Spin effects
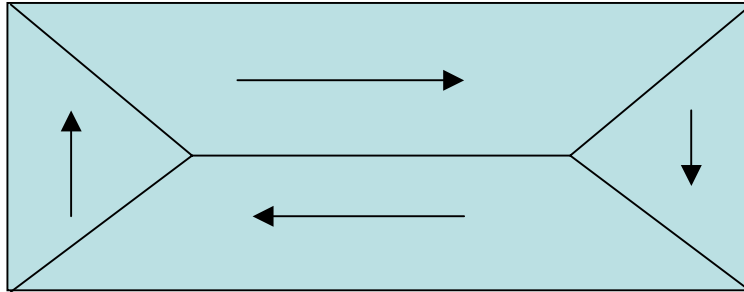## (spin polarized systems, spin-orbit …)

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Macroscopic magnetization

- A crystal can be found in different magnetization states.
- The direction of macroscopic magnetization changes inside the crystal
- This can be observed by the magnetic Kerr effect (rotation of polarized light)

- Under the action of an external field, the magnetization $\mathbf{M}(r)$ changes its direction, not its amplitude. $|M(r)| = M_s$

- Under a very intense magnetic field $\mathbf{M} = M_s \dfrac{\mathbf{B}}{B}$

- When the magnetic field is turned off, the magnetization distribution is reestablished.

- The domain distribution has an energetic origin (and is not related to defects for instance)

Macroscopic Magnetism

- Magnetic energy

- Landau-Ginzburg like functional

$$E\left[\mathbf{M}(\mathbf{r})\right] = E_{an}\left[\mathbf{M}(\mathbf{r})\right] + E_{ech}\left[\nabla\mathbf{M}(\mathbf{r})\right]$$
$$+ E_{ms}\left[\mathbf{M}(\mathbf{r})\right] - \mathbf{M}(\mathbf{r}).\mathbf{B}_{ext}(\mathbf{r})$$

- The observed magnetization minimizes this functional.
- The first two terms are of microscopic origin
- The third term depends upon the shape of the sample.
- The fourth one describes the interaction with the external field.
- NB: If time is reversed, $M(r) \to -M(r), B(r) \to -B(r)$ but the energy Is constant

Macroscopic Magnetism

- Different terms in the magnetic energy

- Magnetic anisotropy energy depends upon orientation
- Can exist only if there is a coupling between the lattice and magnetization, through the spin-orbit coupling.

$$\Delta E_{an}\left[M(r)\right] \approx 1\mu\, eV / atom$$

Macroscopic Magnetism

Anisotropy energy respects the symmetries of the crystal

- Cubic ($K_1>0$, [100], $K_1<0$ [111] etc..)

$$E_{an} = K_1(m^2_x m^2_y + m^2_x m^2_z + m^2_z m^2_y) + K_2 m^2_x m^2_y m^2_z + \cdots \qquad \vec{m} = \vec{M}/|M|$$

- Hexagonal

$$E_{an} = K_1(m^2_x + m^2_y) + K_2(m^2_x + m^2_y) + \frac{K_4}{2}\left((m_x + im_y)^6 + (m_x - im_y)^6\right)\cdots \qquad \vec{m} = \vec{M}/|M|$$

Objectives of a magnetic calculation

1. Microscopic determination of the saturation magnetization
   - It might be non uniform inside the crystal cell (non-collinear magnetism)

2. Microscopic determination of the magneto crystalline anisotropy
   – Its most important contribution from the spin-orbit coupling
     - Other an isotropic interactions: spin-spin, spin-other orbits neglected

3. Exchange terms

Some Classes of Magnetic Systems

- Paramagnetism is favored by the presence of bands, which are doubly occupied. But some systems exhibit spontaneous magnetization.

- Collinear ferromagnets :3d Metals : Fe, Co, Ni. Mostly due to spin (orbital moment ~0) Stoner criterion: xc X D(Ef) large

- Antiferromagnet (anti parallel orientation): Cr, Mn (some phases), ordered alloys: Fe_3Mn …, insulating compounds MnO, NiS …: different sublattices with opposite orientations.

- In case the moments do not compensate: ferrimagnetism yields a net magnetic moment. Magnetite: Fe_3O_4, $NiFe_2O_4$ Complicated structures: exchange mediated by oxygen

- Helimagnetism: some 4f Rare earth (RKKY interaction), $MnAu_2$

- More complex non collinear structure: Mn, fcc Fe etc….

