: ↑(full) ↓(empty)

s or s-p state of conduction band

U d-d interaction

Vdk covalent mixing of conduction band with d states



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Decrease of the number of electrons with spin (↑) and increase of those with spin (↓)

$\mathcal{H}=\mathcal{H}0+\mathcal{H}sd$

$\mathcal{H}0=\mathcal{H}0k+\mathcal{H}0d+\mathcal{H}cor$ Coulomb interaction between electrons with spin ↑ and ↓

nonperturbed states

electrons in conduction band

Density of mixing states, $\eta d\sigma$ has half width $\Gamma/2$

For S=1/2

$$S\cong\frac{1}{2}\left[1-\frac{1}{\pi xy(1-x)}\right] \qquad x=\frac{E_F-E_O}{U} \qquad y=U/(\Gamma/2);$$

Kondo model:

Anomalous temperature dependence of the electrical resistivity

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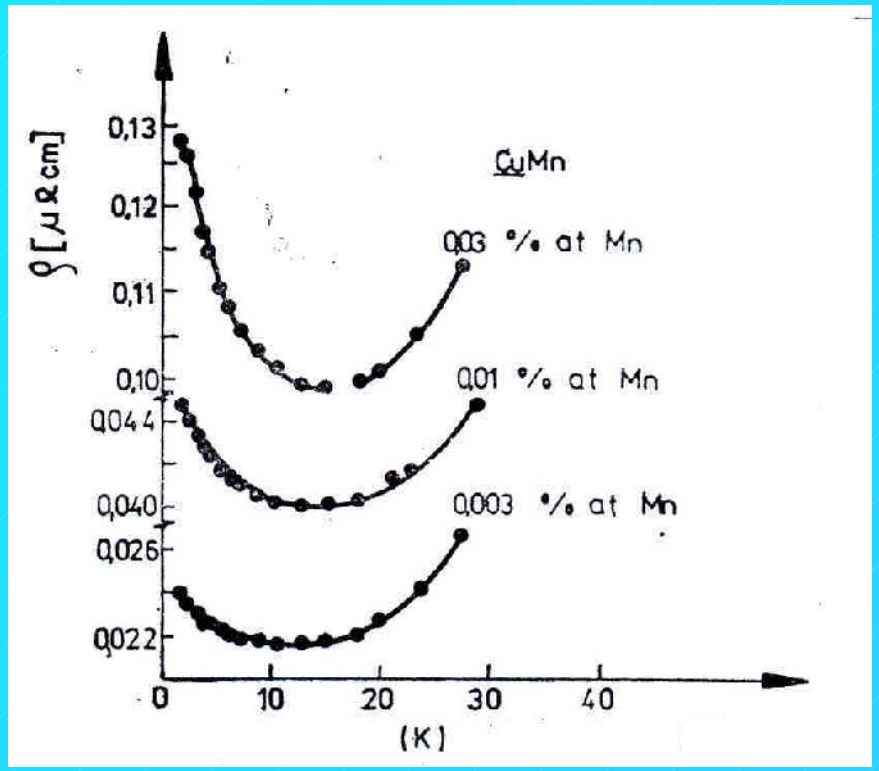
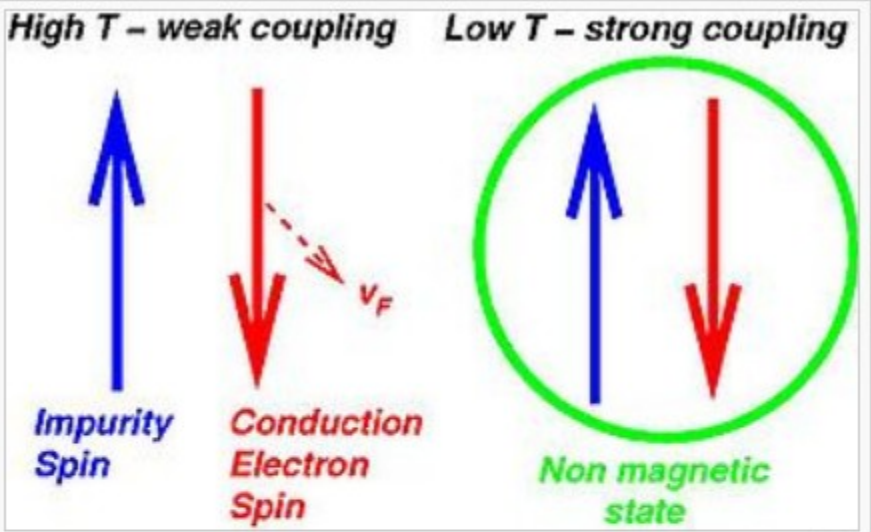
Interaction between the localized magnetic impurities and the itinerant electrons.

