Spin-orbit coupling in Wien2k

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Dirac Hamiltonian

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

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

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

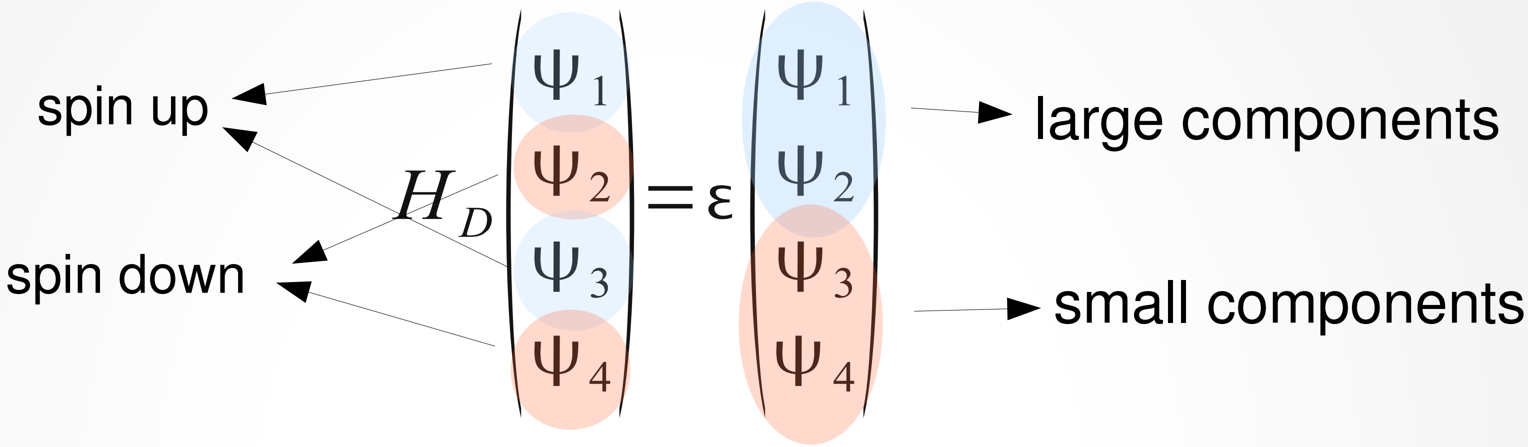
Pauli matrices:

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

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

H_D and the wave function are 4-dimensional objects

Dirac Hamiltonian



$$H_D \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

spin up

spin down

large components

small components

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):

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

spin up spin down

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

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 spinor

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

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

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.

