Magnetism

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ABINIT Hands-on 2019

Outline

- Origin of magnetism:
    - A bit of history
    - Inside an atom
    - Between 2 atoms
    - Interaction with ligands
    - Interaction through ligands
    - Spin-orbit coupling and spin orientation
- Collinear magnetism in DFT
- Non-collinear magnetism in DFT
- Constrained magnetic moments
- Finite magnetic field

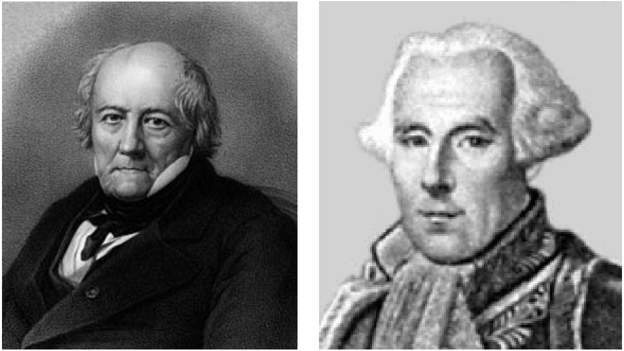
History of magnetism

1819: Hans Christian Oersted

First experimental evidence of the link between electric current and magnetic field.

History of magnetism

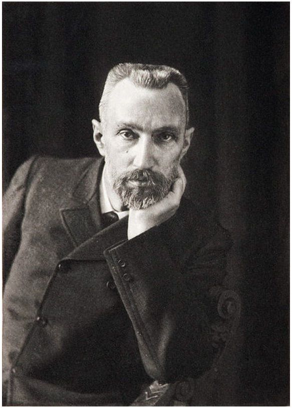
1820: Jean-Baptiste Biot and Felix Savart

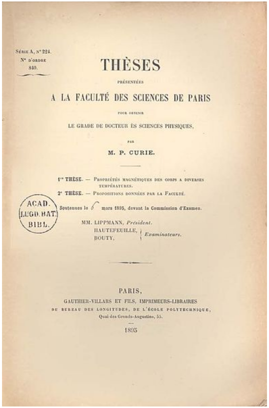


Mathematical expression of the magnetic field generated by an electric current flowing through a wire.

History of magnetism

1895: Pierre Curie





Série A, n° 224.
N° d'ordre
840.

THÈSES

présentées

A LA FACULTÉ DES SCIENCES DE PARIS

pour obtenir

LE GRADE DE DOCTEUR ÈS SCIENCES PHYSIQUES,

par

M. P. CURIE.

1re THÈSE. — Propriétés magnétiques des corps a diverses températures.
2e THÈSE. — Propositions données par la Faculté.

Soutenues le 6 mars 1895, devant la Commission d'Examen.

MM. LIPPMANN, *Président.*
HAUTEFEUILLE, BOUTY, *Examinateurs.*

PARIS,
GAUTHIER-VILLARS ET FILS, IMPRIMEURS-LIBRAIRES
DU BUREAU DES LONGITUDES, DE L'ÉCOLE POLYTECHNIQUE,
Quai des Grands-Augustins, 55.

1895

Effect of temperature on paramagnetic susceptibilities (Curie's law).

History of magnetism

1907: Pierre-Ernest Weiss

First microscopic model to explain magnetism (molecular field).

History of magnetism

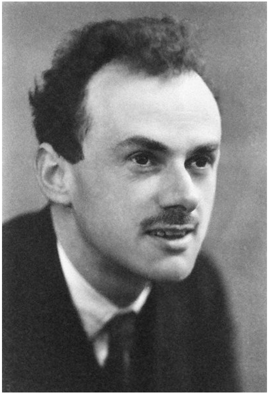
1930: Louis Néel

Extension of Weiss model to antiferromagnetism and ferrimagnetism.

However, no explanation of the high temperature magnetic phase transitions.

History of magnetism

Pauli, Dirac, Heisenberg


Magnetism cannot be explained without quantum mechanics!