Extended to lattice of magnetic impurities, the Kondo effect is belied to underlay the formation of heavy fermions in intermetallic compounds based particularly on rare-earth.





Schematic of the weakly coupled high temperature situation in which the magnetic moments of conduction electrons in the metal host pass by the impurity magnetic moment at speeds of v_F, the Fermi velocity, experiencing only a mild antiferromagnetic correlation in the vicinity of the impurity. In contrast, as the temperature tends to zero the impurity magnetic moment and one conduction electron moment bind very strongly to form an overall non-magnetic state.

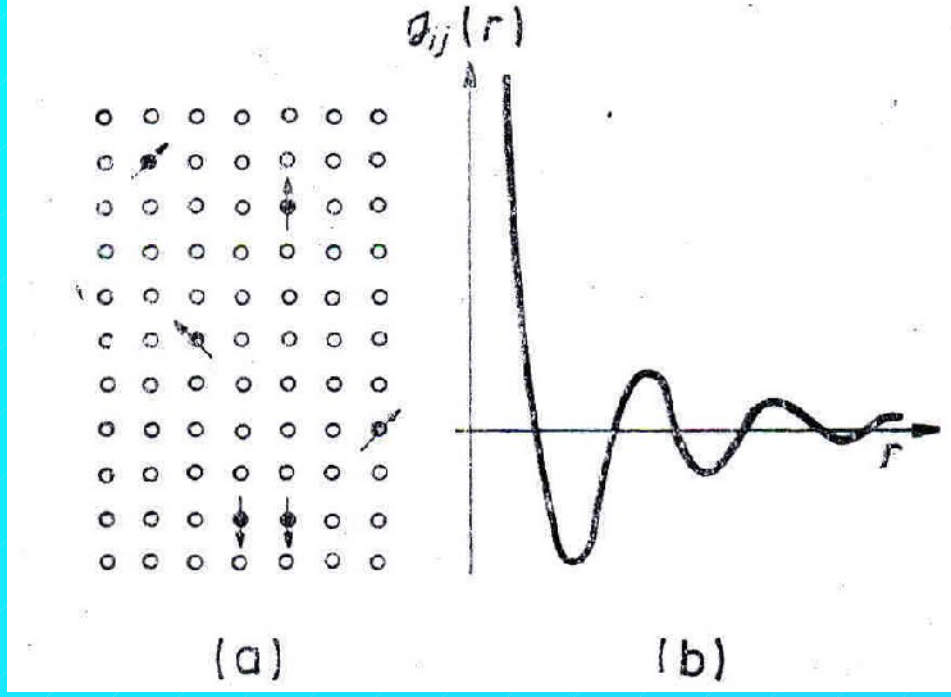
Schrieffer-Wolff (1966): Anderson Hamiltonian can be of a similar form as the Kondo one, considering an antiferromagnetic interaction $J(\mathbf{k},\mathbf{k}')$ energy dependent

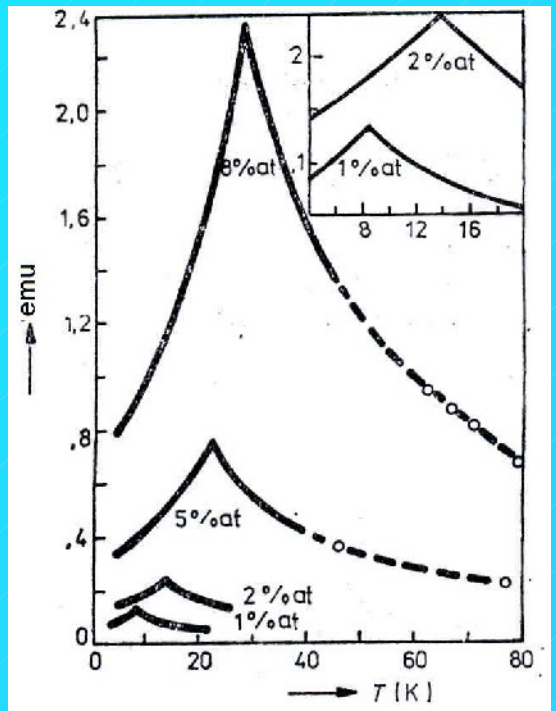
Spin glass, Mictomagnets:

Dilute alloy with random distribution of 3d atoms

Oscillatory polarization can direct the moments in different directions.