Example: Ferromagnetism of 3d metals

- Iron, Nickel and Cobalt: ferromagnets
  - These are 3d elements, for which the atomic 3d WF strongly overlap and form a band of a given width W
  - A qualitative understanding of the existence of magnetism is given by the Stoner criterion.
    - Assume a constant DOS (D), and decompose the energy as band+exchange contributions
    - Correlation effects has a structure: $U n_\uparrow n_\downarrow$
    - If $DU > 1$, then one spin channel will be filled at the expense of the other.

$$E = E_B + E_{XC} = \int_0^{\varepsilon_\uparrow} \varepsilon D(\varepsilon) d\varepsilon + \int_0^{\varepsilon_\downarrow} \varepsilon D(\varepsilon) d\varepsilon + U n_\uparrow n_\downarrow$$
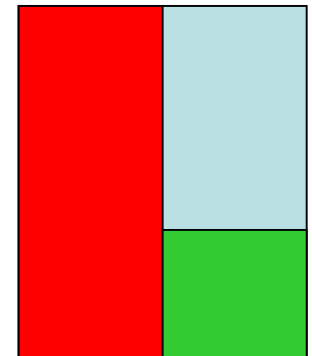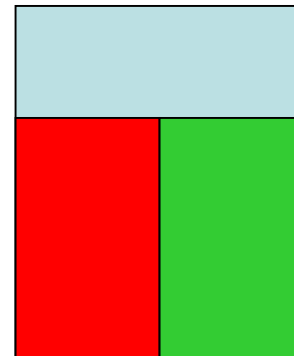
$$= \frac{1}{2D}(n_\uparrow^2 + n_\downarrow^2) + U n_\uparrow n_\downarrow = \frac{n^2}{2D} + (-\frac{1}{D} + U)n_\uparrow n_\downarrow = \frac{n^2}{2D} + (-\frac{1}{D} + U)\frac{n^2(1-\zeta^2)}{4}$$

$$D(\varepsilon) = D = Cste$$

$$D\varepsilon_\uparrow = n_\uparrow$$

$$n_\uparrow + n_\downarrow = n$$

$$\zeta = \frac{n_\uparrow - n_\downarrow}{n}$$

Spin DFT

- In principle, the DFT is an exact theory and so there is no need for a particular consideration for spin.
- But, the usual approximations generalize easily if we consider spin explicitly
- One complements the external potential V, with a magnetic field B along z (next for **B**)
- The system will polarize, and one gets a up and a down electron density: $n_\uparrow(\mathbf{r}), n_\downarrow(\mathbf{r})$
- The energy of the system will be a functional of the density and the magnetization (supposed along z).

$$E = K\left[n_\uparrow\right] + K\left[n_\downarrow\right] + E_H\left[n\right] + E_{xc}\left[n_\uparrow, n_\downarrow\right]$$

$$+ \int d\mathbf{r}\, n(\mathbf{r}) V_{ext}(\mathbf{r}) - \int d\mathbf{r}\, m(\mathbf{r}) B_{ext}(\mathbf{r})$$

$$n(\mathbf{r}) = n_\uparrow(\mathbf{r}) + n_\downarrow(\mathbf{r})$$

$$m(\mathbf{r}) = n_\uparrow(\mathbf{r}) - n_\downarrow(\mathbf{r}), \text{ in units of } \mu_\mathbf{B}$$

The Kohn-Sham equations

- If we minimize the energy, we obtain two equations, one for each spin channel (we set $B_{ext}=0$)

$$\left\{-\frac{\Delta}{2}+V^{\sigma}{}_{eff}(\mathbf{r})\right\}\Psi^{i}{}_{\sigma}=\varepsilon^{i}{}_{\sigma}\Psi^{i}{}_{\sigma} \qquad \sigma=\uparrow\downarrow$$

$$n^{\sigma}(\mathbf{r})=\sum_{i}f(\varepsilon^{i}{}_{\sigma})\left|\Psi^{i}{}_{\sigma}(\mathbf{r})\right|^{2}$$

$$V^{\sigma}{}_{eff}(\mathbf{r})=V_{ext}(\mathbf{r})+V_{h}(\mathbf{r})+V^{\sigma}{}_{xc}(\mathbf{r})$$

$$V^{\sigma}{}_{xc}(\mathbf{r})=\frac{\delta E_{xc}(n_{\downarrow},n_{\uparrow})}{\delta n_{\sigma}}$$

