Spin-orbit coupling in Wien2k

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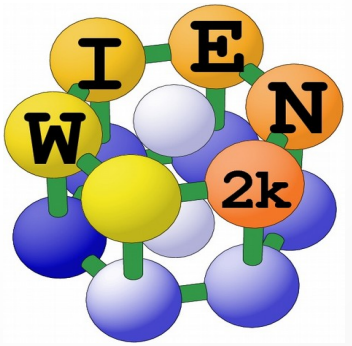


Dirac Hamiltonian

Quantum mechanical description of electrons, consistent with the theory of special relativity.

$$H_D = c\,\vec{\alpha}\cdot\vec{p} + \beta\, m c^2 + V$$

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \qquad \beta_k = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{-1} \end{pmatrix}$$

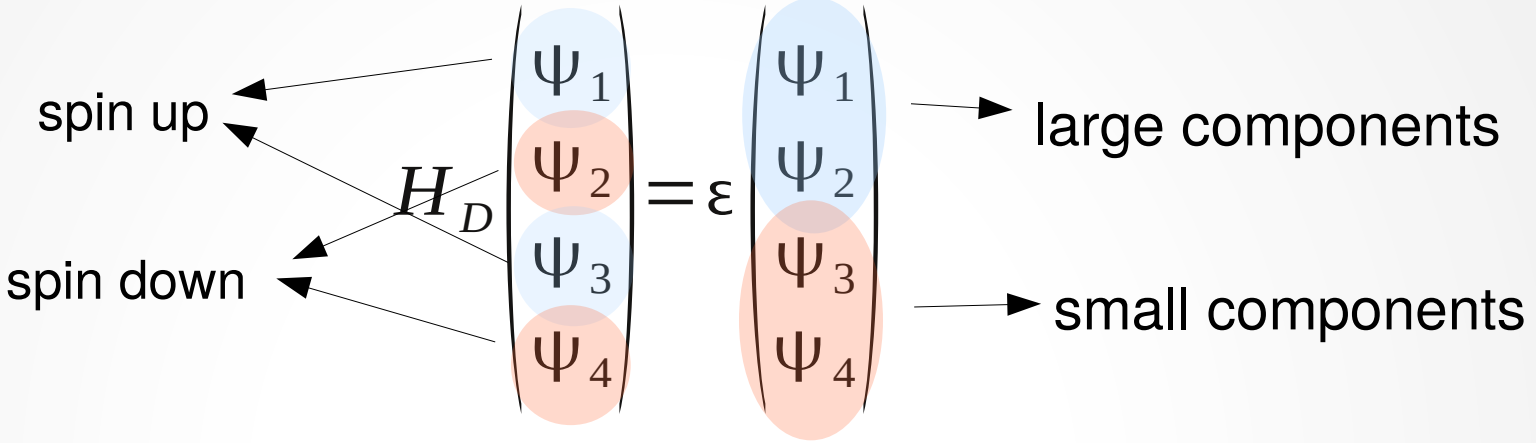
Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

H_D and the wave function are 4-dimensional objects

Dirac Hamiltonian



free particle:

$$\begin{pmatrix} \varepsilon - mc^2 & 0 & -\hat{p}_z & -(\hat{p}_x - i\hat{p}_y) \\ 0 & \varepsilon - mc^2 & -(\hat{p}_x + i\hat{p}_y) & \hat{p}_z \\ -\hat{p}_z & -(\hat{p}_x - i\hat{p}_y) & \varepsilon + mc^2 & 0 \\ -(\hat{p}_x + i\hat{p}_y) & \hat{p}_z & 0 & \varepsilon + mc^2 \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{pmatrix} = 0$$

slow particle limit (p=0):

$mc^2, \begin{pmatrix} \Psi \\ 0 \\ 0 \\ 0 \end{pmatrix}$ $mc^2, \begin{pmatrix} 0 \\ \Psi \\ 0 \\ 0 \end{pmatrix}$

spin up spin down

$-mc^2, \begin{pmatrix} 0 \\ 0 \\ \Psi \\ 0 \end{pmatrix}$ $-mc^2, \begin{pmatrix} 0 \\ 0 \\ 0 \\ \Psi \end{pmatrix}$

antiparticles, up, down

Dirac equation in spherical potential

Solution for spherical potential

$$\Psi = \begin{pmatrix} g_\kappa(r)\chi_{\kappa\sigma} \\ -i\, f_\kappa(r)\chi_{\kappa\sigma} \end{pmatrix}$$

→ combination of spherical harmonics and spinors

$$\kappa = -s\left(j + 1/2\right)$$
$$j = l + s/2$$
$$s = +1, -1$$

$$\frac{dg_\kappa}{dr} = -\frac{(\kappa+1)}{r} g_\kappa + 2\,Mc f_\kappa$$
$$\frac{df_\kappa}{dr} = \frac{1}{c}(V - E)\, g_\kappa + \frac{\kappa - 1}{r} f_\kappa$$

Radial Dirac equation

Dirac equation in spherical potential

Radial Dirac equation

$$\frac{dg_\kappa}{dr} = -\frac{(\kappa+1)}{r} g_\kappa + 2Mcf_\kappa$$
$$\frac{df_\kappa}{dr} = \frac{1}{c}(V-E) g_\kappa + \frac{\kappa-1}{r} f_\kappa$$

κ dependent term, for a constant l, κ depends on the sign of s

substitute f from first eq. into the second eq.

$$-\frac{1}{2M}\left[\frac{d^2 g_\kappa}{dr^2} + \frac{2}{r}\frac{dg_\kappa}{dr} - \frac{l(l+1)}{r^2} g_\kappa\right] - \frac{dV}{dr}\frac{dg_\kappa}{dr}\frac{1}{4M^2c^2} + Vg_\kappa - \frac{\kappa-1}{r}\frac{dV}{dr}\frac{g_\kappa}{4M^2c^2} = Eg_\kappa$$

scalar relativistic approximation

spin-orbit coupling

Implementation: core electrons

Core states are calculated with spin-compensated Dirac equation

For spin polarized potential – spin up and spin down radial functions are calculated separately, the density is averaged according to the occupation number specified in *case.inc* file

$1s^{1/2}$

$2p^{1/2}$

$2p^{3/2}$

```
   9 0.00
1,-1,2          ( N,KAPPA,OCCUP)
2,-1,2          ( N,KAPPA,OCCUP)
2, 1,2          ( N,KAPPA,OCCUP)
2,-2,4          ( N,KAPPA,OCCUP)
3,-1,2          ( N,KAPPA,OCCUP)
3, 1,2          ( N,KAPPA,OCCUP)
3,-2,4          ( N,KAPPA,OCCUP)
3, 2,4          ( N,KAPPA,OCCUP)
3,-3,6          ( N,KAPPA,OCCUP)
```

Core levels configuration (*case.inc* for Ru atom)

Relations between quantum numbers

		j=l+s/2		κ=-s(j+½)		occupation	
	l	s=-1	s=+1	s=-1	s=+1	s=-1	s=+1
s	0		1/2		-1		2
p	1	1/2	3/2	1	-2	2	4
d	2	3/2	5/2	2	-3	4	6
f	3	5/2	7/2	3	-4	6	8

Implementation: valence electrons

Valence electrons inside atomic spheres are treated within scalar relativistic approximation (*Koelling and Harmon, J. Phys C 1977*) if *RELA* is specified in *struct* file

$$\frac{dP}{dr} - \frac{1}{r} P = 2\,McQ$$

$$\frac{dQ}{dr} - \frac{1}{r} Q = \left[l\frac{(l+1)}{2} Mcr^2 + \frac{(V-\epsilon)}{c} \right] P$$