At low T, the moments are freezen in the direction corresponding to polarization (H=0)-spin glass





At higher concentration of magnetic atoms there are.

- random distributed magnetic atoms
- clusters of atoms

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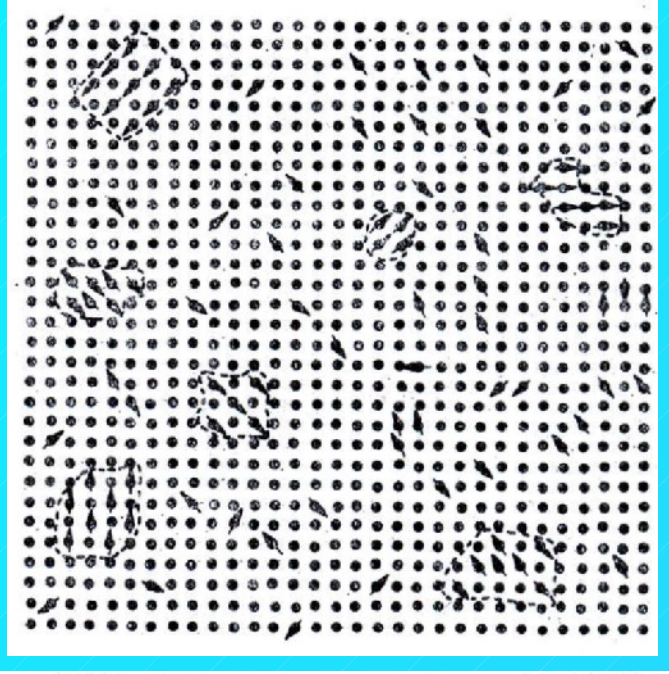
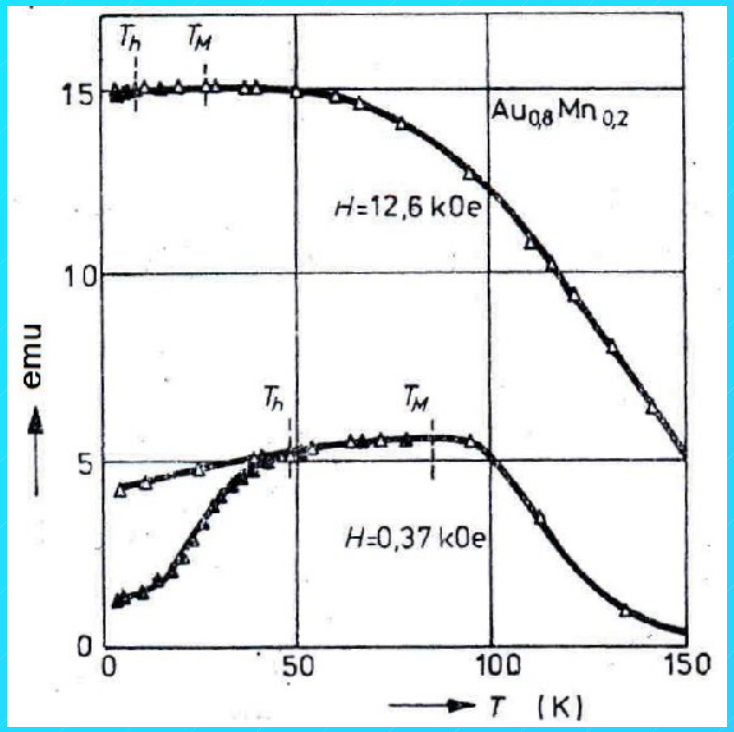
mictomagnetism

Difference in the zero field cooled and field cooled magnetization.