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

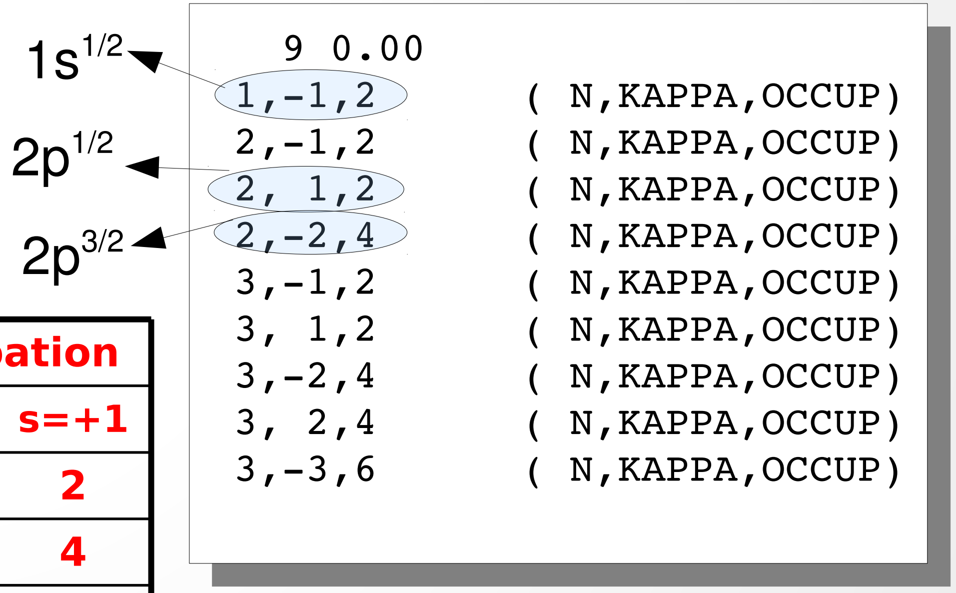
scalar relativistic approximation

spin-orbit coupling

Implementation: core electrons

Core states are calculated with spin-compensated Dirac equation

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



```
  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

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

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

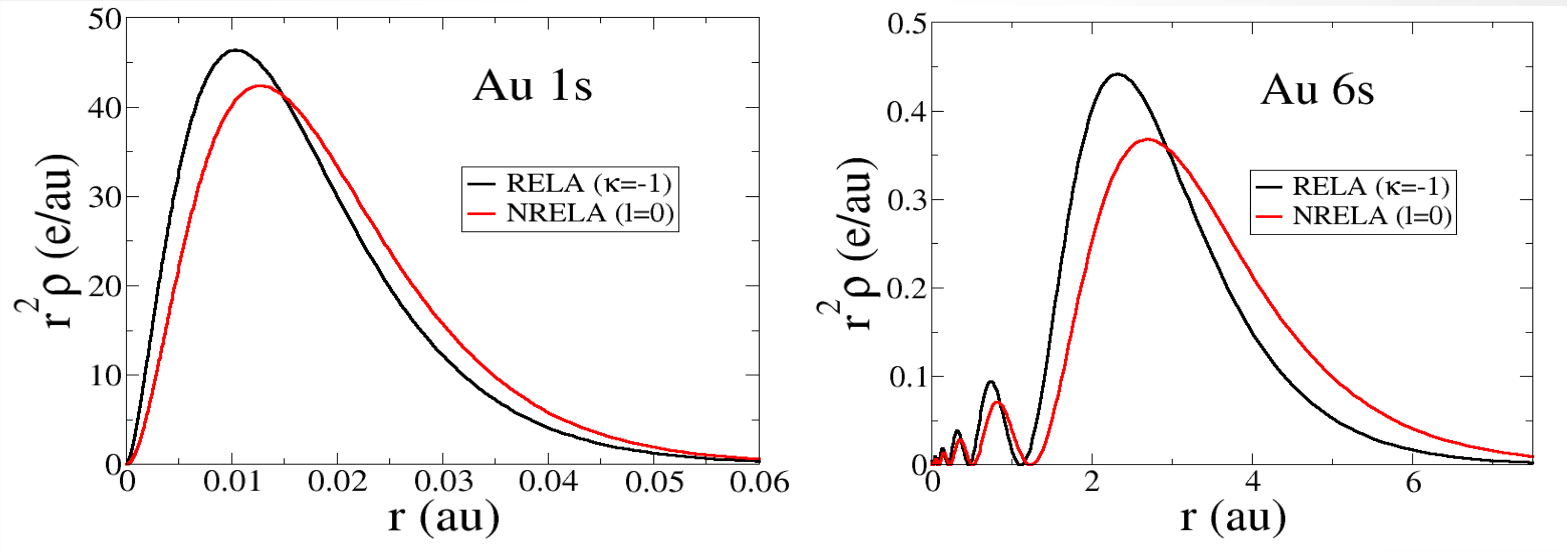
radial equations of Koelling and Harmon (spherical potential)

- 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

$$MV^2/r = Ze/r^2$$

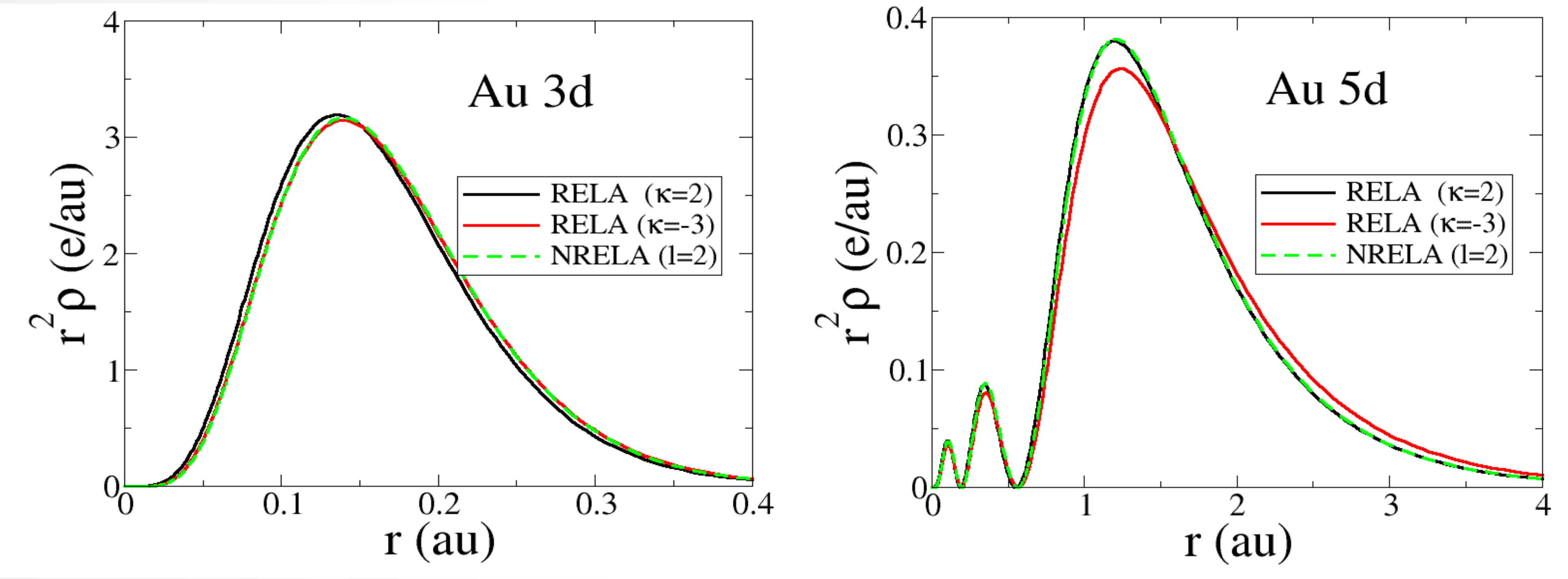
centripetal force

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

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

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

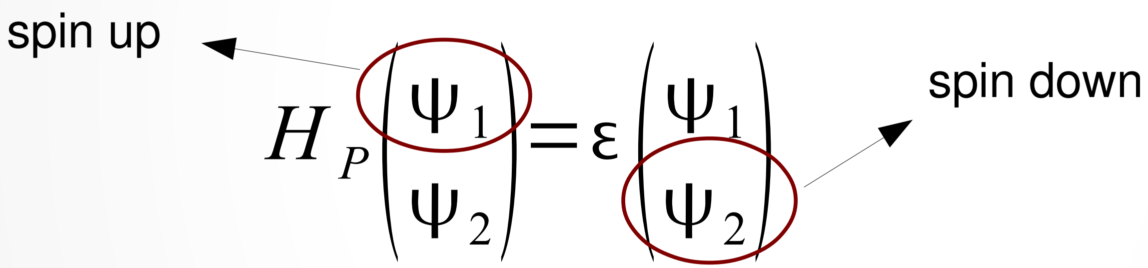
- 2x2 matrix in spin space, due to Pauli spin operators, wave function is a 2-component vector (spinor)

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 up

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

spin down

Spin structure of the Hamiltonian with SOC

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

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, SOC mixes up and down spin states