Origin of magnetism: Inside an atom

2 electrons with the same l but different m_l (Φ_a and Φ_b orbitals):

$$H = H_1 + H_2 + H_{12}$$

$$H_1 = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_1}$$

$$H_2 = -\frac{\hbar^2}{2m}\nabla_2^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_2}$$

$$H_{12} = -\frac{e^2}{4\pi\varepsilon_0 r_{12}}$$

$$\langle\phi_a(r_i)|H_i|\phi_a(r_i)\rangle = E_1$$

$$\langle\phi_b(r_i)|H_i|\phi_b(r_i)\rangle = E_2$$

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}$$

Origin of magnetism: Inside an atom

Each electron can have spin up and down states $\longmapsto$ 4 spin-orbitals:

$$|\uparrow\uparrow\rangle \quad |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \quad |\downarrow\downarrow\rangle$$

Such that we have the following Hamiltonian:

$$H = E_1 + E_2 + \begin{pmatrix} K_{ab} - J_{ab} & 0 & 0 & 0 \\ 0 & K_{ab} & -J_{ab} & 0 \\ 0 & -J_{ab} & K_{ab} & 0 \\ 0 & 0 & 0 & K_{ab} - J_{ab} \end{pmatrix}$$

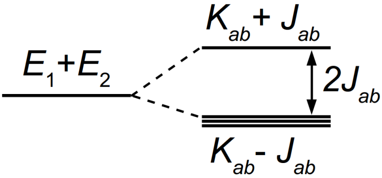
where we have the Coulomb and Exchange integrals:

$$K_{ab} = \frac{e^2}{4\pi\varepsilon_0} \int d^3r_1 \int d^3r_2 \frac{|\phi_a(r_1)|^2 |\phi_b(r_2)|^2}{|r_{12}|} \; (= U)$$

$$J_{ab} = \frac{e^2}{4\pi\varepsilon_0} \int d^3r_1 \int d^3r_2 \frac{\phi_a^*(r_1)\phi_b(r_1)\phi_b^*(r_2)\phi_a(r_2)}{|r_{12}|}$$

Origin of magnetism: Inside an atom

The diagonalization gives a triplet (FM) and a singlet (AFM) states:



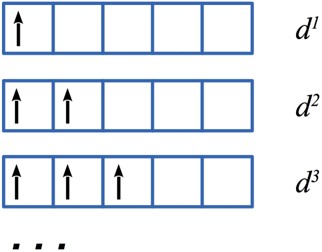
The FM triplet is the ground state.

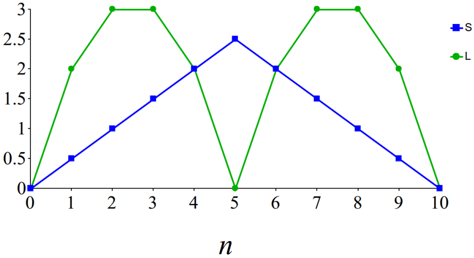
The Hamiltonian can be re-written in the Heisenberg form:

$$H = constant - 2J_{ab}\mathbf{S}_1 \cdot \mathbf{S}_2$$

Origin of magnetism: Inside an atom

To have $\langle S \rangle \neq 0$ one needs partially filed orbitals ex: d^n orbitals



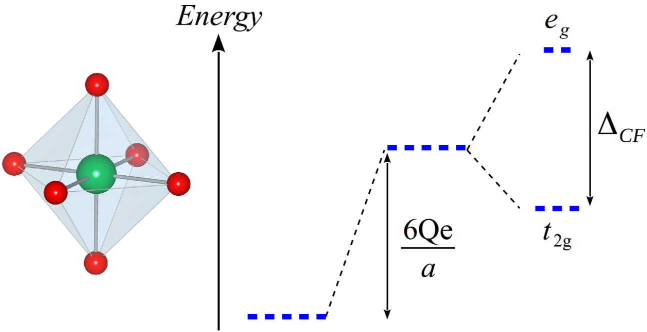


Hund's rules

Most of the crystals are magnetic because they contain Transition-Metal and Rare Earth atoms (*d* and *f* electrons partially filed)

Origin of magnetism: Interaction with ligands

Atom in a solid: Crystal Field Splitting

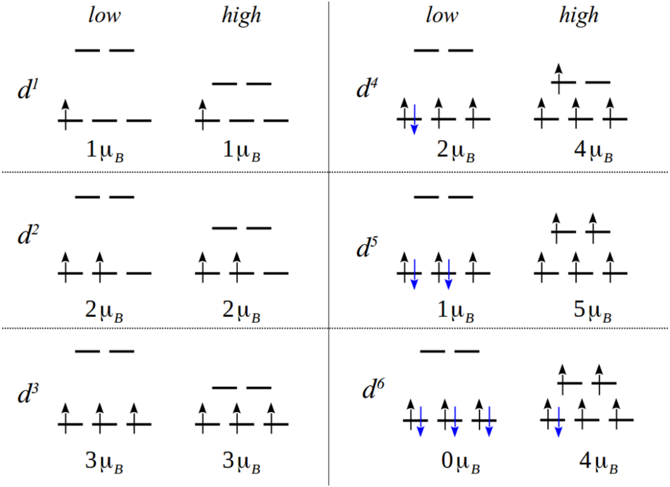


Atomic *d* (or *f*) orbitals splitted due to the surrounding atoms.