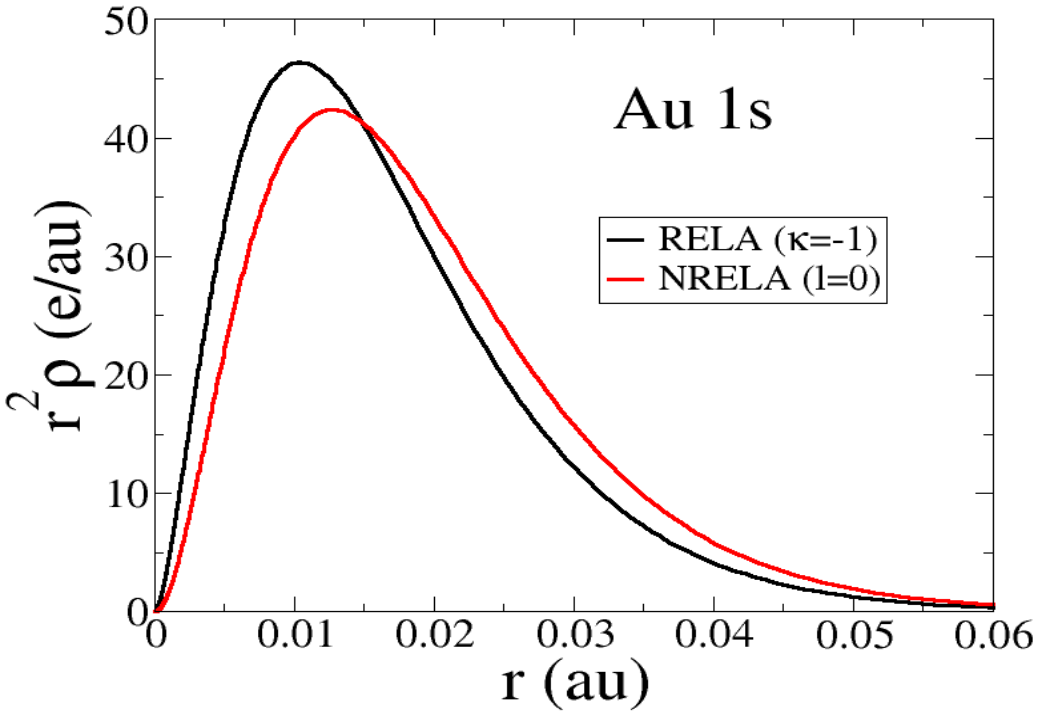
radial equations of Koelling and Harmon (spherical potential)

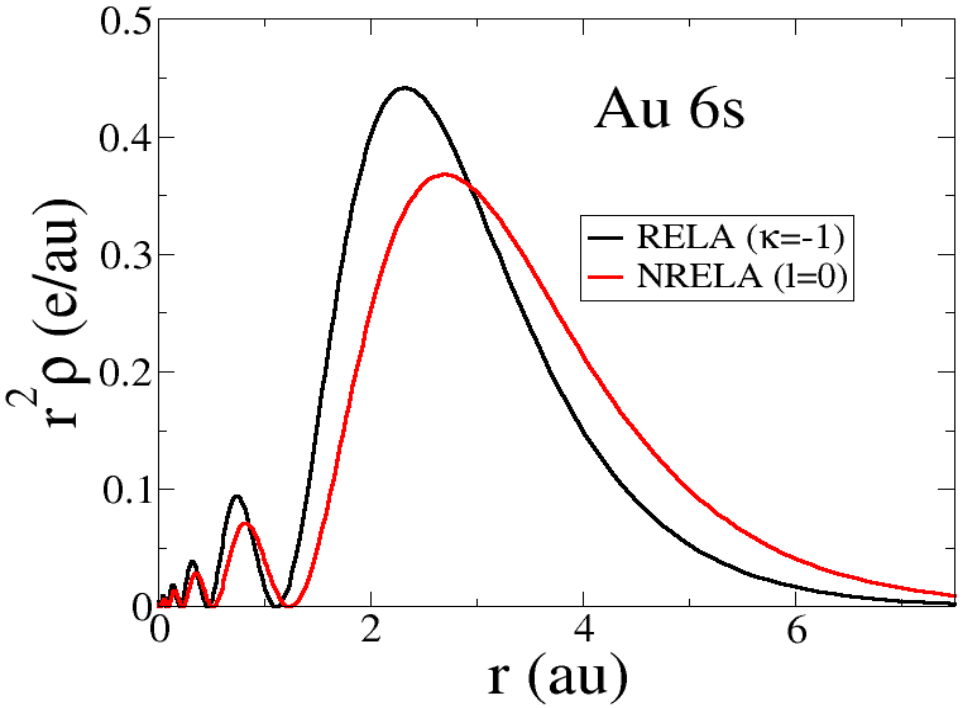
- no κ dependency of the wave function, (l,m,s) are good quantum numbers
- all relativistic effects are included except SOC
- small component enters normalization and calculation of charge inside spheres
- augmentation with large component only
- SOC can be included in “second variation”

Valence electrons in interstitial region are non-relativistic

Effects of *RELA*

- contraction of Au s orbitals





- 1s contracts due to relativistic mass enhancement
- 2s - 6s contract due to orthogonality to 1s

$$M V^2/r = Z e/r^2$$

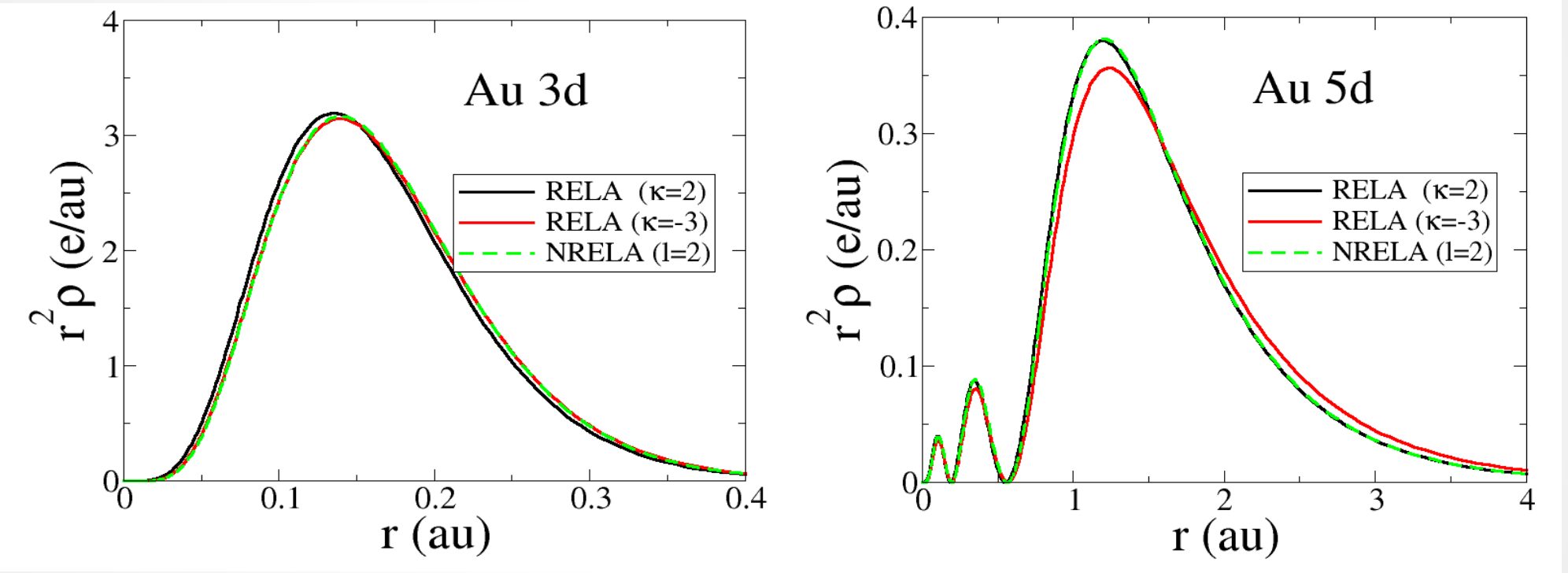
centripetal force

$$M = m/\sqrt{1-(v/c)^2}$$

v ~ Z: Au Z = 79;M = 1.2 m

Effects of *RELA*

orbital expansion of Au d orbitals



Higher l-quantum number states expand due to better shielding of the core charge from contracted s-states (effect is larger for higher states).

Spin orbit-coupling

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \zeta(\vec{\sigma}\cdot\vec{l})\ldots \qquad \zeta = \frac{1}{2Mc^2}\frac{1}{r^2}\frac{dV_{MT}(r)}{dr}$$

- 2x2 matrix in spin space, due to Pauli spin operators, wave function is a 2-component vector (spinor)

spin up

$$H_P\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \varepsilon\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}$$

spin down

Pauli matrices:

$$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$\sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

$$\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

Spin structure of the Hamiltonian with SOC

$$\left(\begin{pmatrix}-\frac{\hbar}{2m}\nabla^2 + V_{ef} & 0\\ 0 & -\frac{\hbar}{2m}\nabla^2 + V_{ef}\end{pmatrix} + \begin{pmatrix}\zeta l_z + \ldots & \zeta(l_x - il_y)\\ \zeta(l_x + il_y) & -\zeta l_z + \ldots\end{pmatrix}\right)\psi = \varepsilon\psi$$