Insulators: magnetic atoms in glasses

perovskites





Dynamical Mean Field Theory (DMFT):

DMFT, a step to develop methods for describing electronic correlations. Depending on the strength of the electronic correlations, the non-perturbative DMFT correctly yields:

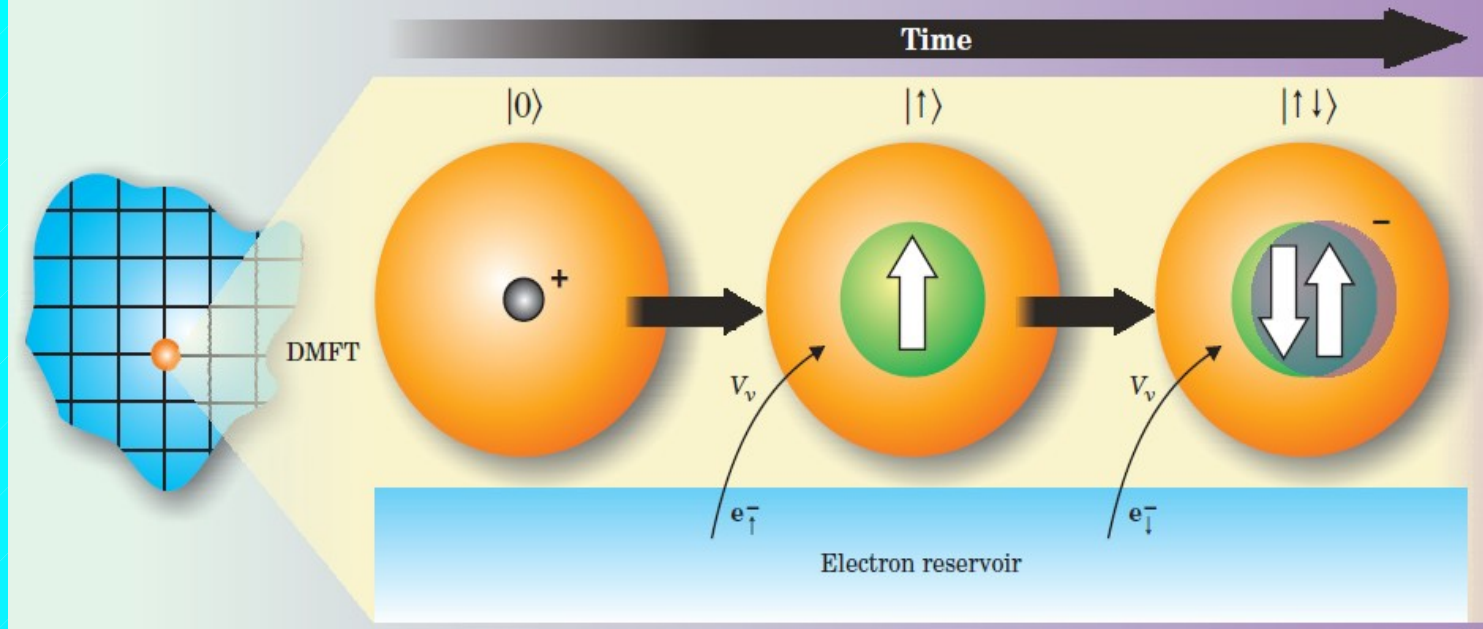
- weakly correlated metal
- strongly correlated metal
- Mott insulator

DMFT+LDA allows a realistic calculation of materials having strong electronic correlations:

transition metal oxides

heavy fermion systems

Theory of everything: kinetic energy, lattice potential, Coulomb interactions between electrons



Dynamical mean-field theory (DMFT) of correlated-electron solids replaces the full lattice of atoms and electrons with a single impurity atom imagined to exist in a bath of electrons. The approximation captures the dynamics of electrons on a central atom (in orange) as it fluctuates among different atomic configurations, shown here as snapshots in time. In the simplest case of an *s* orbital occupying an atom, fluctuations could vary among $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, or $|\uparrow\downarrow\rangle$, which refer to an unoccupied state, a state with a single electron of spin-up, one with spin-down, and a doubly occupied state with opposite spins. In this illustration of one possible sequence involving two transitions, an atom in an empty state absorbs an electron from the surrounding reservoir in each transition. The hybridization V_v is the quantum mechanical amplitude that specifies how likely a state flips between two different configurations.