Hund's rules still apply.

Origin of magnetism: Interaction with ligands

High-spin and low-spin configurations:

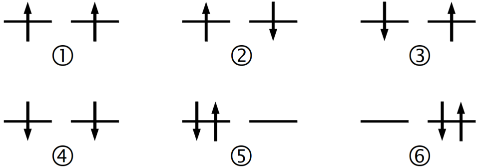


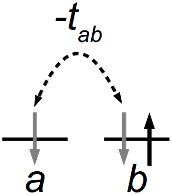
Depending on the size of Δ_{CF} relative to U.

Origin of magnetism: Between two atoms

The FM state is lower in energy inside an iolated atom (Hund's rules).

This is not necessarily the case between atoms, in H_2 molecule:





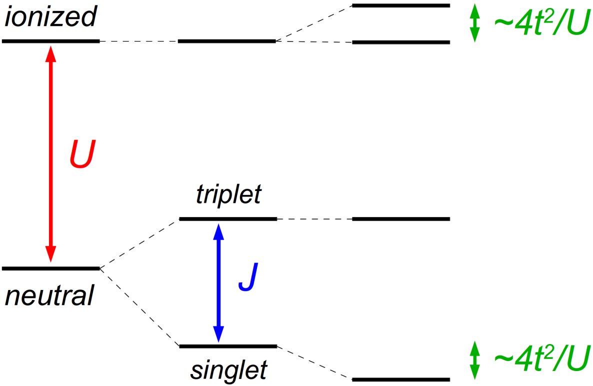
Similar Heisenberg Hamiltonian: $H = constant - 2J_{ab}\mathbf{S}_1 \cdot \mathbf{S}_2$

but with the $1s$ orbital overlap between the 2 atoms: $J < 0$

The singlet AFM state is lower in energy!

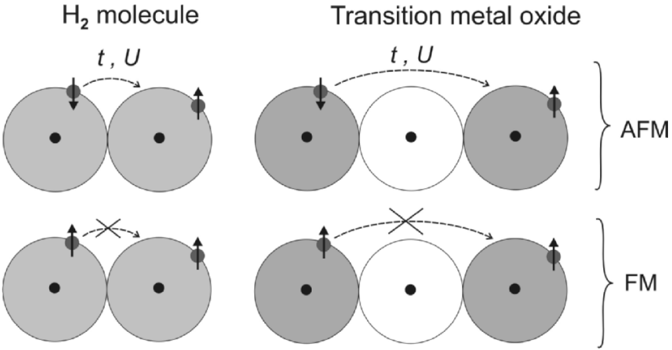
Origin of magnetism: Between two atoms

The hopping process reinforce the AFM state:



Origin of magnetism: Interaction through ligands

Atoms interacting through the ligands: Superexchange



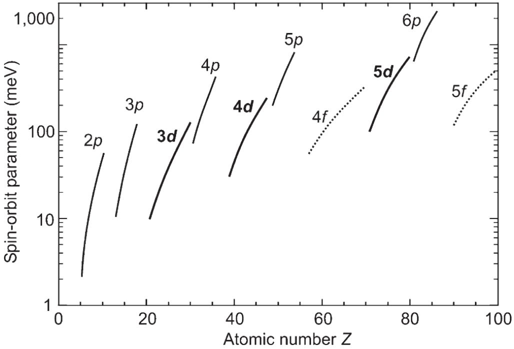
from Stöhr and Siegmann, Magnetism, Springer 2006

Heisenberg picture still holds (localised electrons, $t <<$): $H = JS_1 S_2$

Spin-orbit coupling and spin orientations

Relativistic corrections gives an interaction between S and L:

$$\lambda \mathbf{L}\cdot\mathbf{S} = \frac{\mu_0}{16\pi}\frac{g_s Z e^2}{m^2 r^3}\mathbf{L}\cdot\mathbf{S} \quad or \quad \frac{g_s}{4m^2c^2r}\frac{dV}{dr}\mathbf{L}\cdot\mathbf{S}$$



In crystals, this term drives the easy/hard axis orientation of the spins

It also drives the spin cantings (Dzyaloshinskii-Moriya interaction)