Spin orbit-coupling

- SOC is active only inside atomic spheres, only spherical potential (V_{MT}) is taken into account, in the polarized case spin up and down parts are averaged
- eigenstates are not pure spin states
- off-diagonal term of the spin density matrix do not enter SCF cycle
- SOC is added in a second variation (*lapwso*):

first diagonalization (lapw1)

$$H_1 \psi_1 = \varepsilon_1 \psi_1$$

second diagonalization (lapwso)

$$\left(H_1 + H_{SO}\right)\psi = \varepsilon\,\psi$$

second diagonalization

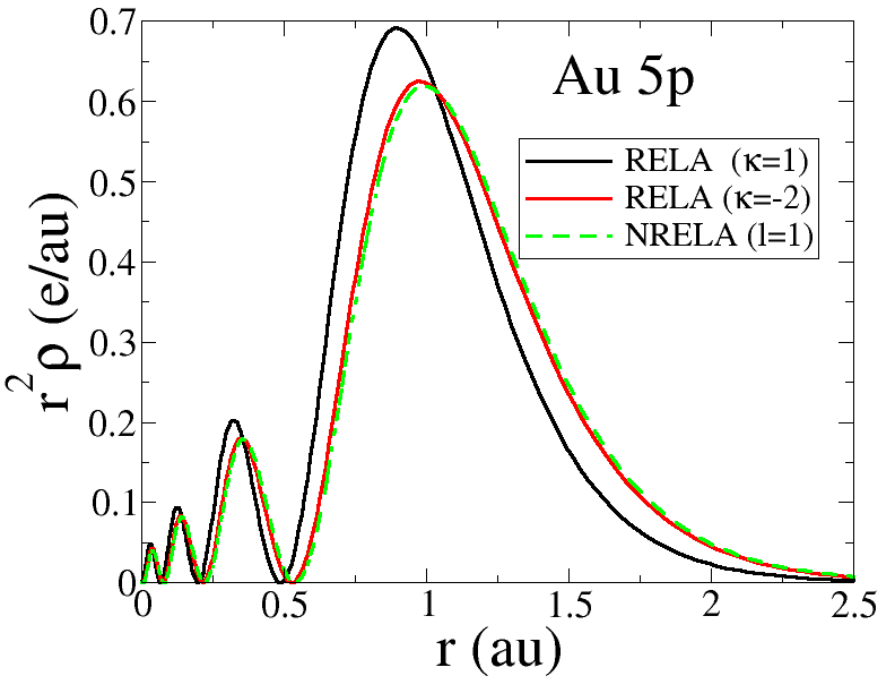
$$\sum_i^N \left(\delta_{ij}\varepsilon_1^j + \left\langle \psi_1^j \middle| H_{SO} \middle| \psi_1^i \right\rangle\right)\left\langle \psi_1^i \middle| \psi \right\rangle = \varepsilon \left\langle \psi_1^j \middle| \psi \right\rangle$$

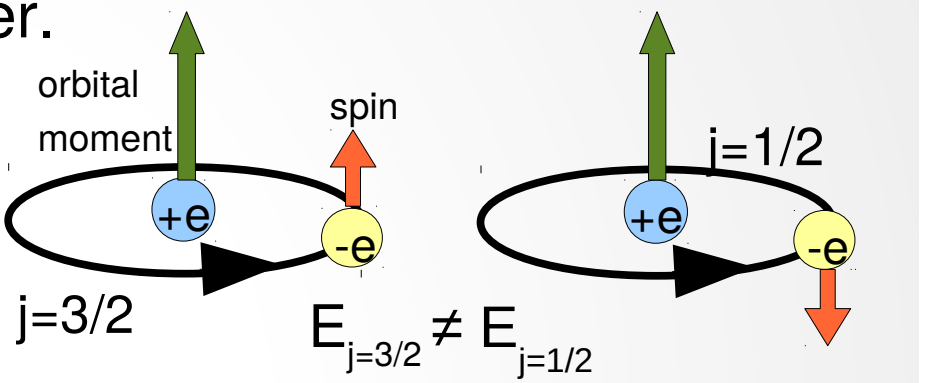
sum includes both up/down spin states

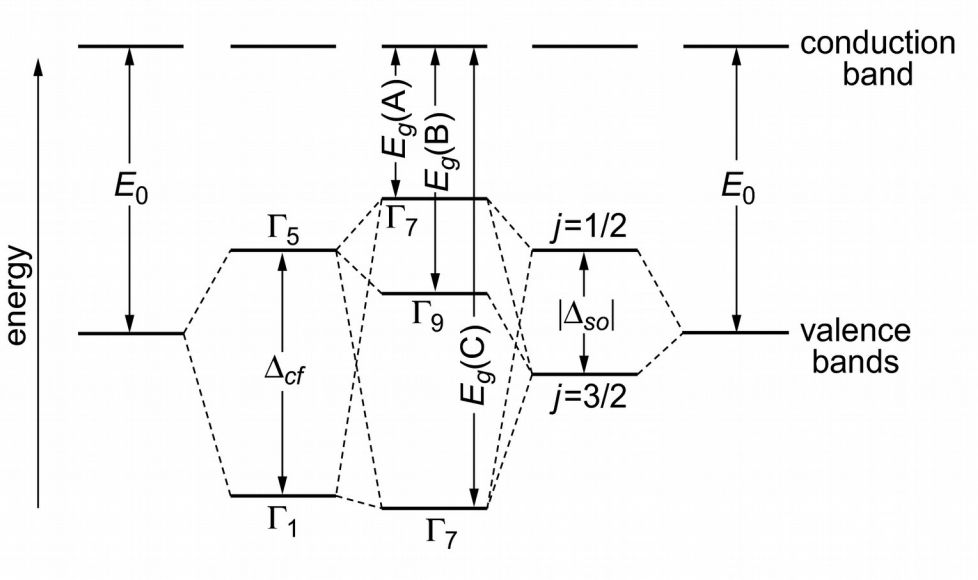
N is much smaller then the basis size in lapw1!!

SOC splitting of p states

Spin Orbit splitting of l-quantum number.







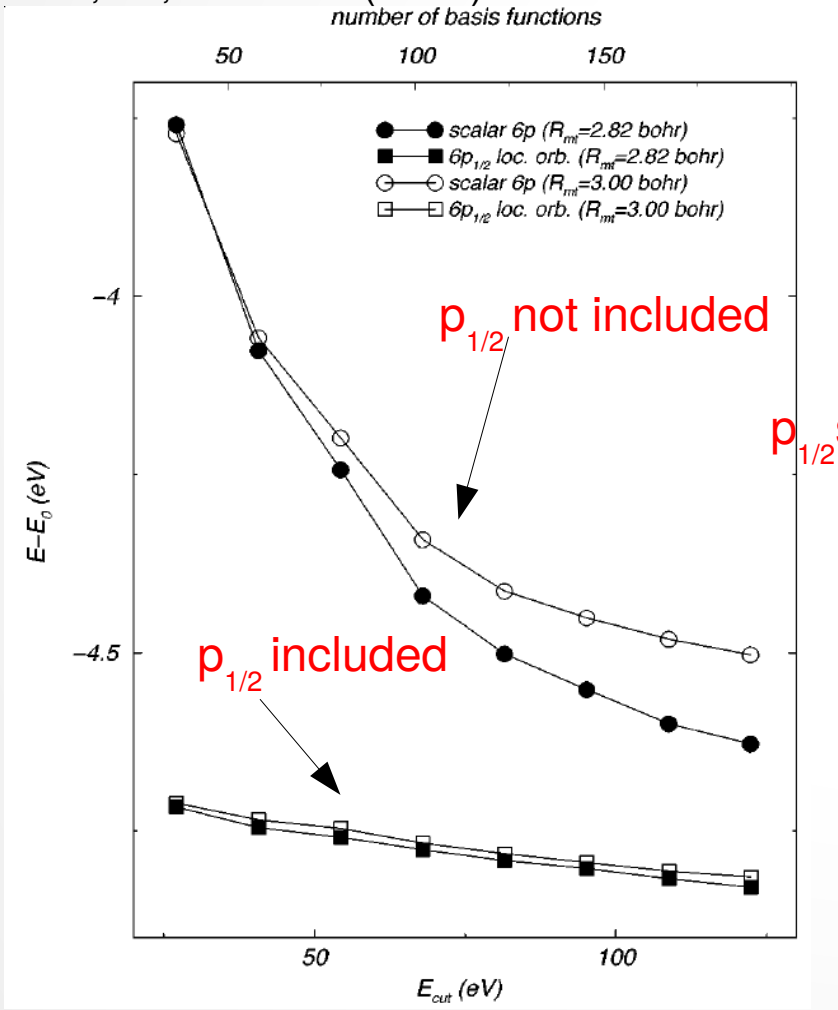
band edge at Γ in ZnO

$p_{1/2}$ (κ=1) different behavior than non-relativistic p-state (density is diverging at nucleus), thus there is a need for extra basis function ($p_{1/2}$ orbital)