$$n(\mathbf{r})=n^{\downarrow}(\mathbf{r})+n^{\uparrow}(\mathbf{r})$$

$$m(\mathbf{r})=n^{\uparrow}(\mathbf{r})-n^{\downarrow}(\mathbf{r})$$

The LSDA

- The total energy is also given by the sum over states:

$$E = \sum_{i,\sigma} \varepsilon_{i,\sigma} - \frac{1}{2}\int d\mathbf{r}\, n(\mathbf{r})V_h(\mathbf{r}) - \sum_\sigma \int d\mathbf{r}\, n_\sigma(\mathbf{r})V_{xc}^\sigma(\mathbf{r}) + E_{xc}\left[n_\uparrow, n_\downarrow\right]$$

- The exchange correlation energy of the electron gas can be written as:

$$E_{xc}^{LDA}\left[n_\uparrow, n_\downarrow\right] \approx \int n(\mathbf{r})\varepsilon_{xc}(n_\uparrow, n_\downarrow)\,d\mathbf{r}$$

$$\varepsilon_{xc}(n_\uparrow, n_\downarrow) = \varepsilon_x(n_\uparrow, n_\downarrow) + \varepsilon_c(n_\uparrow, n_\downarrow)$$

$$\varepsilon_x(n_\uparrow, n_\downarrow) = -3\left(\frac{3}{4\pi}\right)^{1/3}\frac{1}{n}(n_\uparrow^{4/3} + n_\downarrow^{4/3})$$

$$\varepsilon_c(n_\uparrow, n_\downarrow) \quad \text{by QMC}$$

$$E_{xc}^{GGA}\left[n_\uparrow, n_\downarrow\right] \approx \int n(\mathbf{r})\varepsilon_{xc}(n_\uparrow, n_\downarrow, \nabla n_\uparrow, \nabla n_\downarrow)\,d\mathbf{r}$$

Perdew, Burke, Ernzerof PRL,77,3865(1996): PBE

Stoner revisited

- Each spin channel yields a different potential due to the xc term
- To study the stability of the paramagnetic phase, one can expand this potential for a small magnetization term

$$V_{xc}(\mathbf{r}) = V^0_{xc}(\mathbf{r}) \pm m(\mathbf{r})V^1_{xc}(\mathbf{r})$$

$$V_{xc}(\mathbf{r}) = V^0_{xc}(\mathbf{r}) \pm \frac{1}{2}IM \qquad \text{If second term ~constant: rigid shift}$$

$$M = \int^{\varepsilon_f} \left[D^0(\varepsilon + \frac{1}{2}IM) - D^0(\varepsilon - \frac{1}{2}IM) \right] d\varepsilon$$

Non zero solution at small M $\Rightarrow ID^0(\varepsilon_f) > 1$

Stoner revisited

- More rigorously (Janak,1977): compute the spin susceptibility and the criterion is satisfied when it is negative.