Heisenberg Model

For localised moments, the system can be reduced to an effective spin-spin interaction

2^{nd} order Heisenberg model for localised magnetic moments:

$$H = -2\left[J\mathbf{S}\cdot\mathbf{S}' + \mathbf{D}\cdot(\mathbf{S}\times\mathbf{S}') + \mathbf{S}\cdot\Phi\cdot\mathbf{S}'\right]$$

- $J \longmapsto$ Superexchange interaction (favors $S \parallel S'$)
- $\mathbf{D} \longmapsto$ Dzyaloshinskii-Moriya interaction (favors $S \perp S'$)
- $\Phi \longmapsto$ Single Ion Anisotropy (easy/hard spin orientation)

Magnetism in DFT: Collinear case

DFT based on the charge density $\rho(r)$

To enlarge DFT to (collinear) magnetism, decomposition of the density:

$$\rho = \rho(\uparrow) + \rho(\downarrow)$$

The Hohenberg and Kohn theorem generalizes with an energy functional:

$$E = E\left[\rho(\uparrow), \rho(\downarrow)\right]$$

With 2 Kohn-Sham equations to be solved, one for each spin-channel σ:

$$\left(T + V_{Ri}(r) + V_H(r) + V_{xc,\sigma}\right)\phi_{i\sigma}(r) = \varepsilon_{i\sigma}(r)$$

with

$$V_{xc,\sigma} = \frac{\delta E_{xc}\left[\rho(\uparrow), \rho(\downarrow)\right]}{\delta \rho_\sigma(r)}$$

Magnetism in DFT: Collinear case

Then minimizing the K-S equations we get the ground state with:

$$\rho = \rho(\uparrow) + \rho(\downarrow) \quad \text{and magnetization } m = \rho(\uparrow) - \rho(\downarrow)$$

Supposing the magnetic moments are localised around the atoms (this is often the case for *d* and *f* electrons), one can compute magnetization on each atom (*prtdensph* input flag in ABINIT)

Example of Fe bulk BCC:

```
Integrated electronic and magnetization densities in atomic spheres:
---------------------------------------------------------------------
Note: Diff(up-dn) is a rough approximation of local magnetic moment
Atom    Radius    up_density   dn_density  Total(up+dn)  Diff(up-dn)
   1   2.00000     8.152787     5.919175    14.071962     2.233612
---------------------------------------------------------------------
 Sum:              8.152787     5.919175    14.071962     2.233612
Total magnetization (from the atomic spheres):             2.233612
Total magnetization (exact up - dn):                       2.228468
```

about 2.23 μ_B.

Magnetism in DFT: Non-collinear case

Wave functions are described by spinors:

$$\phi_i(r) = \begin{pmatrix} \phi_{i\uparrow} \\ \phi_{i\downarrow} \end{pmatrix}$$

Such as the density is a 2 × 2 matrix:

$$\rho = \begin{pmatrix} \rho^{\uparrow\uparrow} & \rho^{\uparrow\downarrow} \\ \rho^{\downarrow\uparrow} & \rho^{\downarrow\downarrow} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} n + m_z & m_x - im_y \\ m_x + im_y & n - m_z \end{pmatrix}$$

with n the electron density and m_i the magnetization density along the direction i

$$n(r) = \frac{1}{2} Tr\rho(r) = \sum_{\alpha} \rho^{\alpha\alpha}(r) \qquad \mathbf{m}(\mathbf{r}) = \sum_{\alpha\beta} \rho^{\alpha\beta}(\mathbf{r}) \cdot \sigma_{\alpha\beta}$$

with the Pauli matrices $\sigma_{\alpha\beta} = (\sigma_x, \sigma_y, \sigma_z)$:

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

Magnetism in DFT: Non-collinear case

Kohn-Sham equations with spinors:

$$\sum_{\beta} H^{\alpha\beta}|\phi_i^{\beta}\rangle = \varepsilon_i|\phi_i^{\alpha}\rangle$$

where the Hamiltonian is a 2×2 matrix:

$$H^{\alpha\beta} = T\delta_{\alpha\beta} + V(r)\delta_{\alpha\beta} + \int \frac{n(r')}{r-r'}dr'\delta_{\alpha\beta} + V_{xc}^{\alpha\beta}(r)$$

and:

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

$\rho^{\alpha\beta}$ is diagonal when $m = m_z \longmapsto$ collinear case.