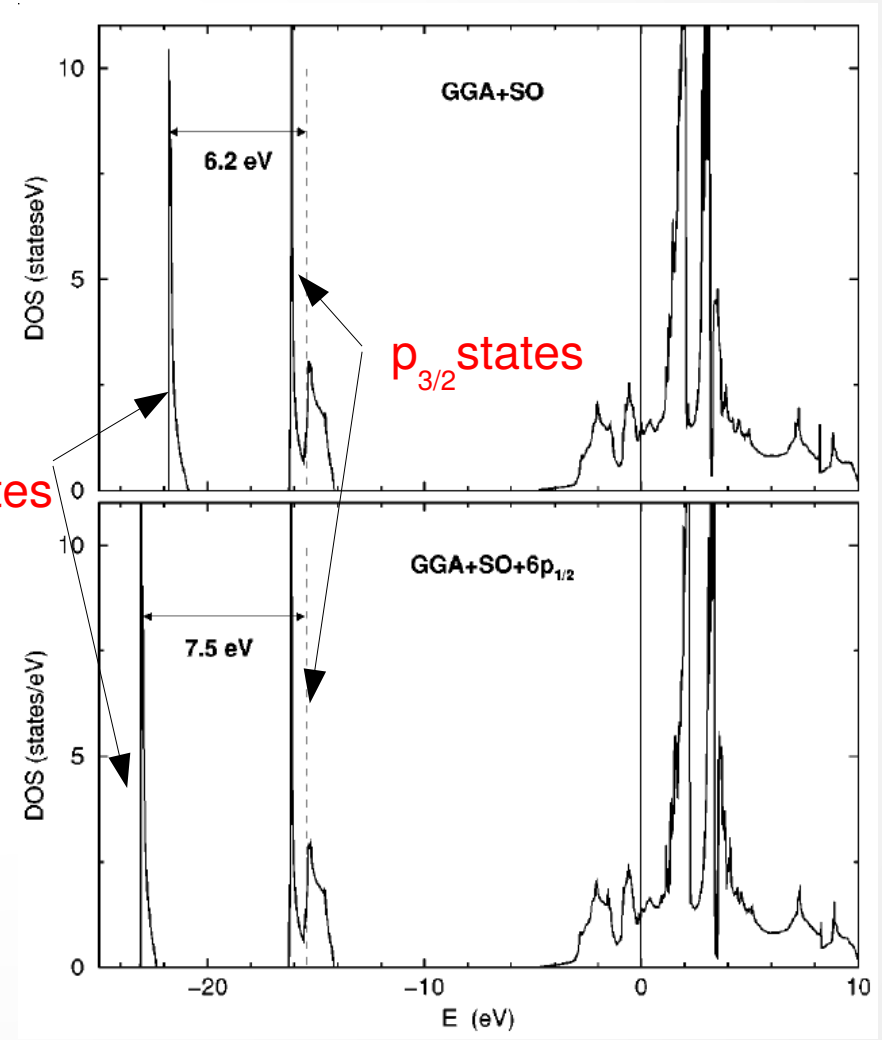
$p_{1/2}$ orbitals

Electronic structure of fcc Th, SOC with $6p_{1/2}$ local orbital

PRB, 64, 1503102 (2001)

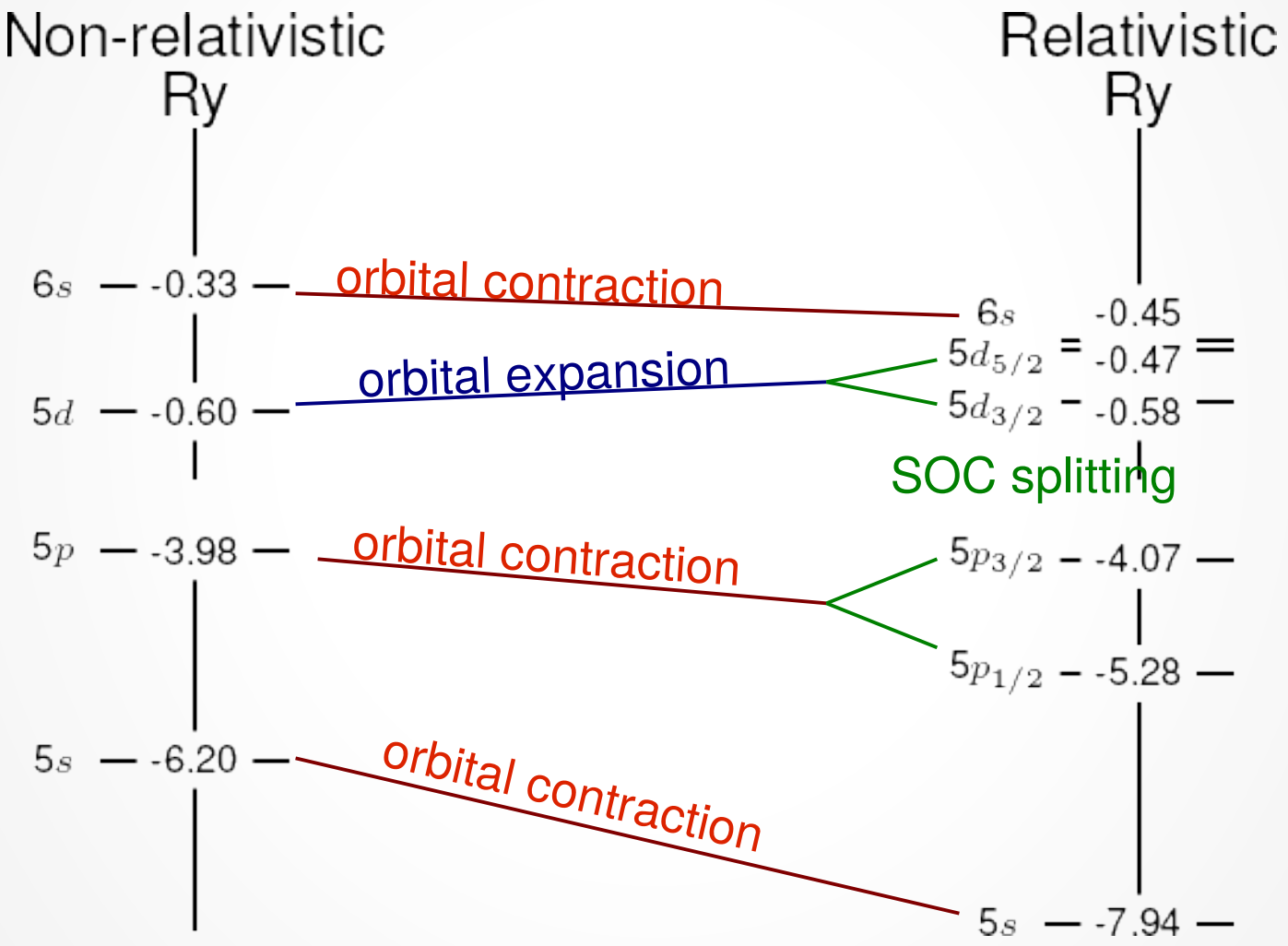


energy vs. basis size



DOS with and without $p_{1/2}$

Au atomic spectra

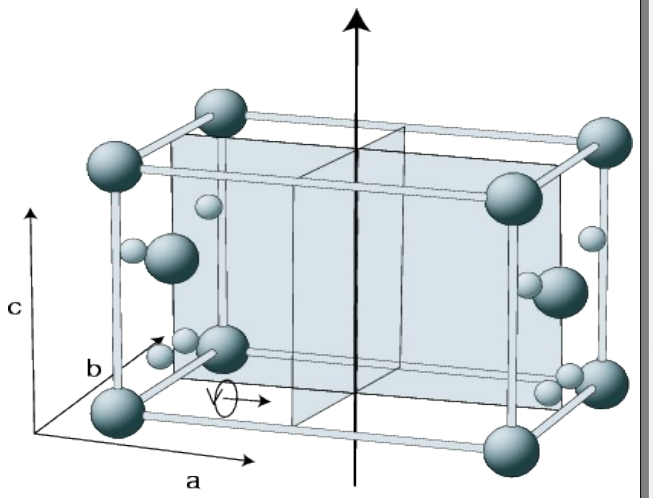


SOC in magnetic systems

- **SOC couples magnetic moment to the lattice**
  - direction of the exchange field matters (input in case.inso)
- **symmetry operations acts in real and spin space**
  - number of symmetry operations may be reduced
  - no *time* inversion
  - ***initso_lapw*** (must be executed) detects new symmetry setting

direction of magnetization

sym. operation	[100]	[010]	[001]	[110]
1	A	A	A	A
m_a	A	B	B	-
m_b	B	A	B	-
2_c	B	B	A	B



SOC in Wien2k

- run(sp)_lapw -so script:

x lapw1 (increase E-max for more eigenvectors in second diag.)

x lapwso (second diagonalization)

x lapw2 -so (SOC ALWAYS needs complex lapw2 version)

`case.inso` file:

```
WFFIL
4  1  0
-10.0000   1.50000
 0.  0.  1.
 1
 2   -0.97      0.005
 0 0 0 0 0
```

llmax,ipr,kpot

emin,emax (output energy window)

direction of magnetization (lattice vectors)

number of atoms for which RLO is added

atom number,e-lo,de (case.in1), repeat NX times

number of atoms for which SO is switched off; list of atoms

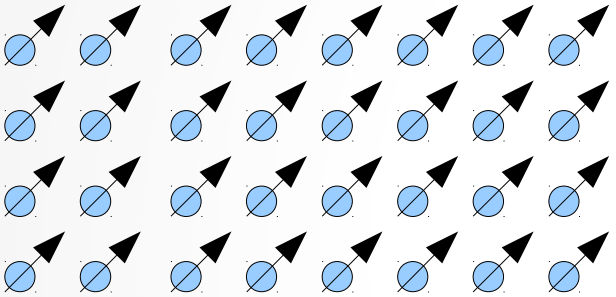
$p_{1/2}$ orbitals, use with caution !!