- off-diagonal term of the spin density matrix is ignored, it means that in each SCF cycle the magnetization is projected on the chosen direction (from *case.inso*)
- 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

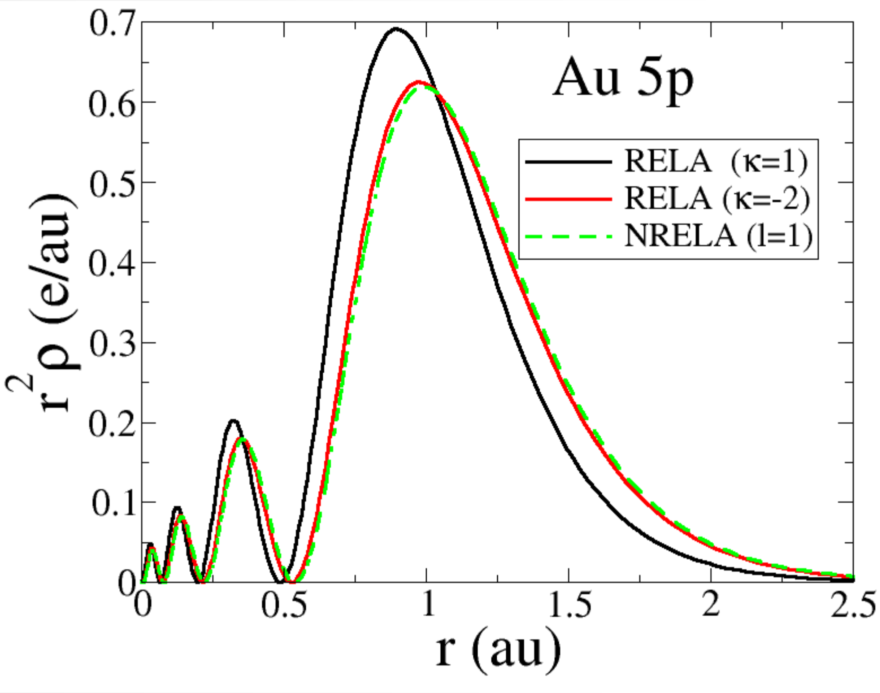
$$\sum_i^N \left(\delta_{ij} \varepsilon_1^j + \left\langle \psi_1^j \middle| H_{SO} \middle| \psi_1^i \right\rangle\right) \left\langle \psi_1^i \middle| \psi \right\rangle = \varepsilon \left\langle \psi_1^j \middle| \psi \right\rangle$$

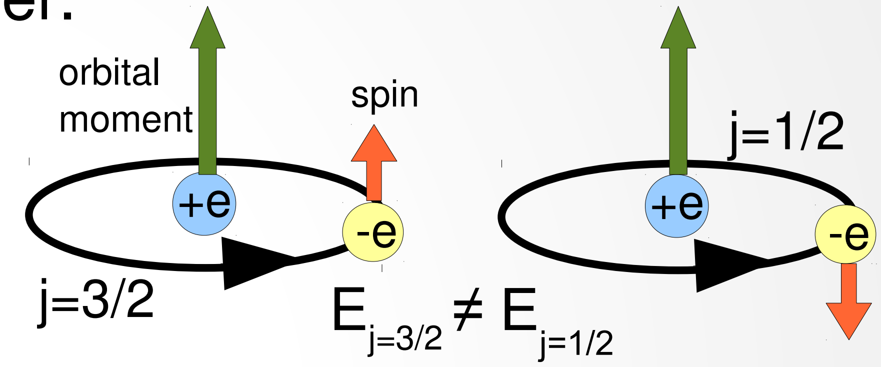
sum includes both up/down spin states

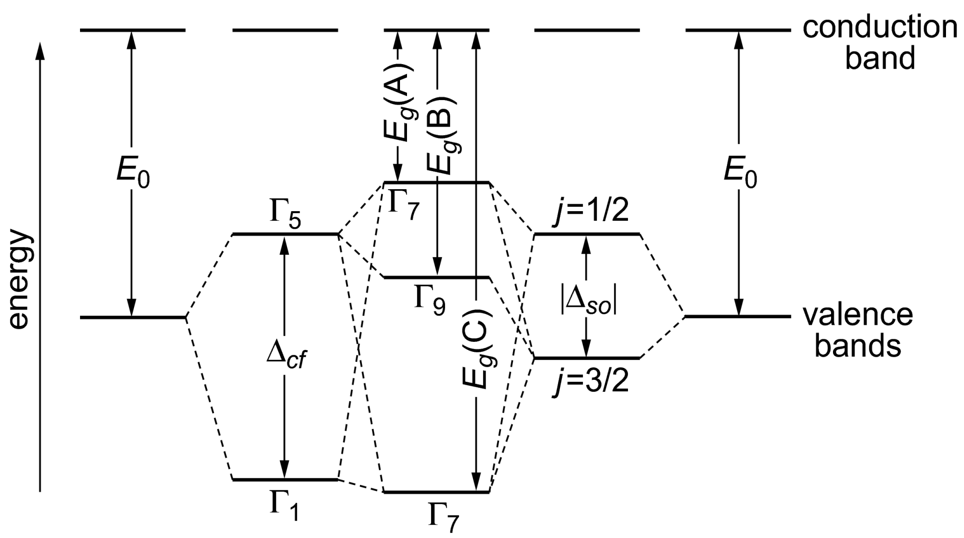
N is much smaller then the basis size in lapw1!!

SOC splitting of p states

Spin Orbit splitting of l-quantum number.







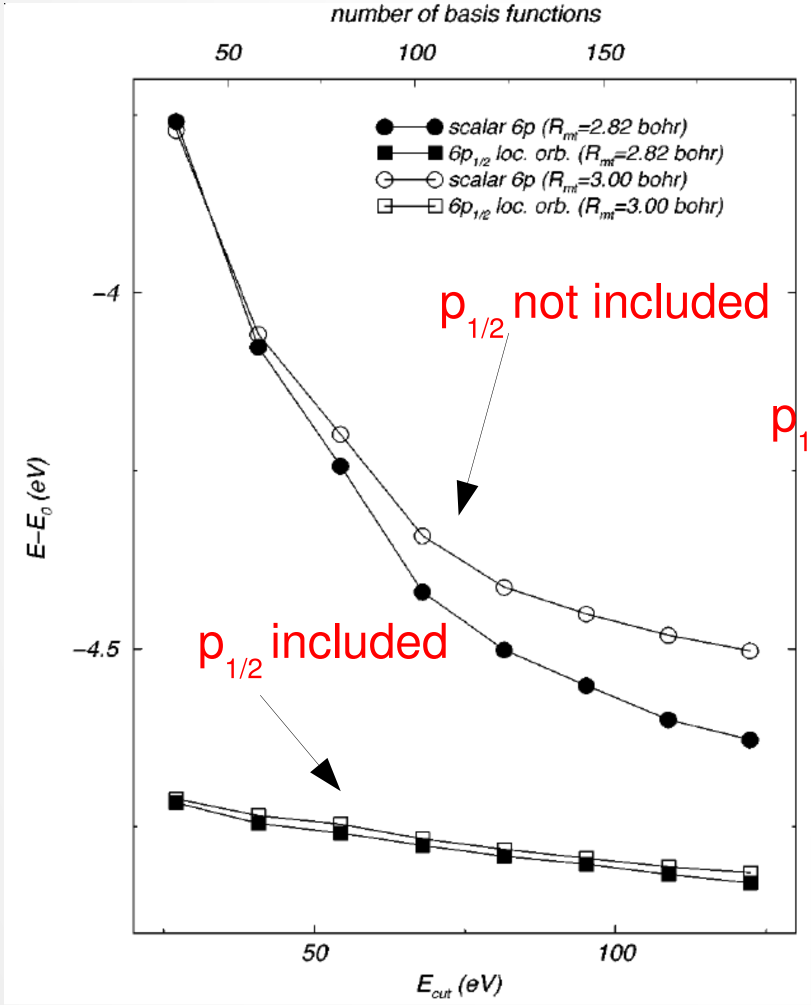
band edge at ?in ZnO

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

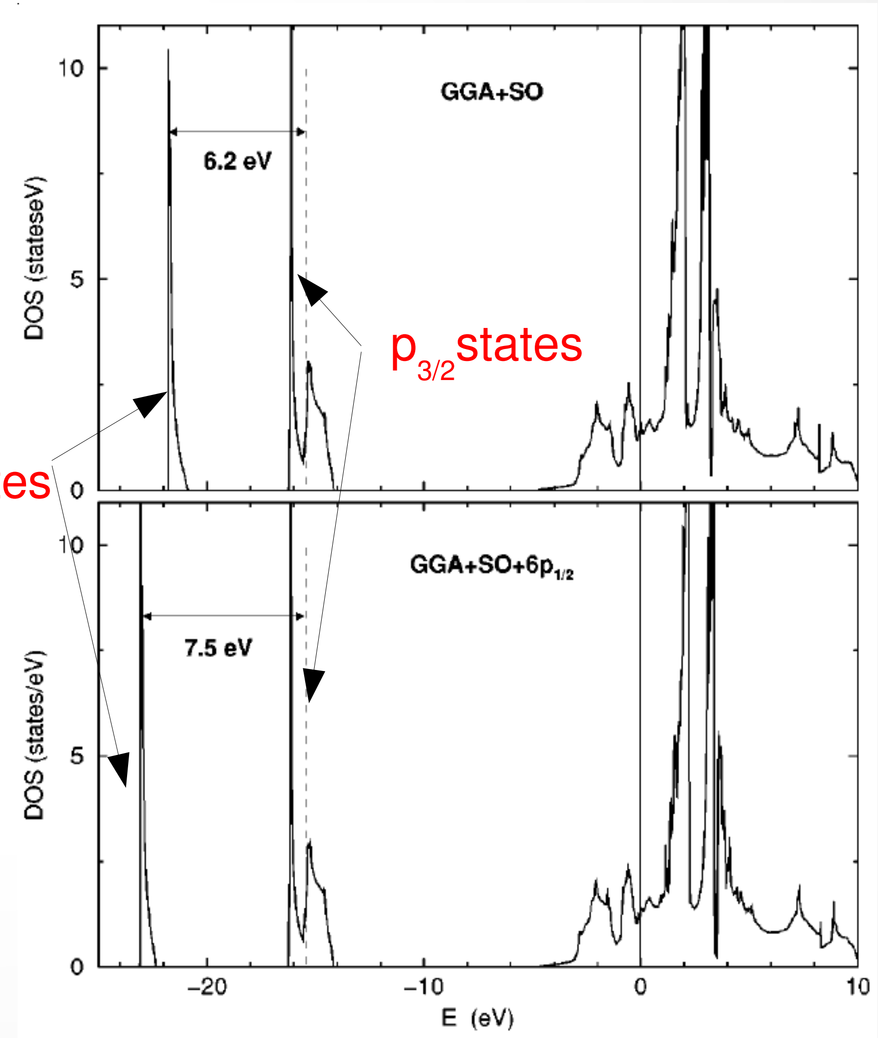
$p_{1/2}$ orbitals

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

PRB, 64, 1503102 (2001)

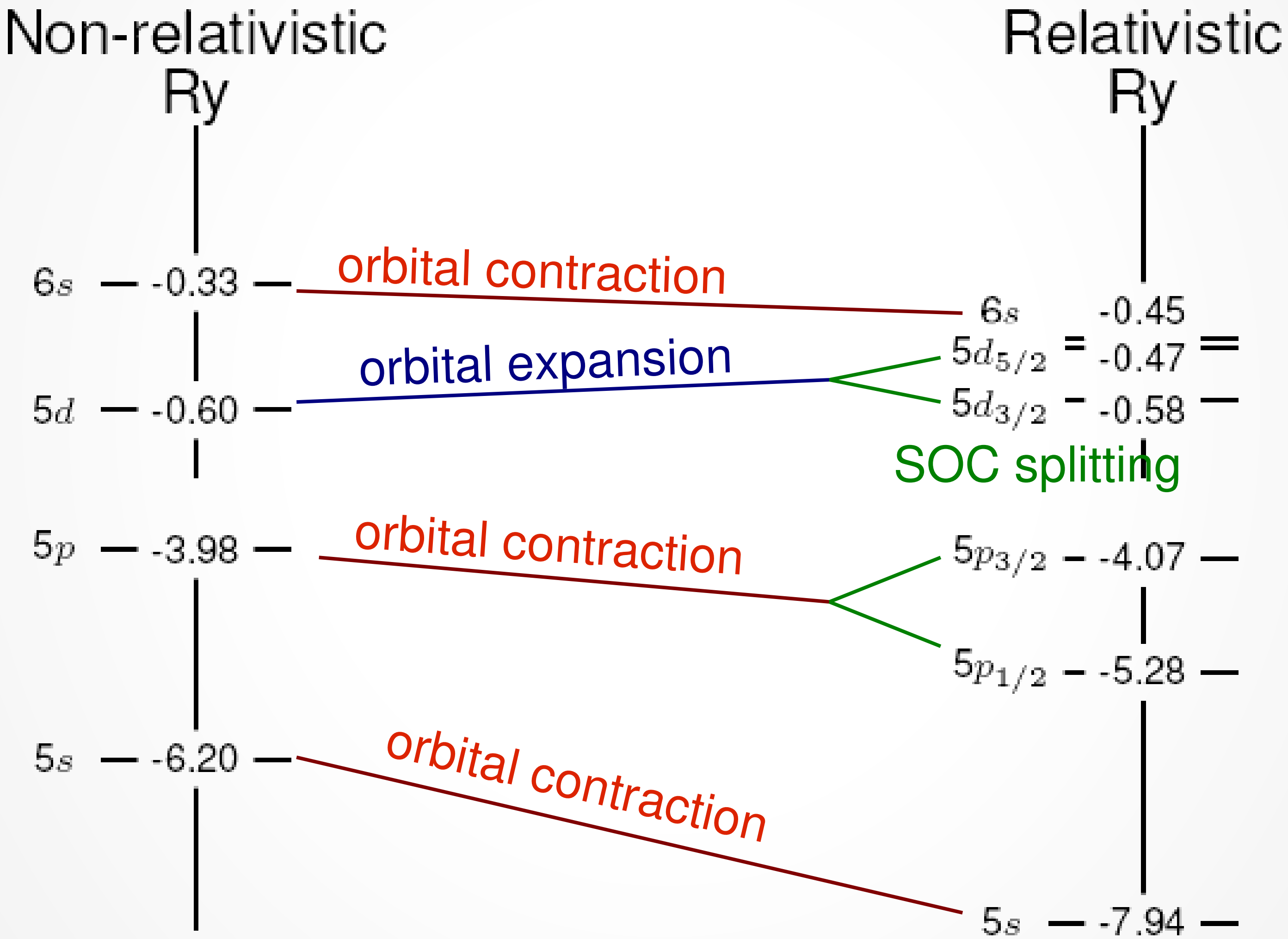


energy vs. basis size



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

Au atomic spectra

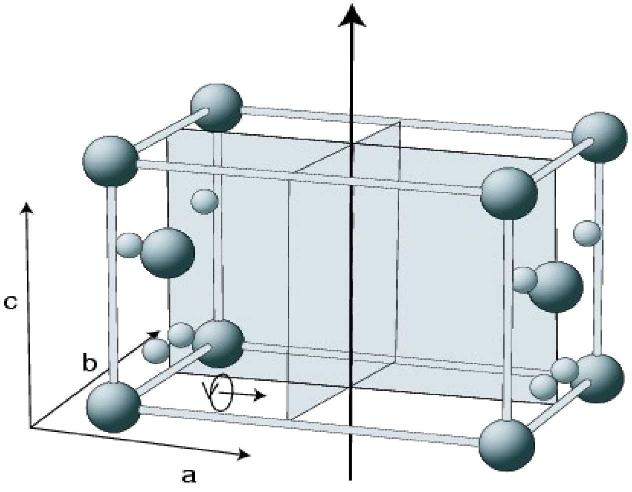


SOC in magnetic systems

- **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 (reflections act differently on spins than on positions)