-

$$\chi = \frac{\chi_0}{1 - \chi_0 I}$$

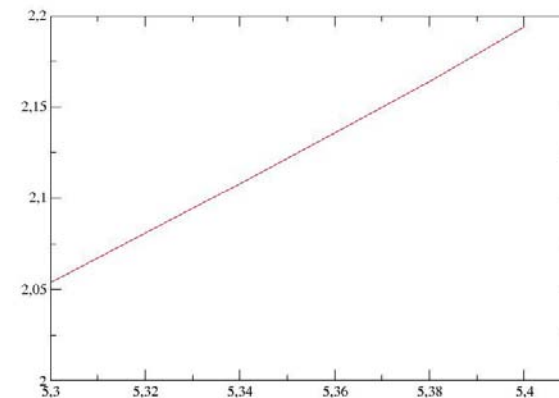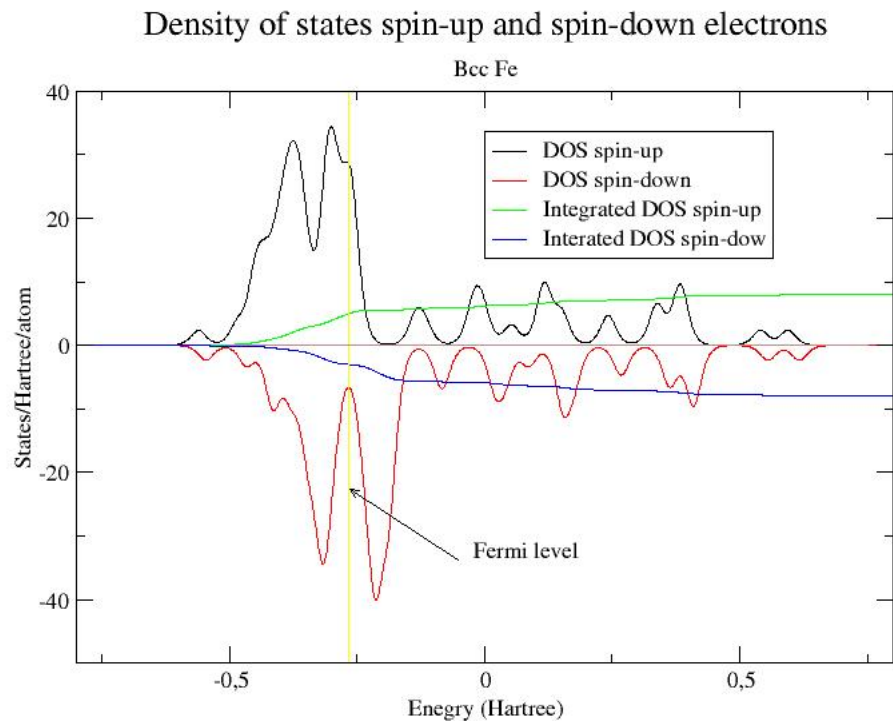$$I = \int d\mathbf{r}\gamma^2(\mathbf{r})|K(\mathbf{r})|$$

$$D^0(\varepsilon_f)\gamma(\mathbf{r}) = \frac{d}{d\varepsilon_f}\rho(\mathbf{r})$$

$$\left\{\delta^2 E_{xc}[\rho,\vec{m}]/\delta m(\mathbf{r})\delta m(\mathbf{r}')\right\} = 2K(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$$

- BCC Fe ~rigid shift of DOS
- Magnetization strongly dependent of cell parameter

Magnetization as a function of cell (a.u.)

Density of states spin-up and spin-down electrons

Bcc Fe

DOS spin-up
DOS spin-down
Integrated DOS spin-up
Interated DOS spin-dow

Fermi level
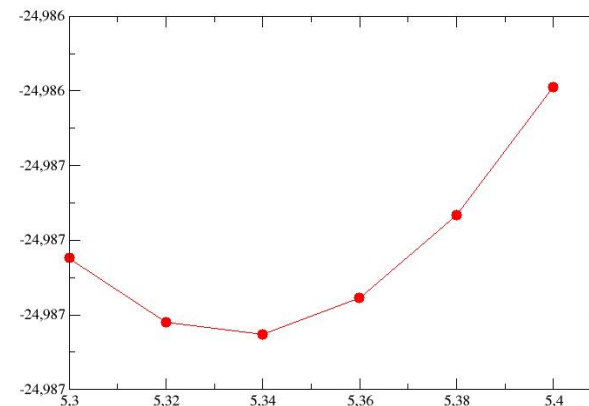
Energy as a function of cell (a.u.)

Calculations using a Pseudo potential

- Iron has been much studied
  - LSDA will predict a correct magnetic moment (2.17 vs 2.22 exp)
  - BUT, the NM fcc structure has a lower energy than the FM bcc
  - This is corrected but using the (PBE) GGA
- Pseudo potentials are generally constructed on non magnetic configurations and used for magnetic systems …
- Also, the use of non local core corrections is essential (exercice: compare magnetization for bcc Fe, using 26fe.pspnc and 26fe.hgh)
- But, best results are obtained with PAW (cf talks by Jollet Torrent): this is an all electron theory with a psp look (and includes nlcc)

Results of calculations

- 3d ferromagnetic elements (Fe, Co, Ni): very good prediction of the magnetization with GGA

- 3d non ferromagnetic elements (Mn, Cr): complicated spin arrangement (e.g. spiral) non compatible with the hypothese of // spins

- Intermetallic compounds (that is compounds of Cu ,Ni, Co, Fe, Mn, Cr), yields good values of magnetization

- Magnetic Oxydes: classical examples of failure of the LSDA (or GGA)

- This failure is presumably due to a neglect of the on site correlation (U term) of localized orbital.