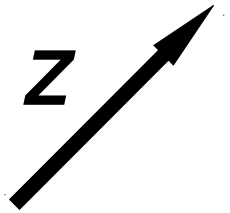
Summary: relativistic effects

- core electrons - Dirac equation using spherical part of the total potential (dirty trick for spin polarized systems)
- valence electrons - scalar relativistic approximation is used as default (RELA switch in *case.struct*),
- SOC for valence electrons - ***lapwso*** has to be included in SCF cycle (***run -so/run_sp -so***), atomic spheres only
- limitations: not all programs are compatible with SOC, for instance: no forces with SOC (yet)

magnetism, non-collinear case

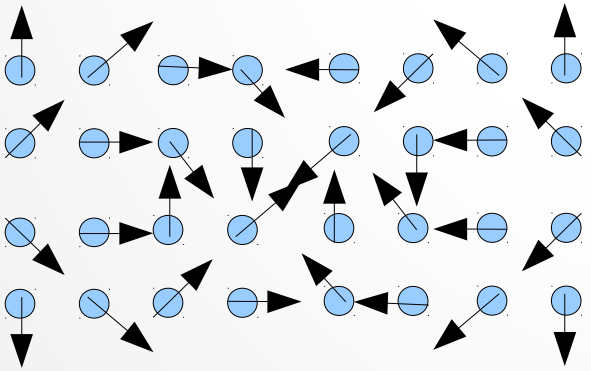
- WIEN2k can do only nonmagnetic or collinear magnetic structures

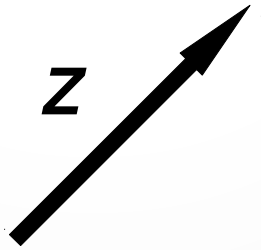




$$\psi_{\uparrow}=\begin{pmatrix}\psi_1\\0\end{pmatrix},\ \psi_{\downarrow}=\begin{pmatrix}0\\\psi_2\end{pmatrix}$$

- noncollinear magnetic structures, use WIENNCM



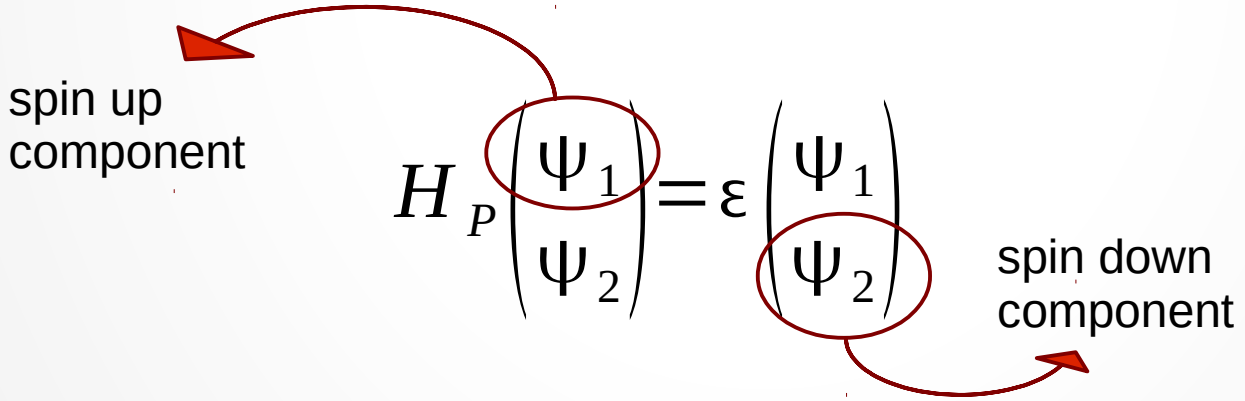


$$\psi=\begin{pmatrix}\psi_1\\\psi_2\end{pmatrix},\quad \psi_1,\psi_2\neq 0$$

Pauli Hamiltonian

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \zeta(\vec{\sigma}\cdot\vec{l})\ \ldots$$

- 2x2 matrix in spin space, due to Pauli spin operators
- wave function is a 2-component vector (spinor)



Pauli matrices:

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$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Pauli Hamiltonian

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \zeta(\vec{\sigma}\cdot\vec{l})\ldots$$

electrostatic potential

magnetic field

spin-orbit coup.

$$V_{ef} = V_{ext} + V_H + V_{xc}$$

Hartee term

exchange-correlation potential

$$B_{ef} = B_{ext} + B_{xc}$$

exchange-correlation field

- exchange-correlation potential V_{xc} and magnetic field B_{xc} are defined within DFT LDA or GGA

Exchange and correlation

- from DFT LDA exchange-correlation energy:

$$E_{xc}(n,\vec{m}) = \int n\,\epsilon_{xc}(n,\vec{m})\,dr^3$$

local function of n and m

- definition of V_{cx} and B_{xc}:

$$V_{xc} = \frac{\partial E_{xc}(n,\vec{m})}{\partial n} \qquad \vec{B}_{xc} = \frac{\partial E_{xc}(n,\vec{m})}{\partial \vec{m}}$$

functional derivatives

- LDA expression for V_{cx} and B_{xc}:

$$V_{xc} = \epsilon_{xc}(n,\vec{m}) + n\frac{\partial \epsilon_{xc}(n,\vec{m})}{\partial n}$$

B_{xc} and m are parallel

$$\vec{B}_{xc} = n\frac{\partial \epsilon_{xc}(n,\vec{m})}{\partial m}\hat{m}$$

Non-collinear case

$$H_P = -\frac{\hbar}{2\mathrm{m}}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \zeta(\vec{\sigma}\cdot\vec{l})\ \ldots$$

- direction of magnetization vary in space

- spin-orbit coupling is present

$$\begin{pmatrix} -\frac{\hbar}{2\mathrm{m}}\nabla^2 + V_{ef} + \mu_B B_z + \ldots & \mu_B\left(B_x - iB_y\right) \\ \mu_B\left(B_x + iB_y\right) & -\frac{\hbar}{2\mathrm{m}}\nabla^2 + V_{ef} + \mu_B B_z + \ldots \end{pmatrix} \psi = \varepsilon\psi$$

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad \psi_1, \psi_2 \neq 0$$

- solutions are not pure spinors
- non-collinear magnetic moments

Collinear case

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \cancel{\zeta(\vec{\sigma}\cdot\vec{l})} \ldots$$

- magnetization in Z direction, B_x and B_y=0
- spin-orbit coupling is not present

$$\begin{pmatrix} -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B B_z + \ldots & 0 \\ 0 & -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B B_z + \ldots \end{pmatrix} \psi = \varepsilon\,\psi$$

$$\psi_\uparrow = \begin{pmatrix} \psi_1 \\ 0 \end{pmatrix},\ \psi_\downarrow = \begin{pmatrix} 0 \\ \psi_2 \end{pmatrix},\quad \varepsilon_\uparrow \neq \varepsilon_\downarrow$$

- solutions are pure spinors
- collinear magnetic moments

Non-magnetic case

$$H_P = -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \mu_B \vec{\sigma}\cdot\vec{B}_{ef} + \zeta(\vec{\sigma}\cdot\vec{l})\ldots$$

- no magnetization present, B_x, B_y and B_z=0
- spin-orbit coupling is not present

$$\begin{pmatrix} -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \ldots & 0 \\ 0 & -\frac{\hbar}{2m}\nabla^2 + V_{ef} + \ldots \end{pmatrix} \psi = \varepsilon\,\psi$$

$$\psi_\uparrow = \begin{pmatrix} \psi \\ 0 \end{pmatrix},\ \psi_\downarrow = \begin{pmatrix} 0 \\ \psi \end{pmatrix},\quad \varepsilon_\uparrow = \varepsilon_\downarrow$$