  - no time inversion (do not add an inversion for k-list)
  - ***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	llmax,ipr,kpot
-10.0000 1.50000	emin,emax (output energy window)
0. 0. 1.	direction of magnetization (lattice vectors)
1	number of atoms for which RLO is added
2 -0.97 0.005	atom number,e-lo,de (case.in1), repeat NX times
0 0 0 0 0	number of atoms for which SO is switched off; list of atoms

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

Summary

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

NCM

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)

spin up component

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

spin down component

Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

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

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

Hartee term

exchange-correlation potential

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

exchange-correlation field

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}:

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

B_{xc} and m are parallel

Non-magnetic case

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

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

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

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

- solutions are pure spinors
- degenerate spin solutions

Non-magnetic calculation

- spin up and spin down part of the electronic spectrum is the same
- formally only one spin channel needs to be solved

run_lapw script:

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

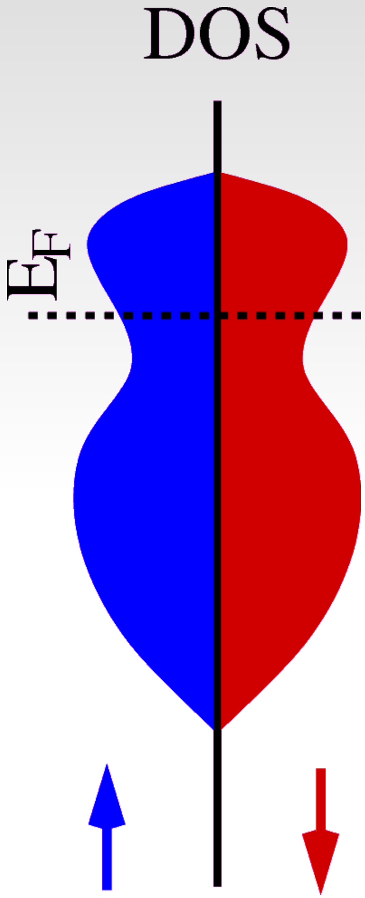
calculate potential

calculate valence wave-functions

calculate valence densities

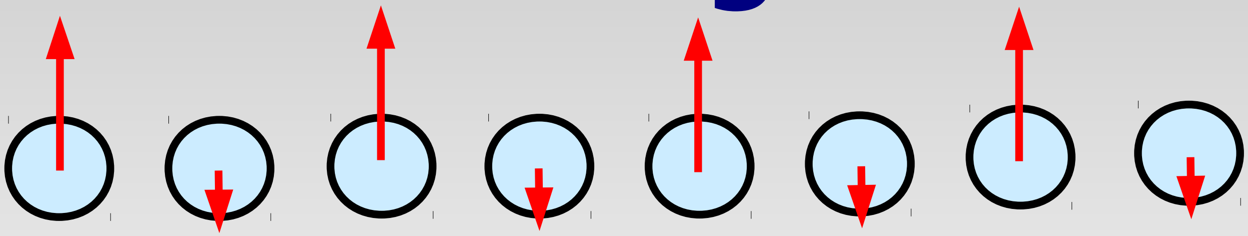
calculate core states

generete new density



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

Collinear magnetism



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

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

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

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

- solutions are pure spinors

Collinear magnetic calculation

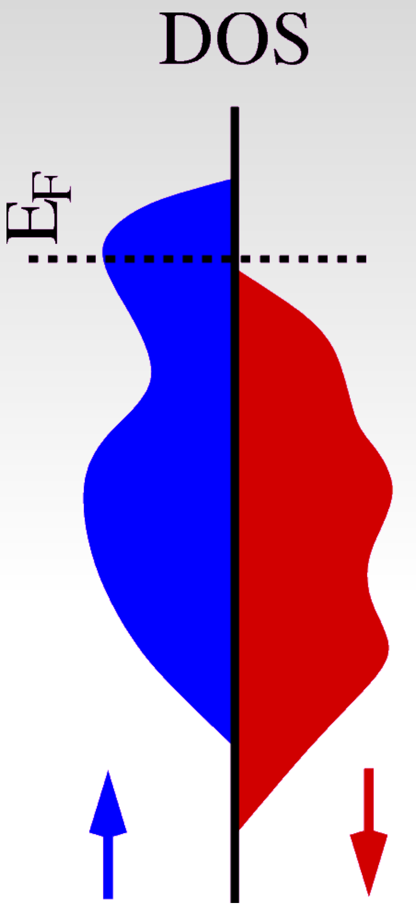
- due to the exchange field the potential is different for up and down spin channels
- Pauli Hamiltonian is diagonal in spin space, thus up and down spin channels are solved separately

$$\left(-\frac{\hbar}{2m}\nabla^2+V_{ef}+\mu_B B_z+\dots\right)\psi_\uparrow=\varepsilon_\uparrow\psi_\uparrow$$

$$\left(-\frac{\hbar}{2m}\nabla^2+V_{ef}-\mu_B B_z+\dots\right)\psi_\downarrow=\varepsilon_\downarrow\psi_\downarrow$$

`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
```