Magnetism in DFT: Non-collinear case

One needs SOC to couple directions (space rotations) to the spins:

- controlled by *so_psp* flag for norm-conserving pseudopotential
- controlled by *pawspnorb* flag for PAW

(necessary to probe magnetic anisotropies or spin cantings)

Magnetization on each atom can also be estimated through *prtdensph* flag, example of Fe bulk BCC:

```
Integrated electronic and magnetization densities in atomic spheres:
---------------------------------------------------------------------
Note:      this is a rough approximation of local magnetic moments
Atom   Radius      Total density     mag(x)      mag(y)      mag(z)
   1   2.00000       14.078578     -0.000039   -0.000023    2.274108
---------------------------------------------------------------------
Total magnetization (spheres)      -0.000039   -0.000023    2.274108
Total magnetization (exact)        -0.000039   -0.000023    2.270315
```

Magnetism in practice with Abinit

nsppol, *nspinor* and *nspden* input flags:

	nsppol	nspinor	nspden
Non-magnetic	1	1	1
Collinear FM	2	1	2
Collinear AFM	1	1	2
Non-Collinear	1	2	4

Initialize *spinat* = (m_x, m_y, m_z) for each atom,

(only *spinat* = (0, 0, m) for collinear calculations).

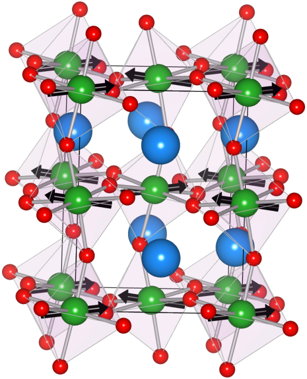
SOC coupling controlled by *so_psp* (norm-conserving) or *pawspnorb* for PAW (PAW SOC coupling amplitude can be artificially tuned with *spnorbscl* flag).

With SOC do not use time-reversal symmetry (*kptopt* = 3 or 4, nsym$\neq$1 and *kptopt* =4 is under dev.).

Example of $YCrO_3$

$YCrO_3$ has a distorted perovskite structure (*Pnma* space group)

$YCrO_3$ is a non-collinear AFM (wFM and wAFM)



Collinear case of $YCrO_3$ (input)

```
natom  20
ntypat 3
znucl  39 24 8
typat  4*1 4*2 12*3

acell 5.518 7.54 5.247  Angstrom
xred
  0.07064  0.75000  0.48013 # Y
  0.42935  0.25000  0.98013 # Y
  0.57064  0.75000  0.01986 # Y
  0.92935  0.25000  0.51986 # Y
  0.00000  0.00000  0.00000 # Cr
  0.50000  0.00000  0.50000 # Cr
  0.00000  0.50000  0.00000 # Cr
  0.50000  0.50000  0.50000 # Cr
  0.46054  0.75000  0.61179 # O
  0.03945  0.25000  0.11179 # O
  0.96054  0.75000  0.88820 # O
  0.53945  0.25000  0.38820 # O
  0.30409  0.55780  0.19616 # O
  0.19590  0.44219  0.69616 # O
  0.80409  0.94219  0.30383 # O
  0.69590  0.05780  0.80383 # O
  0.69590  0.44219  0.80383 # O
  0.80409  0.55780  0.30383 # O
  0.19590  0.05780  0.69616 # O
  0.30409  0.94219  0.19616 # O
```

```
nspden  2 (Collinear)
nsppol  1 (AFM)
nspinor 1
spinat
12*0 # Y
0.0 0.0  5.0 # Cr1 (d^3)
0.0 0.0 -5.0 # Cr2 (d^3)
0.0 0.0 -5.0 # Cr3 (d^3)
0.0 0.0  5.0 # Cr4 (d^3)
36*0 # O
```

