Low dimensional magnetism : the role of the electronic structure

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I. Introduction :

Low dimensional systems : - OD (clusters) / 1D (chains) /2D(films) /3D (multilayers)
Due to reduced dimension, new properties can appear.
Particularly the magnetic moments are widely studied for fondamental and applied research.

The key point of this lecture is the determination of the electronic structure of the material of interest. Once the Schrödinger equation is solved (in a reasonable way), one can expect to describe all interesting physical properties with the help of appropriate theoretical frameworks.

Two different approaches are used to describe the magnetism of materials :
- localized magnetism (for Rare earths for instance) => Heisenberg type Hamiltonian
- itinerant magnetism (for transition metals) we will focus on in this lecture

II. Itinerant magnetism at T=0K

1. *The Density Fonctional Theory (DFT)* – Proposed by W. Kohn (1964)

The starting point is the fact that the total energy is a fonctional of the electronic density n(**r**).
The main problem is to treat the exchange-correlation term.

2. *An alternative : the semi-empical tight-binding scheme*

Not ab initio but faster and very efficient to get general trends

3. *The local densities of states (LDOS)*

$H \Psi_v = E_v \Psi_v$

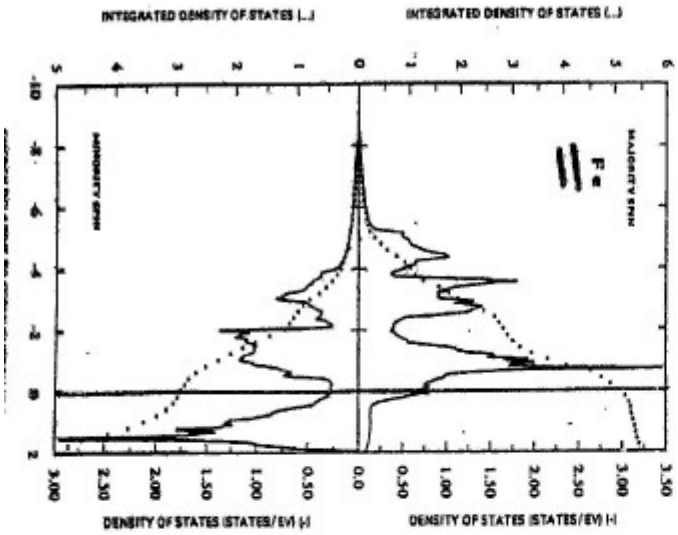
=> total density of states : $n(E) = \delta(E-E_v)$

By projection for each atom (and even orbital), the LDOS $n_i(E)$ is obtained
μ_i the local magnetic moment is obtained as the difference of occupation in bands of different spins

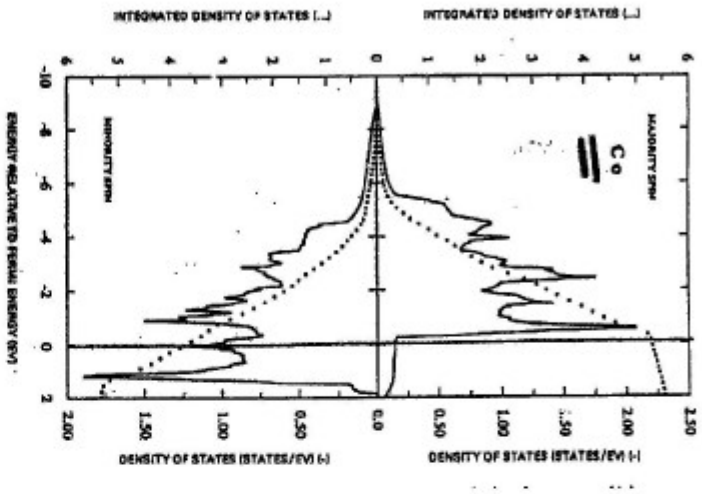
$$\mu_i = \int^{E_F} (n_i^+(E) - n_i^-(E)) \, dE$$

For a ferromagnetic atom, the main difference between the LDOS for the two directions of spins is a shift of the center of gravity of the sub-bands :