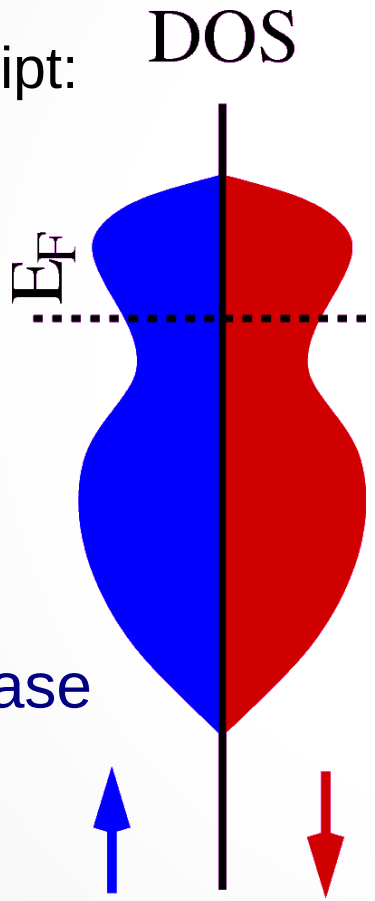
- solutions are pure spinors
- degenerate spin solutions

Magnetism and Wien2k

- Wien2k can only handle collinear or non-magnetic cases

run_lapw script:

```
x lapw0
x lapw1
x lapw2
x lcore
x mixer
```

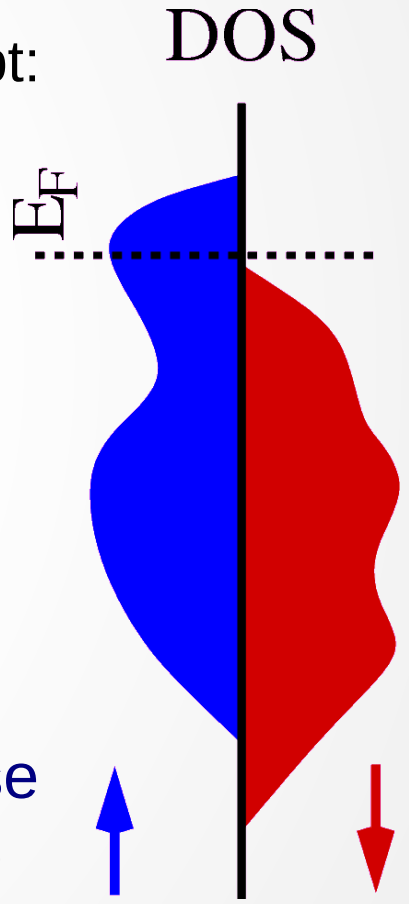


non-magnetic case

$m = n_\uparrow - n_\downarrow = 0$

runsp_lapw script:

```
x lapw0
x lapw1 -up
x lapw1 -dn
x lapw2 -up
x lapw2 -dn
x lcore -up
x lcore -dn
x mixer
```



magnetic case

$m = n_\uparrow - n_\downarrow \neq 0$

Magnetism and Wien2k

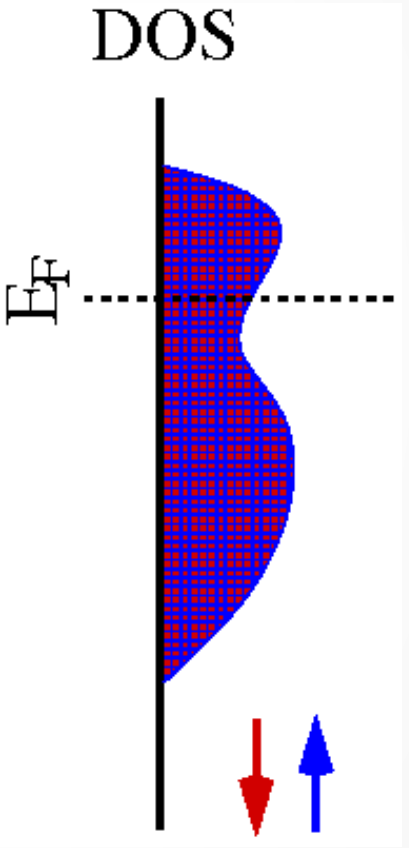
- in NCM case both part of the spinor are treated simultaneously

$$\hat{n} = \sum_{nk} \begin{pmatrix} \Psi_{\uparrow nk} \\ \Psi_{\downarrow nk} \end{pmatrix}^{*} \begin{pmatrix} \Psi_{\uparrow nk} \Psi_{\downarrow nk} \end{pmatrix}$$

$$m_z = n_{\uparrow\uparrow} - n_{\downarrow\downarrow} \neq 0$$

$$m_x = \frac{1}{2}\left(n_{\uparrow\downarrow} + n_{\downarrow\uparrow}\right) \neq 0$$

$$m_x = i\frac{1}{2}\left(n_{\uparrow\downarrow} - n_{\downarrow\uparrow}\right) \neq 0$$



Non-collinear calculations

- **in the case of non-collinear arrangement of spin moment WienNCM (Wien2k clone) has to be used**
  - code is based on Wien2k (available for Wien2k users)
  - structure and usage philosophy similar to Wien2k
  - independent source tree, independent installation
- **WienNCM properties:**
  - real and spin symmetry (simplifies SCF, less k-points)
  - constrained or unconstrained calculations (optimizes magnetic moments)
  - SOC is applied in the first variational step, LDA+U

WienNCM - implementation

- **basis set – mixed spinors** (Yamagami, PRB (2000); Kurtz PRB (2001)

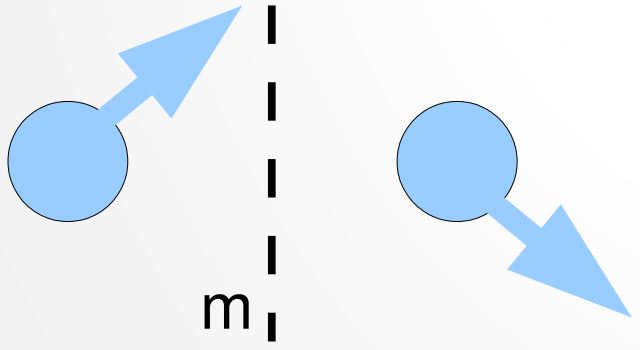
interstities: $\varphi_{\vec{G}\sigma} = e^{i\left(\vec{G}+\vec{k}\right)\cdot\vec{r}}\chi_\sigma \qquad \chi_\sigma = \begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$

spheres:

$$\varphi^{APW}_{\vec{G}\sigma} = \sum_{\sigma_\alpha}\sum_{lm}\left(A^{\vec{G}\sigma\sigma_\alpha}_{lm}u_l^{\sigma_\alpha} + B^{\vec{G}\sigma\sigma_\alpha}_{lm}\dot{u}_l^{\sigma_\alpha}\right)Y_{lm}\chi_{\sigma_\alpha}$$

$$\varphi^{APW}_{\vec{G}\sigma_\alpha} = \left(A^{\vec{G}\sigma\sigma_\alpha}_{lm}u_l^{\sigma_\alpha} + B^{\vec{G}\sigma\sigma_\alpha}_{lm}\dot{u}_l^{\sigma_\alpha} + C^{\vec{G}\sigma\sigma_\alpha}_{lm}u_{2,l}^{\sigma_\alpha}\right)Y_{lm}\chi_{\sigma_\alpha}$$

- **real and spin space parts of symmetry op. are not independent**



- symmetry treatment like for SOC always on
- tool for setting up magnetic configuration
- concept of magnetic and non-magnetic atoms

WienNCM implementation

- Hamiltonian inside spheres:

$$\hat{H} = -\frac{\hbar}{2\mathrm{m}}\nabla^2 + \hat{V} + \hat{H}_{so} + \hat{H}_{orb} + \hat{H}_c$$

AMA and full NC calculation

$$\hat{V}_{FULL} = \begin{pmatrix} V_{\uparrow\uparrow} & V_{\downarrow\uparrow} \\ V_{\uparrow\downarrow} & V_{\downarrow\downarrow} \end{pmatrix} \qquad \hat{V}_{AMA} = \begin{pmatrix} V_{\uparrow\uparrow} & 0 \\ 0 & V_{\downarrow\downarrow} \end{pmatrix}$$

SOC in first diagonalization

$$\hat{H}_{so} = \xi\,\vec{\sigma}\cdot\vec{l} = \xi \begin{pmatrix} \hat{l}_z & \hat{l}_x - i\,\hat{l}_y \\ \hat{l}_x + i\,\hat{l}_y & -\hat{l}_z \end{pmatrix}$$