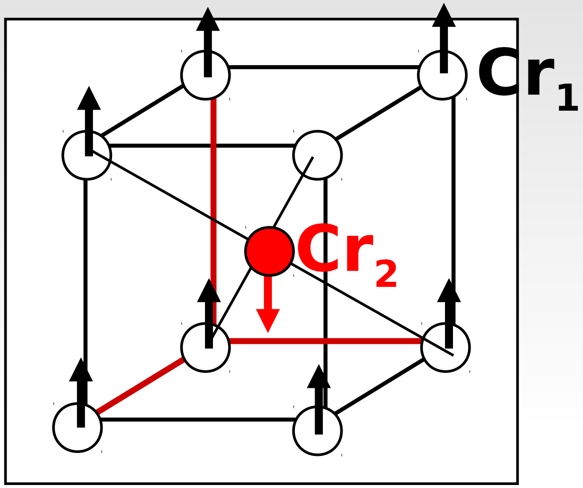


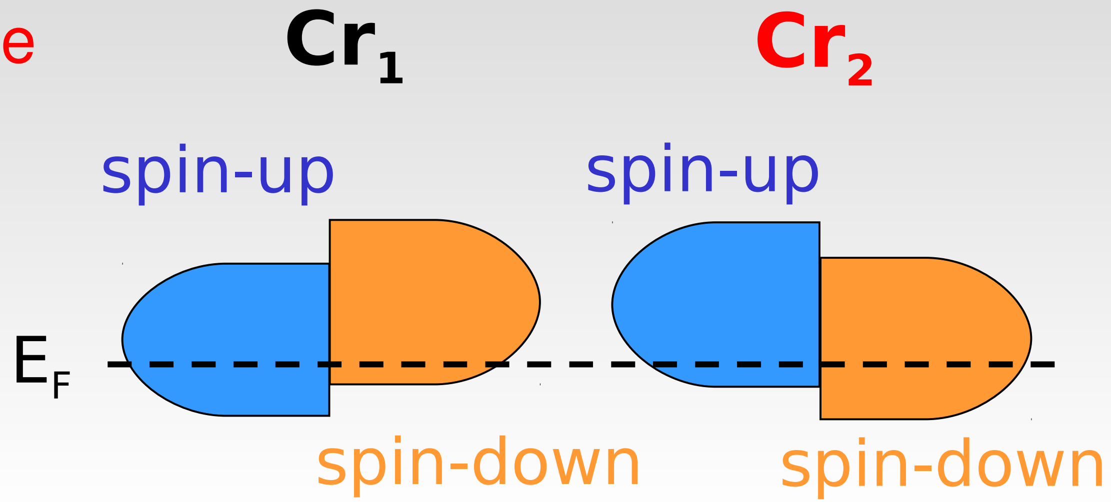
$$m=n_\uparrow-n_\downarrow\neq 0$$

$$\psi_\uparrow\Rightarrow\begin{pmatrix}\psi_\uparrow\\0\end{pmatrix},\quad\psi_\downarrow\Rightarrow\begin{pmatrix}0\\\psi_\downarrow\end{pmatrix},\quad\varepsilon_\uparrow\neq\varepsilon_\downarrow$$

anti-ferromagnetic systems

- Cr has AFM bcc structure



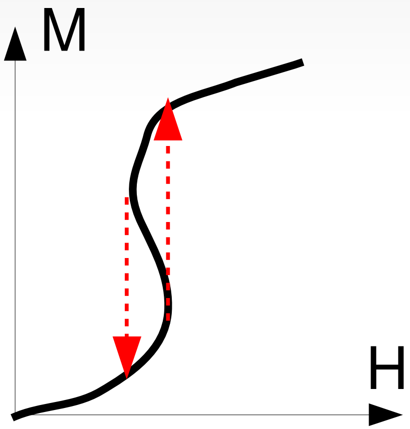


- there is a symmetry relation between spin up and spin down densities (one atoms spin up is another atoms spin down)
- therefore it is enough to do the spin-up calculation, the spin-down results can be generated afterwards
- use *runafm_lapw* script in such cases (stabilizes and speeds up the SCF convergence)

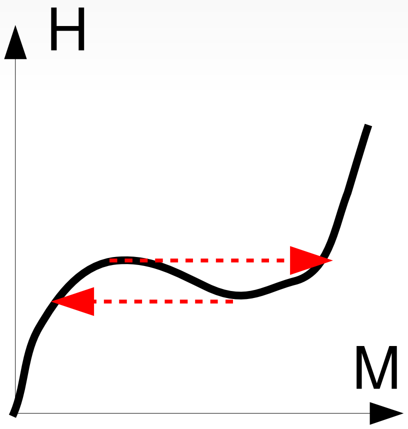
fix spin moment calculations

- constrain value of magnetic moments and dependence of energy on magnetic moment

A.R.Williams, V.L.Moruzzi, J.Kübler, K.Schwarz, Bull.Am.Phys.Soc. **29**, 278 (1984)
K.Schwarz, P.Mohn J.Phys.F **14**, L129 (1984)
P.H.Dederichs, S.Blügel, R.Zoller, H.Akai, Phys. Rev, Lett. **53**,2512 (1984)



- under certain conditions magnetization can be multivalued function of H



- interchanging the dependent and independent variable makes this function is single valued (unique)