- LDA includes this only on average (cf the example of Ce)

- This failure is the source of many improvements of LDA, GGA: LDA+U, SIC, Hybrids functionals (HF+LDA), etc…

Non collinear Magnetism

- Up to now, we considered moments all parallel along a given axis
- But there are cases where it is not justified:
  - In some systems, the ground state is non collinear: in Mn, in solid oxygen, in Mn_4N, in fcc Fe etc…
  - Spin excitations ("spin waves") must take into account non parallel configurations
  - The exchange coupling parameter of the Heisenberg Hamiltonian requires a non collinear arrangement
- This requires a generalization of spin DFT to account for a vector **m(r)**

Spin ½ reminder

- Spin state

$$|s\rangle = a|+\rangle + b|-\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

- Magnetic moment along *x*

$$S_x = \mu_B \langle s|\sigma_x|s\rangle$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The WF as a two component spinor

- In each point in space, the wave function posses two spin components, and the KS principle is generalized towards a duality between (density, magnetization) and external fields (potential, magnetic field)

$$\psi\ (\ r\ ) = \begin{bmatrix} \psi_\uparrow(\ r\ ) \\ \psi_\downarrow(\ r\ ) \end{bmatrix}$$

- The electronic density can be written:

$$\rho(r) = \begin{bmatrix} \psi_\uparrow(r) & \psi_\downarrow(r) \end{bmatrix}^* I \begin{bmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{bmatrix} = |\psi_\uparrow(r)|^2 + |\psi_\downarrow(r)|^2$$

- The magnetization along x, for instance:

$$M_x(r) = \begin{bmatrix} \psi_\uparrow(r) & \psi_\downarrow(r) \end{bmatrix}^* S_x \begin{bmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{bmatrix}$$

$$= \mu_B \begin{bmatrix} \psi_\uparrow(r) & \psi_\downarrow(r) \end{bmatrix}^* \sigma_x \begin{bmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{bmatrix}$$

$$= \mu_B \begin{bmatrix} \psi_\uparrow(r) & \psi_\downarrow(r) \end{bmatrix}^* \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{bmatrix}$$

$$= \mu_B (\psi_\uparrow(r)^* \psi_\downarrow(r) + \psi_\uparrow(r)\psi_\downarrow(r)^*)$$

- Magnetization

$$\vec{M}(r) = \begin{bmatrix} \psi_\uparrow(r) & \psi_\downarrow(r) \end{bmatrix}^* \vec{S} \begin{bmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{bmatrix}$$

- Spin density matrix

$$\rho^{\alpha\beta}(r) = \psi^*_\alpha(r)\psi_\beta(r) \rightarrow \rho^{\alpha\beta}(r) = \sum_{kj} f_{kj} \psi^{*kj}_\alpha(r)\psi^{kj}_\beta(r)$$

- We can equivalently use each object:

$$\vec{m}(r) = \sum_{\alpha\beta} \rho^{\alpha\beta}(r)\vec{\sigma}_{\alpha\beta} \qquad \rho(\mathrm{r}) = \sum_{\alpha\beta} \rho^{\alpha\alpha}(r)$$

$$2\rho^{\alpha\beta}(r) = \rho(r)\delta_{\alpha\beta} + \vec{\mathrm{m}}(\mathrm{r}).\vec{\sigma}^{*}_{\alpha\beta}$$

- Note the *

Energy functional (GLSDA)

- Energy is now a functional of energy and magnetization vector **m**

$$E\left[\rho^{\alpha\beta}(r)\right] = T\left[\rho^{\alpha\beta}(r)\right] + E_H\left[\rho(r)\right] + E_{xc}\left[\rho^{\alpha\beta}(r)\right] + \int V_{ext}(r)\rho(r)dr$$

$$T\left[\rho^{\alpha\beta}(r)\right] = -\frac{\hbar^2}{2m}\sum_{jk}\int f_{kj}(\psi_{kj}^{*\alpha}(r)\Delta\psi_{kj}^{*\alpha}(r) + \psi_{kj}^{*\beta}(r)\Delta\psi_{kj}^{*\beta}(r))dr$$

$$E_{xc}\left[\rho^{\alpha\beta}(r)\right] = E_{xc}\left[\rho(r), \mathbf{m}(r)\right]$$

- One can equivalently use the spin density matrix.
- The variational principle applied to it leads to the new Hamiltonian
- As usual, one needs to construct the exchange correlation

The « local spin density approximation »(LSDA)