$\Delta_i = J.\ \mu_i$ where J is the exchange integral



Fe bulk ferromagnetic LDOS



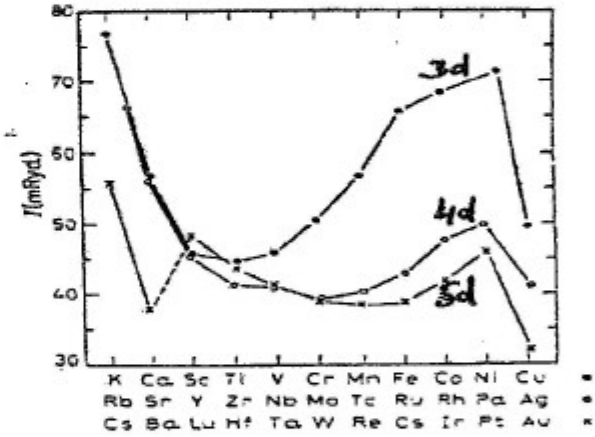
Co bulk ferromagnetic LDOS

<u>Stoner criterion for onset of ferromagnetism</u> :

$J.\ n(E_F) > 1$

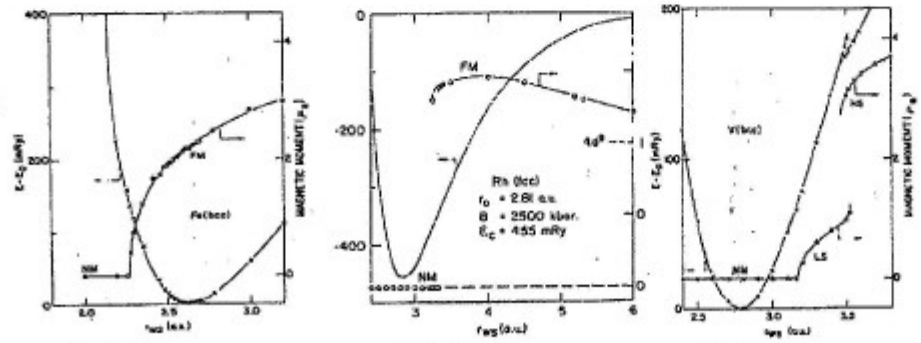
$n(E_F)$ is the paramagnetic LDOS at Fermi level
J is almost an atomic quantity
+ the band width (w) is increasing when going from 3d to 5d transition metals

=> Only Fe, Co and Ni are bulk ferromagetic



III. The magneto-volumic effects

1. Transition para-ferromagnetism

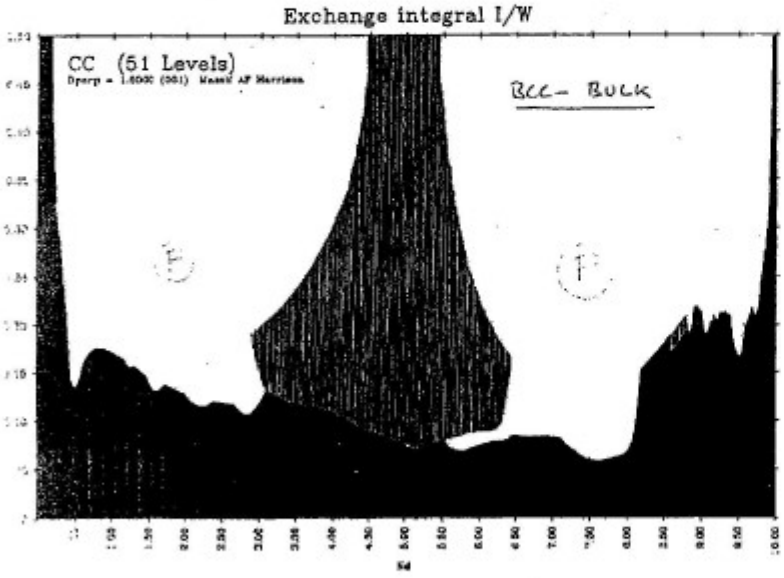


Fe Bulk Rh Bulk V Bulk

Variation of the magnetic moment versus the interatomic distance : different behaviours.
Can be undertood in a simple d tight-binding model

The Stoner criterion gives only an upper limit for the onset of ferromagnetism

2. Competition ferro-antiferromagnetism



Bulk bcc (for an example)
As function of the d band filling versus I/W (or equivently the interatomic distances).
Ground state :
In black : paramagnetic
In grey : Antiferromagnetic
In white : ferromagnetic

General behaviour at any dimension

IV. Local Spin Magnetic moments distribution:

1. Influence of the dimensionality

General trend: An increase (decrease) of the coordination number induces a decrease (increase) of the local magnetic moments.