Fixed spin moment (FSM) method

- Conventional scheme

$$E_F^{\uparrow} = E_F^{\downarrow}$$

$$Z_v = N^{\uparrow} + N^{\downarrow}$$

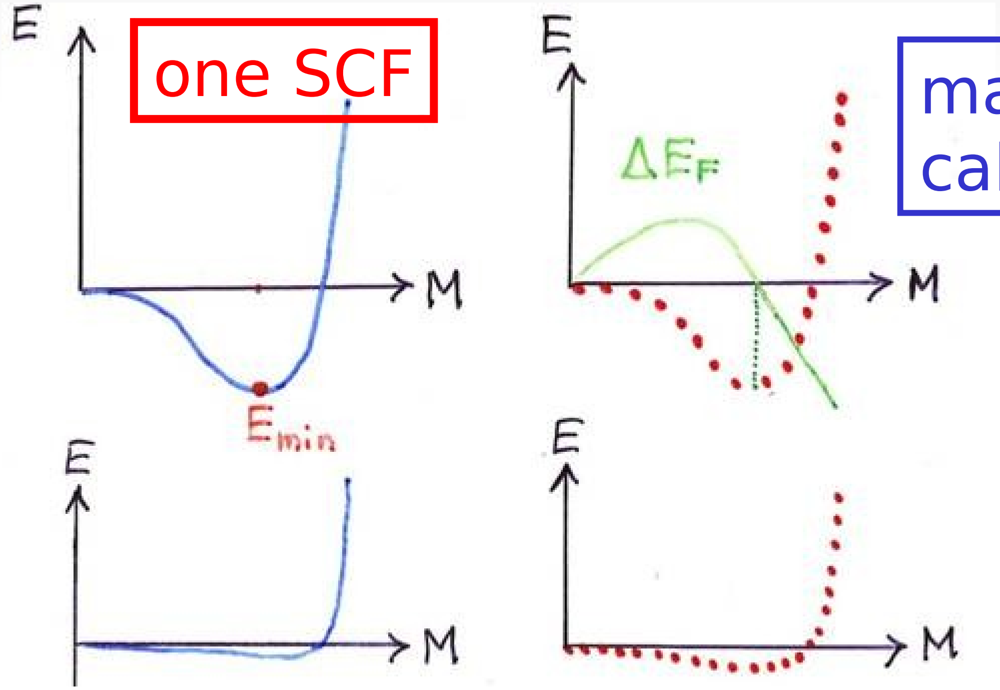
output $\boxed{M = N^{\uparrow} - N^{\downarrow}}$

constrained (FSM) method

$\boxed{M = N^{\uparrow} - N^{\downarrow}}$ input

$$Z_v = N^{\uparrow} + N^{\downarrow}$$

$E_F^{\uparrow} \neq E_F^{\downarrow}$ output



one SCF

many calculations

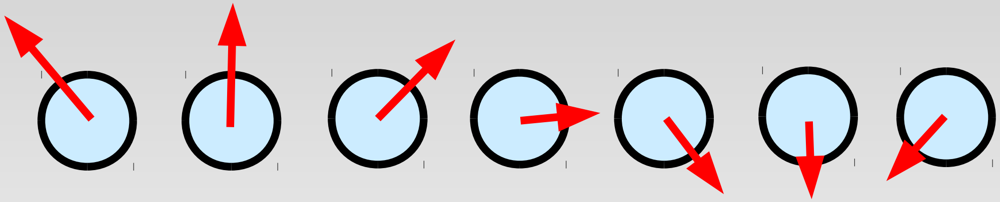
Simple case:
bcc Fe

difficult case:
Fe_3Ni

poor convergence

good convergence

Non-collinear magnetism



- direction of magnetization vary in space and/or spin-orbit coupling is present

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

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

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad \psi_{1,}\psi_2 \neq 0$$

- solutions are non-pure spinors

Non-collinear magnetism

- Wien2k can only handle collinear or non-magnetic cases
- in NCM case both spin channels have to be considered simultaneously

`runncm_lapw` script:

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

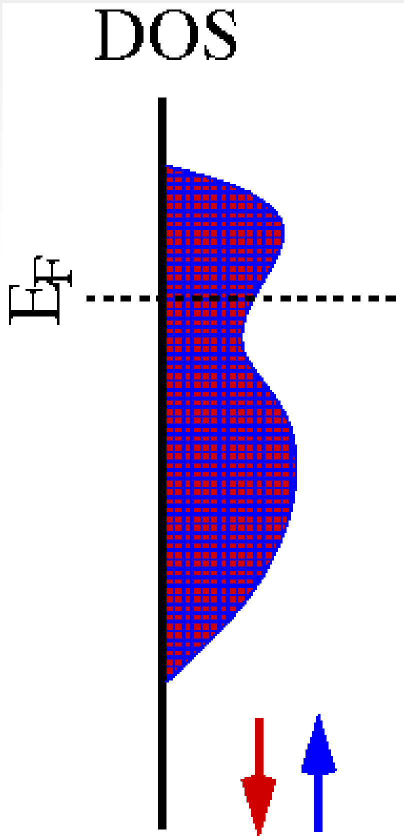
$$\hat{n} = \sum_{nk} \begin{pmatrix} \Psi_{\uparrow nk} \\ \Psi_{\downarrow nk} \end{pmatrix}^* \begin{pmatrix} \Psi_{\uparrow nk} & \Psi_{\downarrow nk} \end{pmatrix}$$

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

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

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

relation between spin density matrix and magnetization



NCM case

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 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
  - spin spirals are available

WienNCM - implementation

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

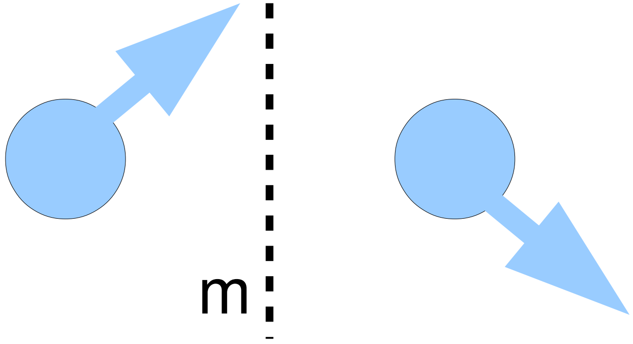
interstitities: $\varphi_{\vec{G}\sigma} = \mathrm{e}^{i(\vec{G}+\vec{k})\cdot\vec{r}}\chi_\sigma$ $\qquad \chi_\sigma = \begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$

spheres:

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

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

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



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

WienNCM implementation

- Hamiltonian inside spheres:

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

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

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

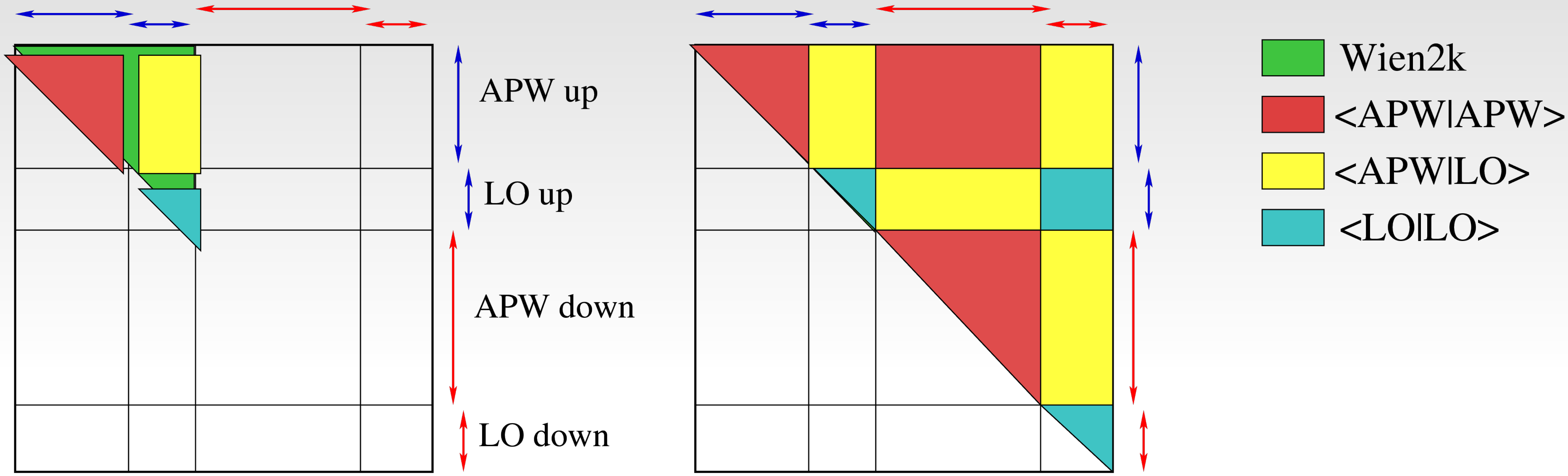
diagonal orbital field

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

constraining field

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

NCM (SOC) Hamiltonian



Wien2k

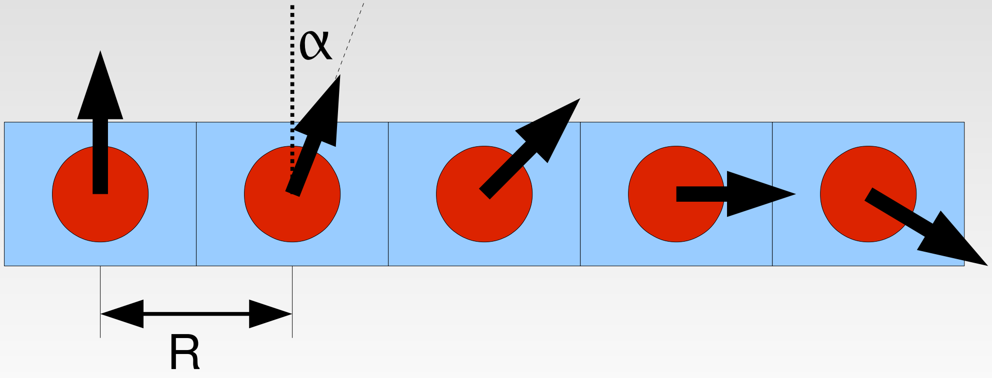
WienNCM

- 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

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

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

group of T_n is Abelian

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

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

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**, ...

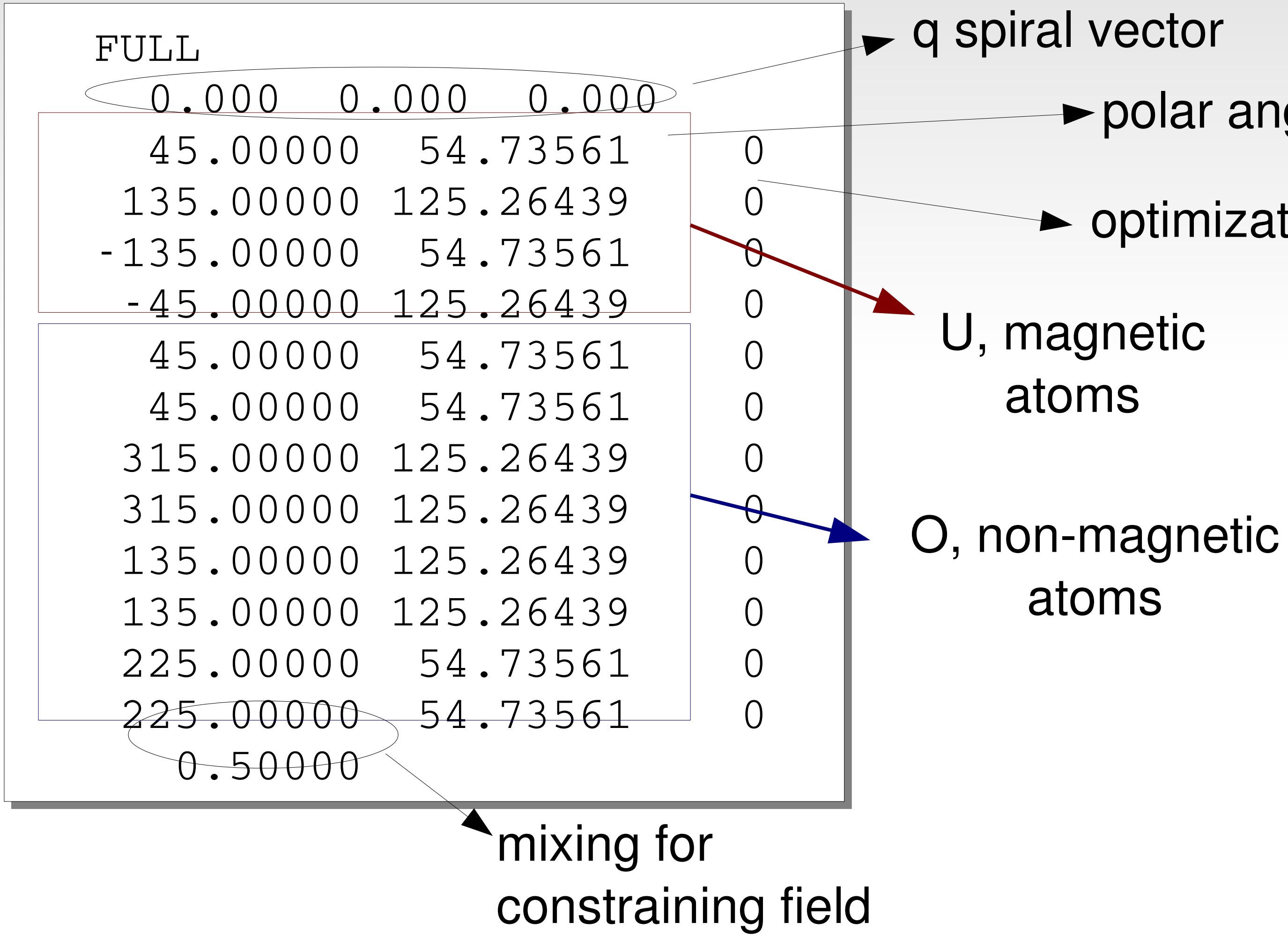
- run **initncm** (initialization script)
- **xncm** (WienNCM version of **x** script)
- **runncm** (WienNCM version of **run** script)
- find more in manual

runncm_lapw script:

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

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