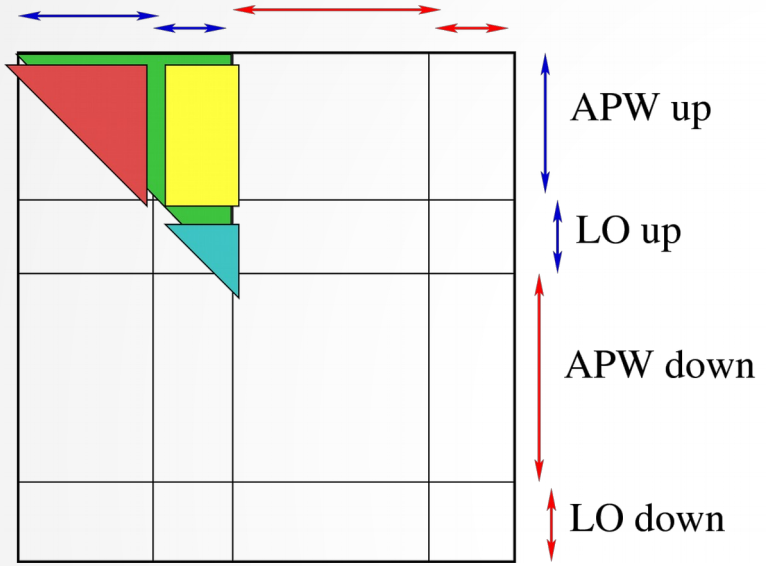
diagonal orbital field

$$\hat{H}_{orb} = \sum_{m\,m'} \begin{pmatrix} |m\rangle V^{\uparrow}_{mm'} \langle m'| & 0 \\ 0 & |m\rangle V^{\downarrow}_{mm'} \langle m'| \end{pmatrix}$$

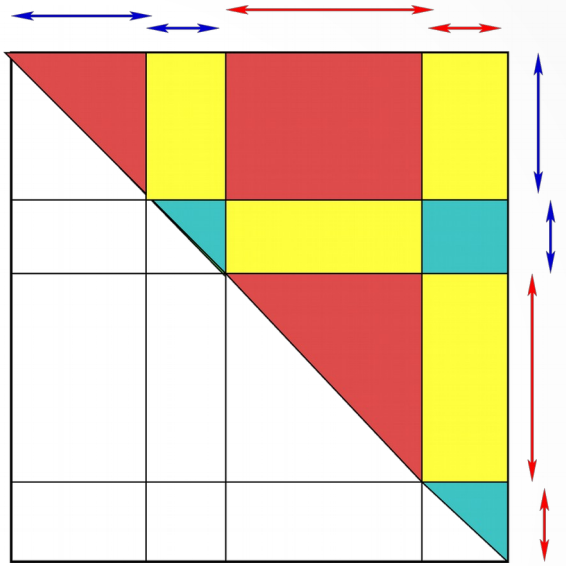
constraining field

$$\hat{H}_c = \mu_B\,\vec{\sigma}\cdot\vec{B}_c = \begin{pmatrix} 0 & \mu_B\left(B_{cx} - iB_{cy}\right) \\ \mu_B\left(B_{cx} + iB_{cy}\right) & 0 \end{pmatrix}$$

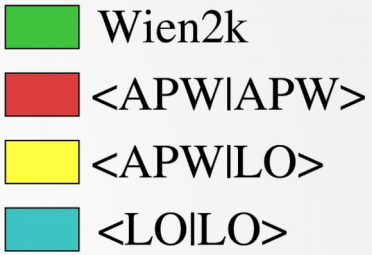
NCM Hamiltonian



Wien2k



WienNCM

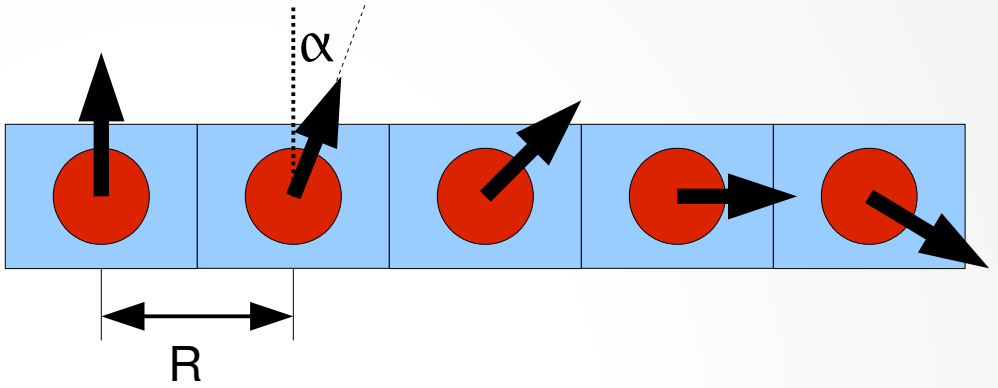


- size of the Hamiltonian/overlap matrix is doubled comparing to Wien2k
- computational cost increases !!!

WienNCM – spin spirals

- transverse spin wave

$$\alpha = \vec{R} \cdot \vec{q}$$



$$\vec{m}^n = m\left(\cos(\vec{q}\cdot\vec{R}^n), \sin(\vec{q}\cdot\vec{R}^n)\sin(\theta), \cos(\theta)\right)$$

- spin-spiral is defined by a vector **q** given in reciprocal space and,
- an angle **Θ** between magnetic moment and rotation axis
- rotation axis is arbitrary (no SOC), hard-coded as Z

Translational symmetry is lost !!!

WienNCM – spin spirals

- generalized Bloch theorem
  - generalized translations are symmetry operation of the H

$$T_n = \left\{ -\vec{q}\cdot\vec{R}_n \middle| \epsilon \middle| \vec{R}_n \right\}$$

$$T_n^{\dagger} H(\vec{r}) T_n = U^{\dagger}(-\vec{q}\cdot\vec{R}_n) H(\vec{r}+\vec{R}_n) U(-\vec{q}\cdot\vec{R}_n)$$

group of T_n is Abelian

$$\psi_{\vec{k}}(\vec{r}) = e^{i(\vec{k}\cdot\vec{r})} \begin{pmatrix} e^{\frac{i\vec{q}\cdot\vec{r}}{2}} u^{\uparrow}(\vec{r}) \\ e^{\frac{-i\vec{q}\cdot\vec{r}}{2}} u^{\downarrow}(\vec{r}) \end{pmatrix}$$

$$T_n \psi_{\vec{k}}(\vec{r}) = U(-\vec{q}\cdot\vec{R}) \psi_{\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{r}} \psi_{\vec{k}}(\vec{r})$$

1-d representations, Bloch Theorem

- efficient way for calculation of spin waves, only one unit cell is necessary for even incommensurate wave

Usage

- generate atomic and magnetic structure

  1) create atomic structure
  2) create magnetic structure

  need to specify only directions of magnetic atoms
  use utility programs: **ncmsymmetry**, **polarangles**, ...
- run **initncm** (initialization script)
- **xncm** (WienNCM version of **x** script)
- **runncm** (WienNCM version of **run** script)
- find more in manual

WienNCM – case.inncm file

- `case.inncm` – magnetic structure file

```
FULL
  0.000  0.000  0.000
 45.00000  54.73561    0
135.00000 125.26439    0
-135.00000  54.73561    0
 -45.00000 125.26439    0
  45.00000  54.73561    0
  45.00000  54.73561    0
 315.00000 125.26439    0
 315.00000 125.26439    0
 135.00000 125.26439    0
 135.00000 125.26439    0
 225.00000  54.73561    0
 225.00000  54.73561    0
   0.50000
```