- One extends the usual (LDA) exchange correlation term to include the presence of vector magnetization

$$E_{xc} = \int \rho(r)\varepsilon_{xc}(\rho(r),|\mathbf{m}(r)|)dr = \int \rho(r)\varepsilon_{xc}(\rho^{\alpha\beta}(r))dr$$

- If one uses the electron gas as a reference, the magnetization direction is immaterial (note, this is easy to express with the help of the magnetization vector)
- We can use the same formula for the LDA as the usual collinear magnetic case, since it only depends on $|\mathbf{m}|$
- In principle, the GGA should include the rotationally invariant parts of $\nabla\mathbf{m}$, but is not yet done…

Kohn-Sham Hamiltonian

$$H^{\alpha\beta} = -\frac{1}{2}\Delta\delta_{\alpha\beta} + V^{\alpha\beta}{}_{eff} = \frac{\delta E}{\delta\rho^{\alpha\beta}(r)}$$

$$V^{\alpha\beta}{}_{eff} = V_H(\rho(r))\delta_{\alpha\beta} + V^{\alpha\beta}_{xc}(\rho^{\alpha\beta}(r)) + V_{ext}(r)$$

$$V_{xc}^{\alpha\beta}(\rho^{\alpha\beta}(r)) = \frac{\delta E_{xc}(\rho^{\alpha\beta}(r))}{\delta\rho^{\alpha\beta}(r)}$$

$$V_{xc}^{\alpha\beta}(\rho^{\alpha\beta}(r)) = V_{xc}(\rho^{\alpha\beta}(r))\delta_{\alpha\beta} - \mu_B\vec{b}(\rho^{\alpha\beta}(r)).\vec{\sigma}^{\alpha\beta}$$

$$\vec{b}(\rho^{\alpha\beta}(r)) = -\frac{\delta E_{xc}(\rho^{\alpha\beta}(r))}{\delta\mathbf{m}(r)} = \hat{\mathbf{m}}(r)\rho(r)\frac{\partial\varepsilon_{xc}(\rho^{\alpha\beta}(r))}{\partial|m(r)|}$$

Energy functional

$$E\left[\rho^{\alpha\beta}(r)\right] = \sum_{\mathbf{k}j} f(\varepsilon_{\mathbf{k}j})\varepsilon_{\mathbf{k}j} - \int V_{e\!f\!f}(\mathbf{r})\rho(\mathbf{r})d\mathbf{r} + \int \mathbf{B}_{e\!f\!f}(\mathbf{r})\mathbf{m}(\mathbf{r})d\mathbf{r}$$

$$+ \int V_{ext}(\mathbf{r})\rho(\mathbf{r})d\mathbf{r} + E_H\left[\rho(\mathbf{r})\right] + E_{xc}\left[\rho(\mathbf{r}), \mathbf{m}(\mathbf{r})\right]$$

- Dirac's equation (ϕ and ψ two components spinors)

$$\left[E + 2mc^2 - V\right]\phi + c\sigma.p\psi = 0$$

$$\left[E - V\right]\psi + c\sigma.p\phi = 0$$

- Low E: scalar relativistic approximation + spin-orbit coupling

$$\phi \approx (v/c)\psi \quad ordre\ (1/c)^2 = (1/137)^2$$

$$\frac{p^2}{2}F + V(r)\phi$$

$$-\frac{p^4}{8c^2}F - \frac{1}{4c^2}\nabla V(r).\nabla\phi$$

$$+\frac{1}{4c^2}\sigma.(\nabla V(r) \times p\phi) = \varepsilon\phi$$

- Spherical potential

$$\nabla V(r) = \frac{1}{r}\frac{dV}{dr}\mathbf{r}$$

$$\frac{1}{4c^2}\boldsymbol{\sigma}.(\nabla V(r)\times\mathbf{p}) = \frac{1}{r}\frac{dV}{dr}\boldsymbol{\sigma}.(\mathbf{r}\times\mathbf{p}) = \frac{1}{r}\frac{dV}{dr}\boldsymbol{\sigma}.\mathbf{l}$$