* Can be understood in a simple model where $W \sim Z^{1/2}$

* Obtained in various calculations for Fe-bcc, Co-hcp and Ni-fcc (FLAPW, LMTO, TB....) and observed experimentally.
A significative exception : Palladium => Need to compute the electronic structure

2. Influence of the direct neighbouring

- interface with noble metal : few changes
- interface with transition metal : possible induced magnetization
  Example : V on Fe : the first layer of V at the interface is widely polarized

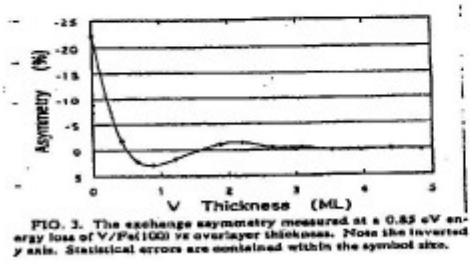


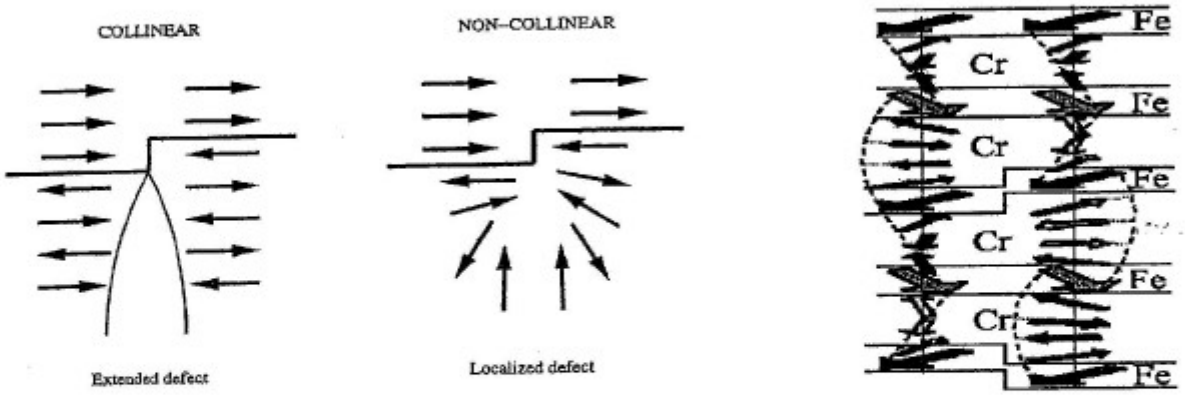
FIG. 3. The exchange asymmetry measured at a 0.85 eV energy loss of V/Fe(100) vs overlayer thickness. Note the inverted y axis. Statistical errors are contained within the symbol size.

+ variation of the interatomic distances / Atomic relaxations
+ different band widths
+ type of magnetic coupling
==> **possible complicate arrangements**

(from Walker and Hopster)

V. Non-collinear spin arrangement

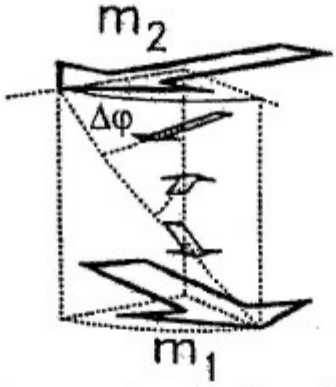
Role of the frustrations (Fe-Fe : Ferro, Fe-Cr and Cr-Cr Antiferro)



Schreyer *et al.* PRL 79, 4914 (1997).

Fe on Cr :Two possibles mechanisms to overcome the magnetic frustrations.
Defects indicate magnetic arrangement different of the bulk with at the interface possible small values.

- Phenomenogical model of Slonczewski (Proximity model : JMMM **150** (1995) 13)



Exchange coupling energy between ferromagnetic layers separated by an antiferromagnetic spacer :

$\mathbf{E(\Delta\phi) = J_+ \Delta\phi^2}$ or $\mathbf{J_-(\Delta\phi - \pi)^2}$

FM coupling AFM coupling

- Biquadratic coupling

$$\mathbf{E = A\cos\phi + B\cos^2\phi}$$

More complex situation with Mn (which has a spiral ground state)