Collinear case $YCrO_3$ (output)

```
Integrated electronic and magnetization densities in atomic spheres:
---------------------------------------------------------------------
Note: Diff(up-dn) is a rough approximation of local magnetic moment
Atom    Radius    up_density   dn_density  Total(up+dn)  Diff(up-dn)
   1   2.21000     4.011174     4.011174      8.022348     -0.000000
   2   2.21000     4.011174     4.011174      8.022348     -0.000000
   3   2.21000     4.011174     4.011174      8.022348     -0.000000
   4   2.21000     4.011174     4.011174      8.022348     -0.000000
   5   2.10818     7.280490     4.827179     12.107670      2.453311
   6   2.10818     4.827179     7.280490     12.107670     -2.453311
   7   2.10818     4.827179     7.280490     12.107670     -2.453311
   8   2.10818     7.280490     4.827179     12.107670      2.453311
   9   1.41465     2.281923     2.281923      4.563846      0.000000
  10   1.41465     2.281923     2.281923      4.563846      0.000000
  11   1.41465     2.281923     2.281923      4.563846      0.000000
  12   1.41465     2.281923     2.281923      4.563846      0.000000
  13   1.41465     2.273977     2.274262      4.548239     -0.000285
  14   1.41465     2.274262     2.273977      4.548239      0.000285
  15   1.41465     2.273977     2.274262      4.548239     -0.000285
  16   1.41465     2.274262     2.273977      4.548239      0.000285
  17   1.41465     2.273977     2.274262      4.548239     -0.000285
  18   1.41465     2.274262     2.273977      4.548239      0.000285
  19   1.41465     2.273977     2.274262      4.548239     -0.000285
  20   1.41465     2.274262     2.273977      4.548239      0.000285
---------------------------------------------------------------------
 Sum:             67.580681    67.580681    135.161363     -0.000000
Total magnetization (from the atomic spheres):             -0.000000
Total magnetization (exact up - dn):                       -0.000000
```

Non-collinear case of $YCrO_3$ (input with spins along z)

```
natom  20
ntypat 3
znucl  39 24 8
typat  4*1 4*2 12*3

acell 5.518 7.54 5.247  Angstrom
xred
  0.07064  0.75000  0.48013 # Y
  0.42935  0.25000  0.98013 # Y
  0.57064  0.75000  0.01986 # Y
  0.92935  0.25000  0.51986 # Y
  0.00000  0.00000  0.00000 # Cr
  0.50000  0.00000  0.50000 # Cr
  0.00000  0.50000  0.00000 # Cr
  0.50000  0.50000  0.50000 # Cr
  0.46054  0.75000  0.61179 # O
  0.03945  0.25000  0.11179 # O
  0.96054  0.75000  0.88820 # O
  0.53945  0.25000  0.38820 # O
  0.30409  0.55780  0.19616 # O
  0.19590  0.44219  0.69616 # O
  0.80409  0.94219  0.30383 # O
  0.69590  0.05780  0.80383 # O
  0.69590  0.44219  0.80383 # O
  0.80409  0.55780  0.30383 # O
  0.19590  0.05780  0.69616 # O
  0.30409  0.94219  0.19616 # O
```

```
nspden  4 (Non-collinear)
nsppol  1
nspinor 2
so_psp 3*1 (SOC for norm-conserving)
spinat
12*0 # Y
0.0 0.0  5.0 # Cr1 (d^3)
0.0 0.0 -5.0 # Cr2 (d^3)
0.0 0.0 -5.0 # Cr3 (d^3)
0.0 0.0  5.0 # Cr4 (d^3)
36*0 # O
```

Non-collinear case $YCrO_3$ (output from spinat along z)

```
Atom   Radius      Total density     mag(x)      mag(y)      mag(z)
   1   2.00000        7.451331     -0.000000    0.000277   -0.000000
   2   2.00000        7.451331      0.000000    0.000277   -0.000000
   3   2.00000        7.451331     -0.000000    0.000277   -0.000000
   4   2.00000        7.451331     -0.000000    0.000277   -0.000000
   5   2.00000       11.787209     -0.072667    0.067117    2.434474
   6   2.00000       11.787209     -0.074021    0.066454   -2.434451
   7   2.00000       11.787209      0.072650    0.066488   -2.434491
   8   2.00000       11.787209      0.074038    0.067083    2.434433
   9   2.00000        6.291359      0.000000    0.001070   -0.000000
  10   2.00000        6.291361     -0.000000    0.001070   -0.000000
  11   2.00000        6.291357     -0.000000    0.001070   -0.000000
  12   2.00000        6.291359      0.000000    0.001070    0.000000
  13   2.00000        6.247049      0.001146    0.001165   -0.000078
  14   2.00000        6.247047      0.001146    0.001165    0.000077
  15   2.00000        6.247048     -0.001146    0.001165   -0.000077
  16   2.00000        6.247049     -0.001146    0.001165    0.000077
  17   2.00000        6.247047      0.001146    0.001165   -0.000078
  18   2.00000        6.247049      0.001146    0.001165    0.000077
  19   2.00000        6.247048     -0.001146    0.001165   -0.000077
  20   2.00000        6.247047     -0.001145    0.001165    0.000077
----------------------------------------------------------------------
Total magnetization (spheres)      -0.000001    0.281846   -0.000037
Total magnetization (exact)        -0.000001    0.309096   -0.000041
```