Many body problem ⇨ one site problem

Anderson model

Hybridization function plays the role of the mean field.

Hybridization → small → electron localized

Hybridization → large → electron move throughout crystal

Super exchange and double exchange mechanisms

Two ions separated by diamagnetic ions

Superexchange
⇓
between ions in same valence states

Double exchange
⇓
between ions in different valence states

Superexchange Interactions (Van-Vleck 1951)

Two ions T1,T2 separated by a diamagnetic ion (O2-)

Two p electrons of O2- occupy the same p orbital

T1, T2 have each one d electron

p orbitals axis coincides with T1-T2 axis

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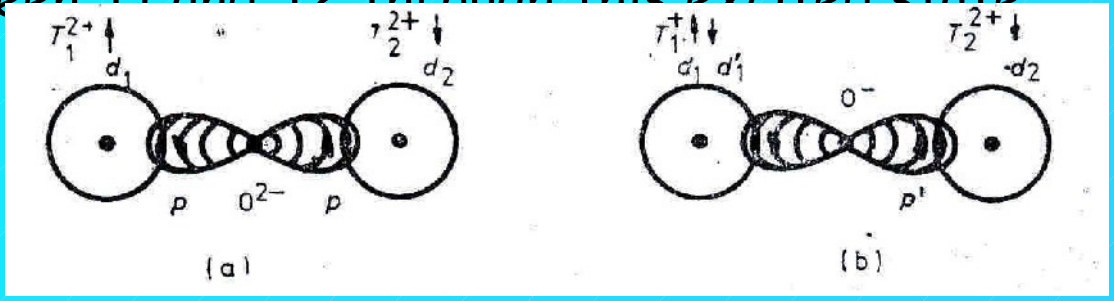
singlet state (no magnetic coupling between T1 and T2

one p electron transferred as d1': coupling between d and d1' on T1 atom

the second p electron of O2- can couple with the d electron of T2 atom. Since of opposite spins of the two O2- electrons will appear an indirect exchange between T1 and T2 through this excited state



Anderson: a more complex model

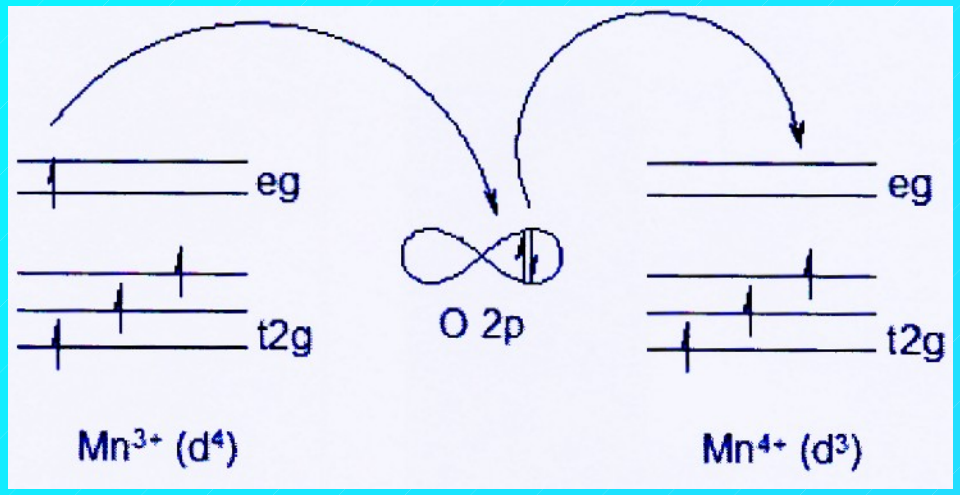
The resultant interaction is given as a sum of two competitive effects having opposite signs:

potential superexchange (Coulomb repulse energy between two magnetic ions) which lead to ferromagnetic coupling

kinetic superexchange (negative)

Double exchange mechanism (Zener 1951)

Mn eg orbitals are directly interacting with the O 2p orbitals: one Mn ion has more electron than other.



If O gives up its spin-up electron to Mn4+, its vacant orbital can be filled by an electron from Mn3+

Electron has moved between the neighbouring metal ions, retaining its spin.

Thank you very much for your attention