- Order of magnitude for a valence orbital

$$a \approx 1/Z, V \approx Z^2$$

$$<\psi\,|\,r^{-1}dV\,/\,dr\,|\psi> \approx (Z\,/\,c)^2$$

- ->Much better for the valence pseudo orbital $\approx (Z_{eff}\,/c)^2$

Spin orbit projector

- ## The **L.S** operator
  - The angular momentum operator has invariant spaces indexed by l and of dimension (2l+1). A projector on this space is denoted

$$\left| l > < l \right|$$

  - The same is true for spin (with l=1/2)

$$\left| s > < s \right|$$

  - A projector on spin and angular momentum space is

$$\left| ls > < ls \right|$$

The L.S operator

- On this space the L+S=J operator has two invariant subspaces

  - Angular momentum l+1/2 and l-1/2 of dimensions 2l+2 and 2l

  - Now, $J^2 = (L+S)^2 = L^2 + S^2 + 2L.S$

  - So we derive the meaning of

$$\left| \mathbf{L.S} ls > < ls \right|$$

  - Project on the ls space, and apply the spin-orbit coupling

How to build Pseudo potentials

- For a potential with a spherical symmetry, the solutions of Dirac's equation have the form:

$$\phi_{l+1/2}(r)\begin{pmatrix} \left(\dfrac{l+m+1}{2l+1}\right)^{1/2} Y_l^m \\[2ex] \left(\dfrac{l-m}{2l+1}\right)^{1/2} Y_l^{m+1} \end{pmatrix} \quad \phi_{l-1/2}(r)\begin{pmatrix} \left(\dfrac{l-m+1}{2l+1}\right)^{1/2} Y_l^{m-1} \\[2ex] -\left(\dfrac{l+m}{2l+1}\right)^{1/2} Y_l^m \end{pmatrix}$$

- One can built a pseudo potential for which the wave functions have the same shape beyond a certain radius, by only adding a spin orbit term to it

$$V_{NL} = \sum_l \left(\sum_m V_l^{SR}(r,r')|ls\rangle\langle ls| + \sum_m V_l^{SO}(r,r')\mathbf{L.S}|ls\rangle\langle ls| \right)$$

$$V_l^{SR(O)}(r,r') = \sum_{ij} \alpha_{ij} P_i(r) P_j(r')$$

How to use a plane wave basis

- Each component is developped on a basis
- For instance, in plane waves, the basis is

$$G\uparrow = \begin{bmatrix} e^{2i\pi G.r} \\ 0 \end{bmatrix} \quad \text{et} \quad G\downarrow = \begin{bmatrix} 0 \\ e^{2i\pi G.r} \end{bmatrix}$$

- The components of the wave function are:

$$\psi(r) = e^{ik.r} \begin{bmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{bmatrix} = e^{ik.r} \begin{bmatrix} \sum_G a_{G\uparrow} e^{iG.r} \\ \sum_G a_{G\downarrow} e^{iG.r} \end{bmatrix}$$

- That is two times more coefficients, and matrices 4 times bigger

Expression in the plane wave basis

- The important term is $\langle G | V_{NL} | G' \rangle$

$$\langle G | Q_i(r) Q_j(r') | ls \rangle \langle ls | G' \rangle = 4\pi(2l+1) f_i(|G|) f_i(|G'|) P_l(\hat{G}.\hat{G}')$$

$$\langle G s_1 | Q_i(r) Q_j(r') \mathbf{L.S} | ls \rangle \langle ls | G' s_2 \rangle = -i4\pi(2l+1) f_i(|G|) f_i(|G'|) P'_l(\hat{G}.\hat{G}') < s_1 | \mathbf{S} | s_2 > . G \times G'$$

$$f_i(|G|) = 4\pi \int_0^{+\infty} Q_i(r) \exp(iGr) r^2 dr$$

- See Gonze at al. Comp. Mat. Sci., 25 (2002)

Effect of spin-orbit coupling upon total energy

- Heavy metals
    - « norm conserving » pseudo potentials
    - Experimental equilibrium phases
    - N. Richard et S. Bernard(PRB,66,2002)

	GGA	GGA+SO	EXP	GGA	GGA+SO	EXP
U	145GPa	132Gpa	135Gpa	19.91	20.33	20.56
Np	180Gpa	165Gpa	120Gpa	18,20	19.83	19.23

Conclusions

- Magnetic moments generally well reproduced by GLSDA
- But magnetic oxides exhibit localized states which are not well described by LDA (Mott insulators e.g. due to correlations are described as metals)
- Anisotropy is well described for "hard" magnets, less well for soft magnets
- Temperature effects on K are nearly untouched
- Spin-orbit coupling has a smaller effect on total energy in a psp context than in all electrons calculations
- But changes the DOS substantially for heavy metals

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