q spiral vector

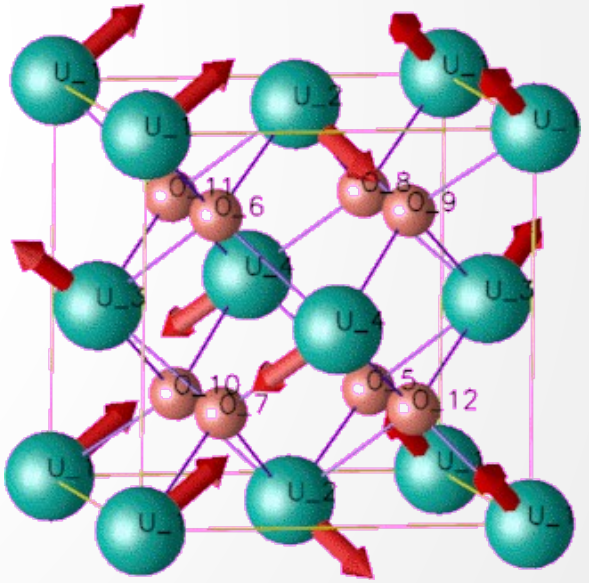
polar angles of mm

optimization switch

U, magnetic atoms

O, non-magnetic atoms

mixing for constraining field



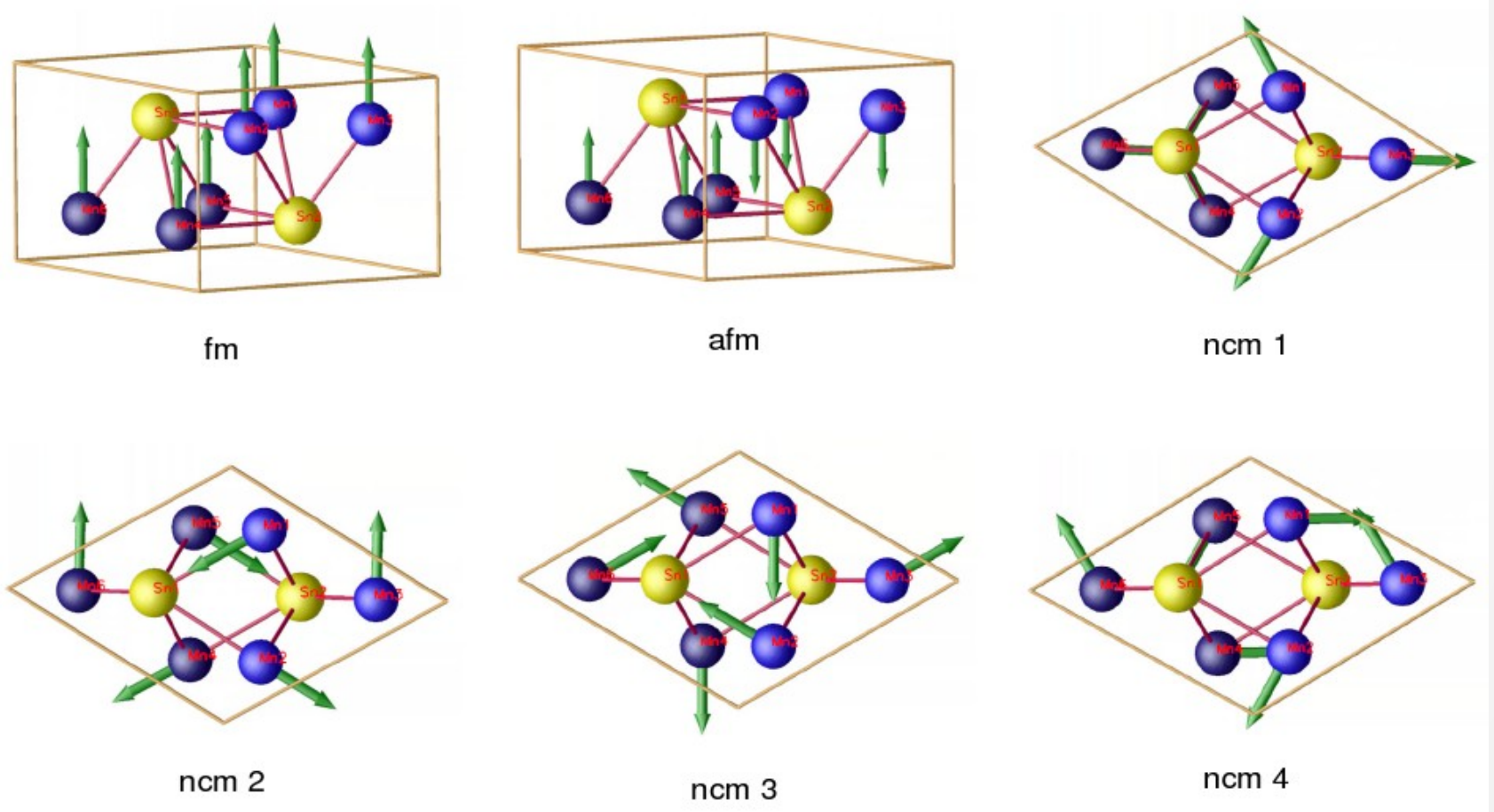
how to run it ?

- similar to WIEN2k (***initncm***, ***runncm***, ***xncm*** ...)

```
runncm_lapw -p -cc 0.0001 ...

xncm lapw0
xncm lapw1
xncm lapw2
xncm lcore
xncm mixer
```

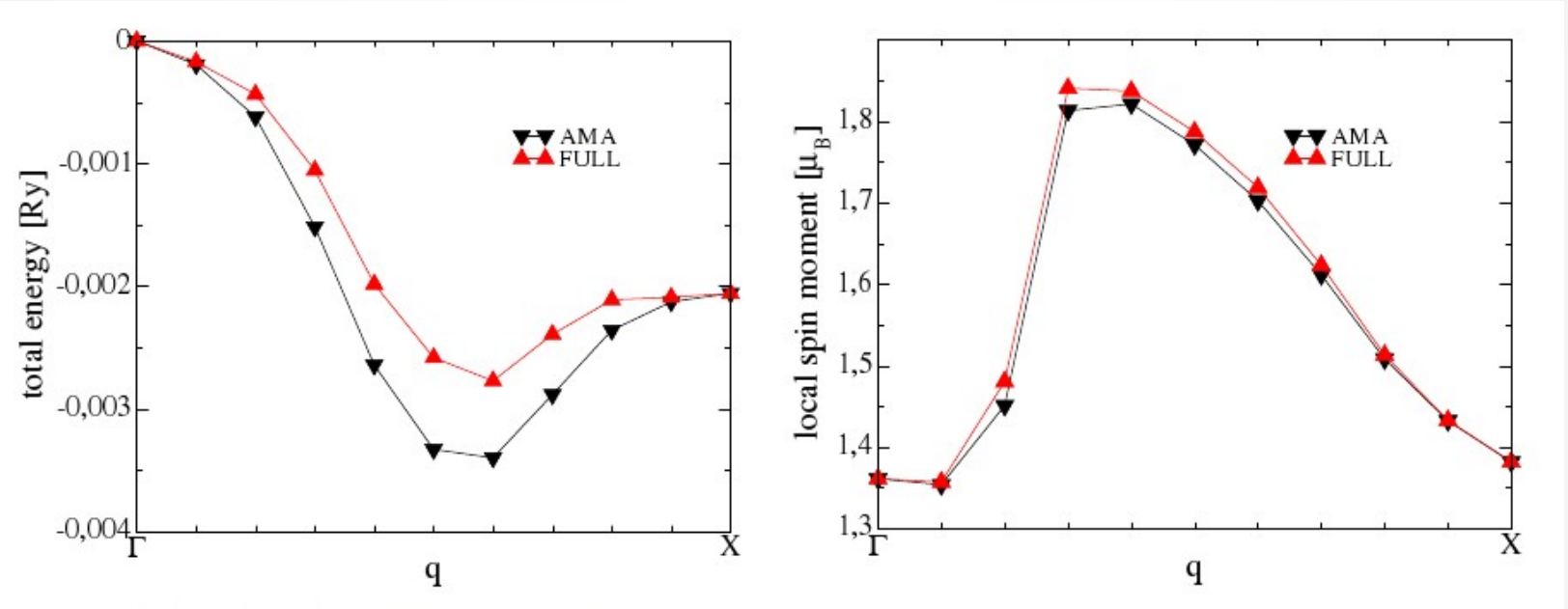
Magnetic structure of Mn_3Sn

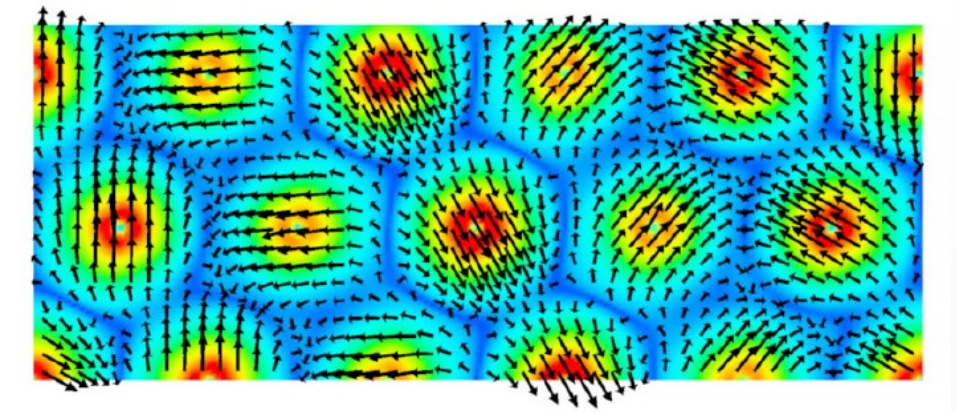


Mn_3Sn cd.

	so	fm	afm	ncm 1	ncm 2	ncm 3	ncm 4
$E_{fm} - E\ [Ry]$	-	0.0	0.0131	0.0444	0.0444	0.0444	0.0444
	+	0.0	0.0133	0.0441	0.0439	0.0444	0.0445
$M_s\ [\mu_B]$	-	3.012	2.684	3.037	3.037	3.037	3.037
	+	3.008	2.679	3.034	3.034	3.038	3.037
efg on Mn	-	-1.657	-2.111	-0.894	-0.894	-0.894	-0.894
$[10^{21}V/m^2]$	+	-1.661	-2.119	-0.892	-0.899	-0.891	-0.894
						-0.898	-0.881
hff on Mn	-	-309.9	-153.1	31.2	31.2	31.2	31.2
$[kGauss]$	+	-309.6	-152.9	31.1	31.5	31.5	30.9
						32.2	32.1

γ Fe, spin spiral





Spin density maps for q = 0.6 (0-Γ, 1-X)