VI. The Magnetic anisotropy

1. The orbital moment : a general trend

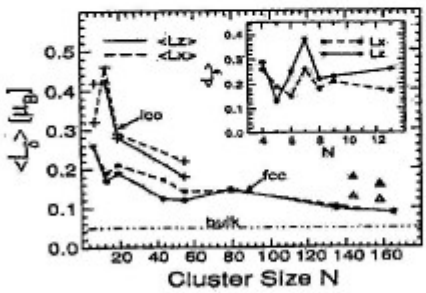


FIG. 1. Average orbital magnetic moment per atom (L_δ) of Ni_N clusters with fcc-like (dots) and icosahedral-like structures (crosses). The magnetization direction δ is a principal C_n symmetry axis ($\delta = z$) or a NN bond perpendicular to z ($\delta = x$). Full (open) triangles refer to coinlike bilayer clusters with perpendicular (in-plane) magnetization. Results for small clusters are given in the inset.

Lowering of the symetry
=> increase of the orbital moment

For instance Ni:
Atom : L = 2 μ_B for $s^1\ d^9$ to solid <L> = 0.05 μ_B

Remarkable enhancement as compared to the bulk value
Strong reduction of L as compared to the atom already for very small clusters
(<--- from Pastor et al)

3. The magnetocristalline Anisotropy Energy

Defined as the difference of energy between two directions of the magnetization
- Much larger as in the bulk (mev instead of tens of μeV)
- Systematic behaviour (based on moments arguments) minimum of nodes versus the band filling

Can be computed from the electronic structure

A simple but very often verified relation (Bruno)

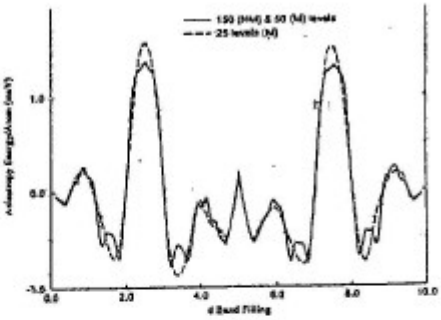


FIG. 2. Magnetic anisotropy energy per atom (meV) vs the *d*-band filling for a (001) monolayer. The results obtained with 150 levels of the continued fraction in the NM *z* basis (full line) practically coincide with those for 50 levels and M basis. The curve obtained with 25 levels of the continued fraction in the M basis is given by the dashed line. Negative values correspond to a favorable perpendicular direction of the magnetization.

$E_{mc} \sim \Delta (m^{//} - m^{\perp})$ where m is taken for the two reference directions

4. The dipolar interaction

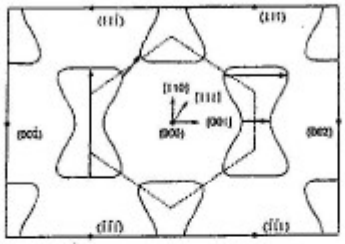
The total Magnetic anisotropy (which will give the direction of the magnetizatin) is the sum of E_{mc} and the dipolar energy E_{dip} also called the shape anisotropy.

E_{dip} is computed generally numerically and tends to align the spin parallel to the surface

5. The sum rules

From XMCD (X Ray Magnetic Circular Dichroïsm) experiment, the spin **and** the orbital moment can be extracted.

VII. The Intelayer Exchange Coupling



Cross-section of the Fermi surface of Cu, parallel to a (110) section. The solid points give the vectors of the reciprocal lattice. The (bulk) first Brillouin zone is indicated by the dashed lines. The horizontal, oblique, and vertical bold arrows, respectively, are the stationary spanning vectors determining the periods of IEC oscillations versus spacer thickness, for the (001), (111) and (110) orientations; from Ref. [88].

Interlayer coupling between two ferromagnetic layers through a non-magnetic spacer can display oscillations.
The period is given by Kohn singularities of the spacer Brillouin Zone (points with antiparallel velocities)

VIII. References

A. General books :
1. Theory of itinerant electron magnetism by J. Kübler, Oxford Science Publications (2000)
2 . Magnetism in the Solid State by P. Mohn, Springer (2002)
B. General papers :
1.Theoretical approaches of magnetism of transition-metal thin films and nanostructures on semi-infinite substrate by H. Dreyssé and C. Demangeat, Surf. Sci. Rep. **28** (1997) 65-122
2.Electronic, magnetic and spectroscopic properties of manganese nanostructures, Rep. Prog Phys. **65** (2002) 1679-1739
3. Theory of interlayer magnetic coupling by P. Bruno, Phys. Rev. B **52** (1995) 411.