$YCrO_3$ spins along the z-axis (AFM G-type); wFM canting along the y axis; wAFM canting along x. Spin-Orbit coupling necessary to describe the canting and easy-axis

Non-collinear case YCrO$_3$ (from spinat along x/y)

starting with spinat along x direction:

```
Atom    Radius       Total density     mag(x)      mag(y)      mag(z)
   5    2.00000        11.787209     2.434622    0.061122    0.072067
   6    2.00000        11.787209    -2.434625   -0.061157    0.071949
   7    2.00000        11.787209    -2.434653    0.059917   -0.072040
   8    2.00000        11.787209     2.434656   -0.059960   -0.071924
 ---------------------------------------------------------------------
Total magnetization (spheres)       -0.000000   -0.000084    0.000057
Total magnetization (exact)         -0.000000   -0.000092    0.000062
```

starting with spinat along y direction:

```
Atom    Radius       Total density     mag(x)      mag(y)      mag(z)
   5    2.00000        11.787205    -0.065491    2.434621   -0.068435
   6    2.00000        11.787205     0.065466   -2.434589   -0.069587
   7    2.00000        11.787205    -0.065497   -2.434588   -0.069588
   8    2.00000        11.787205     0.065542    2.434620   -0.068437
 ---------------------------------------------------------------------
Total magnetization (spheres)        0.000022    0.000067   -0.291274
Total magnetization (exact)          0.000024    0.000073   -0.319436
```

Magnetocrystaline anisotropy (MCA) energy can be calculated:

spin direction	Energy (μeV)
001	0
010	99
100	199

Convergence tips

In case of convergence troubles for magnetic systems:

- *diemixmag* flag can be reduced more than *diemix* (could be down to 0.1 for non-collinear cases).
- Increase *nline*
- Use of *nnsclo*< 0 (useful for non-collinear cases with “noisy” magnetization)
- Use *nnsclo*> 1 (in case *nnsclo*< 0 appears not sufficient)
- (In some systems, it could be necessary to start with a starting moment amplitude (*spinat*) larger than the physical one)

Constrained magnetic moment calculations

Constrain the direction of the magnetic moments (*magconon* flag =1) :

Lagrange multiplier:
$$E = E_{KS} + \sum_i \lambda \left[\mathbf{m}_i - \mathbf{m}_i^0(\mathbf{m}_i^0 \cdot \mathbf{m}_i)\right]^2$$

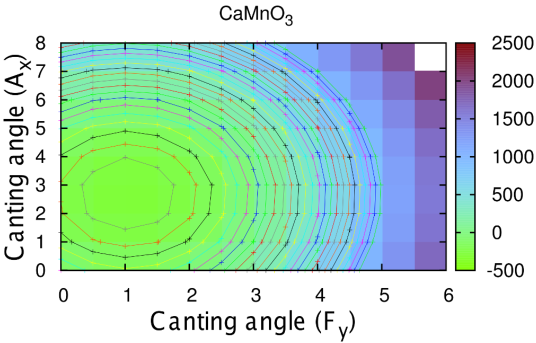
Constrain the direction and the amplitude of the magnetic moments (*magconon* flag =2) :

$$E = E_{KS} + \sum_i \lambda \left[\mathbf{m}_i - \mathbf{m}_i^0\right]^2$$

with λ the strength of the Lagrange multiplier (*magcon_lambda* flag) and m_i^0 the desired magnetic moment on each atom i (given by *spinat*).

Constrained magnetic moment calculations

Useful to explore the spin energy landscape (direction constraint):



And also to compute the magnetocrystaline anisotropy energy.

(For multiple local minima of complex better to use meta-heuristic approach, see J. Chem. Theory Comput. 14, 4455 (2018))

Can be useful to control high/low spin configurations (amplitude constraint).

Applied magnetic field

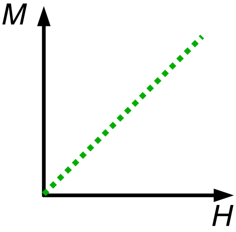
Applying a (Zeeman) magnetic field on the spins gives (*zeemanfield* flag):

$$V_H = -\mu_B\mu_0 \begin{pmatrix} H_z & H_x + iH_y \\ H_x - iH_y & -H_z \end{pmatrix}$$

Allows to access to:

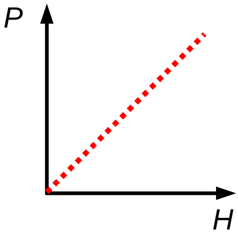
Linear magnetic susceptibility tensor

$\mathbf{M} = \chi\mathbf{H}$



Linear magnetoelectric tensor

$\mathbf{P} = \alpha\mathbf{H}$



As well as non-linear responses!

Conclusions

DFT + spins:

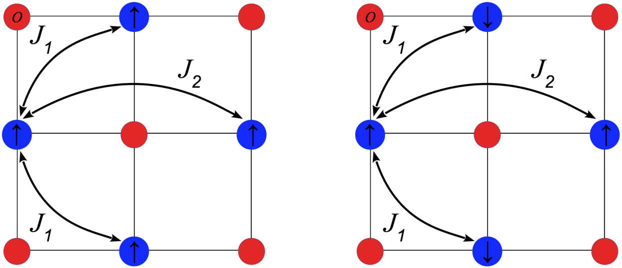
- Collinear magnetism: easy to handle
- Non-Collinear magnetism: often less easy
- DFT+U or Hybrid functionals are often necessary for magnetic systems
- Allows to compute:
  - (Super) Exchange interaction between spins (J).
  - Spin canting / Dzyaloshinsky-Moriya interaction (D)
  - Magnetic anisotropy
  - Response under Zeeman field (magnetic and magnetoelectric susceptibilities)

Other features:

- Orbital magnetism
- DFPT with magnetic field
- Spin dynamics with MULTIBINIT
- . . .

Magnetism in DFT: Collinear case

Superexchange constants J can be estimated. Ex: Rock-Salt oxides



One needs to compute the energy for ferro and antiferro in order to extract J_1 and J_2 from:

$$E = E_0 + S \sum_i J_i S_i$$

Ex. for NiO: $J_1 \simeq 17$ meV and $J_2 \simeq -0.4$ meV (exp: $J_1 \simeq 19$ meV)

PRB 84, p.224429 (2011), PRB 86, 094413 (2012)

Magnetism in DFT: Collinear case

Superexchange constants *J* can also be estimated through Wannier↦Green's functions (PRB 91, 224405 (2015), see TB2J script and related tuto):

$$J_{ij}^{kk'} = -\frac{1}{2\pi}\int_{-\infty}^{E_F} \sum_{kk'} Im(\widetilde{\Delta}_i^{kk} \widetilde{G}_{ij,\downarrow}^{kk'} \widetilde{\Delta}_j^{k'k'} \widetilde{G}_{ji,\uparrow}^{k'k})$$

Ex, $SrMnO_3$:

```
============================================================
Exchange:
i=     0(Mn1  ) , j=     0(Mn1  ), R= ( -1,   0,   0), J=-6.9178 meV, vec=(-3.810,  0.000,  0.000)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  0,  -1,   0), J=-6.9178 meV, vec=( 0.000, -3.810,  0.000)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  0,   1,   0), J=-6.9178 meV, vec=( 0.000,  3.810,  0.000)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  1,   0,   0), J=-6.9178 meV, vec=( 3.810,  0.000,  0.000)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  0,   0,   1), J=-6.8353 meV, vec=( 0.000,  0.000,  3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  0,   0,  -1), J=-6.8353 meV, vec=( 0.000,  0.000, -3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= ( -1,   0,   1), J=-0.5538 meV, vec=(-3.810,  0.000,  3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  1,   0,  -1), J=-0.5538 meV, vec=( 3.810,  0.000, -3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  1,   0,   1), J=-0.5538 meV, vec=( 3.810,  0.000,  3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  0,   1,   1), J=-0.5538 meV, vec=( 0.000,  3.810,  3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  0,  -1,  -1), J=-0.5538 meV, vec=( 0.000, -3.810, -3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  0,  -1,   1), J=-0.5538 meV, vec=( 0.000, -3.810,  3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= ( -1,   0,  -1), J=-0.5538 meV, vec=(-3.810,  0.000, -3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  0,   1,  -1), J=-0.5538 meV, vec=( 0.000,  3.810, -3.810)
i=     0(Mn1  ) , j=     0(Mn1  ), R= ( -1,  -1,   0), J=-0.5314 meV, vec=(-3.810, -3.810,  0.000)
i=     0(Mn1  ) , j=     0(Mn1  ), R= (  1,  -1,   0), J=-0.5314 meV, vec=( 3.810, -3.810,  0.000)
```

Magnetism in DFT: Collinear case

Spin dispersion (magnon) of $SrMnO_3$ in its FM phase: