

Calculation of spin-orbit coupling

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1 Introduction

Relativistic corrections in electron structure calculation are important if:

- the electron velocity is of the same order as velocity of light
- they give rise to the effects not observed otherwise

In the interstitial region relativistic correction may be usually neglected - electron velocity is limited by the cutoff in the k -space.

Within the atomic spheres the importance of relativistic corrections increases with increasing atomic number.

Example of the effect when relativistic corrections are important is magnetocrystalline anisotropy: though dipolar interactions may also contribute, the dominant mechanism usually arises from combined effect of the crystal field and spin-orbit interactions.

2 Dirac equation

Application of the Dirac equation to calculation of the electron structure of atoms may be found in several textbooks. In this section we follow closely the analysis given by: J. Kubler and V. Eyert, *Electronic structure calculations in Materials Science and Technology. Vol. 3A: Electronic and Magnetic Properties of Metals and Ceramics. Part I. Volume Ed.: K.H.J. Buschow. VCH-Verlag, Weinheim 1992, p. 1-145*

Dirac Hamiltonian can be written as (energies are measured relative to the rest energy):

$$H_D = c\vec{\alpha}\vec{p} + (\beta - 1)mc^2 + V(\vec{r}) \quad (1)$$

where $\vec{\alpha}, \beta$ are 4x4 matrices:

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}; \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad (2)$$

$\sigma_x, \sigma_y, \sigma_z$ are the Pauli-spin matrices. Eigenvectors of (1) are four-component functions Ψ which are written in terms of two-component functions Φ, χ :

$$\Psi = \begin{pmatrix} \Phi \\ \chi \end{pmatrix} \quad (3)$$

In case of electrons Φ is the 'large' and χ is the 'small' component of the wave function. (1-3) lead to a set of coupled equations:

$$c(\vec{\sigma}\vec{p})\chi = (\varepsilon - V)\Phi \quad (4)$$

$$c(\vec{\sigma}\vec{p})\Phi = (\varepsilon - V + 2mc^2)\chi \quad (5)$$

From (4-5) we get the equation for the large component:

$$\frac{1}{2m}(\vec{\sigma}\vec{p})\left(1 + \frac{\varepsilon - V}{2mc^2}\right)^{-1}(\vec{\sigma}\vec{p})\Phi + V\Phi = \varepsilon\Phi \quad (6)$$

We now use an approximation:

$$\left(1 + \frac{\varepsilon - V}{2mc^2}\right)^{-1} \approx 1 - \frac{\varepsilon - V}{2mc^2} \quad (7)$$

which, together with:

$$\vec{p}V = V\vec{p} - i\hbar\vec{\nabla}V \quad (8)$$

$$(\vec{\sigma}\vec{\nabla}V)(\vec{\sigma}\vec{p}) = (\vec{\nabla}V\vec{p}) + i\vec{\sigma}[\vec{\nabla}, \vec{p}] \quad (9)$$

leads to an differential equation for Φ :

$$\left[\left(1 - \frac{\varepsilon - V}{2mc^2}\right)\frac{p^2}{2m} + V\right]\Phi - \frac{\hbar^2}{4m^2c^2}(\vec{\nabla}V\vec{\nabla}\Phi) + \frac{\hbar^2}{4m^2c^2}(\vec{\sigma}[\vec{\nabla}V, \vec{p}]\Phi) = \varepsilon\Phi \quad (10)$$

2.1 Dirac equation in central field

If the potential has the spherical symmetry (10) reduces to:

$$\left[\frac{p^2}{2m} + V - \frac{p^4}{8m^3c^2} - \frac{\hbar^2}{4m^2c^2}\frac{dV}{dr}\frac{\partial}{\partial\vec{r}} + \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}(\vec{l}\vec{s})\right]\Phi = \varepsilon\Phi \quad (11)$$

First and second term give nonrelativistic Schrödinger equation. Third and fourth term are mass and Darwin correction, respectively. Finally the last term corresponds to the spin-orbit coupling.

Due to the spin-orbit coupling Ψ is not an eigenfunction of spin or orbital moment. Instead the good quantum numbers are j, j_z and κ

$$\vec{j} = \vec{l} + \vec{s} \quad (12)$$

$\hbar\kappa$ are eigenvalues of an operator:

$$K = \begin{pmatrix} \vec{\sigma}\vec{l} + \hbar & 0 \\ 0 & -\vec{\sigma}\vec{l} - \hbar \end{pmatrix} \quad (13)$$

κ and j are related by $\kappa = \pm(j + \frac{1}{2})$.

The four-component function Ψ is now written as:

$$\Psi = \begin{pmatrix} \Phi \\ \chi \end{pmatrix} = \begin{pmatrix} g(r)\mathcal{Y}_{jl}^{j_z} \\ if(r)\mathcal{Y}_{j'l'}^{j_z} \end{pmatrix} \quad (14)$$

where g and f are the radial function, $\mathcal{Y}_{jl}^{j_z}$ is the r -independent eigenfunction of j^2, j_z, l^2 and s^2 formed by the combination of the Pauli spinor with the spherical harmonics.

The coupled systems of equations for f, g is:

$$\hbar c\left[\frac{df}{dr} + \frac{1 - \kappa}{r}f\right] + (\varepsilon - V)g = 0 \quad (15)$$

$$\hbar c\left[\frac{dg}{dr} + \frac{1 + \kappa}{r}g\right] - (\varepsilon - V + 2mc^2)f = 0 \quad (16)$$

By eliminating f we obtain:

$$-\frac{\hbar^2}{2Mr^2} \frac{d}{dr} \left(r^2 \frac{dg}{dr} \right) + \left[V + \frac{\hbar^2}{2Mr^2} \frac{l(l+1)}{r^2} \right] g - \frac{\hbar^2}{4M^2c^2} \frac{dV}{dr} \frac{dg}{dr} - \frac{\hbar^2}{4M^2c^2} \frac{dV}{dr} \frac{1+\kappa}{r} g = \varepsilon g \quad (17)$$

where we introduced relativistically enhanced mass

$$M = m + \frac{\varepsilon - V}{2c^2} \quad (18)$$

and used that

$$\kappa(\kappa + 1) = l(l + 1) \quad (19)$$

Function f is given by

$$f = \frac{\hbar}{2Mc} \left(\frac{dg}{dr} + \frac{1+\kappa}{r} g \right) \quad (20)$$

The scalar relativistic approximation is obtained by omitting in (17, 20) the terms which depend on κ . Clear advantage of this approximation is that l and s are good quantum numbers - this is especially important in spin-polarized calculations. The spin-orbit coupling may be then taken into account using the method described below.

We denote the scalar relativistic approximation to f, g by \tilde{f}, \tilde{g} :

$$-\frac{\hbar^2}{2Mr^2} \frac{d}{dr} \left(r^2 \frac{d\tilde{g}}{dr} \right) + \left[V + \frac{\hbar^2}{2Mr^2} \frac{l(l+1)}{r^2} \right] \tilde{g} - \frac{\hbar^2}{4M^2c^2} \frac{dV}{dr} \frac{d\tilde{g}}{dr} = \varepsilon \tilde{g} \quad (21)$$

and \tilde{f}, \tilde{g} satisfy the set of equations:

$$\tilde{f} = \frac{\hbar}{2Mc} \frac{d\tilde{g}}{dr} \quad (22)$$

$$\tilde{g} = -\frac{\hbar c}{\varepsilon - V} \frac{d\tilde{f}}{dr} \quad (23)$$

The four-component wave function is now written as:

$$\tilde{\Psi} = \begin{pmatrix} \tilde{\Phi} \\ \tilde{\chi} \end{pmatrix} \quad (24)$$

where $\tilde{\Phi}$ is a pure spin state:

$$\tilde{\Phi} = \tilde{g} Y_{lm} \chi_s \quad (25)$$

while $\tilde{\chi}$ contains mixture of up and down spin functions and it is obtained from (4)

$$\tilde{\chi} = i \frac{\vec{\sigma} \vec{r}}{r} \left(-\tilde{f} + \frac{\tilde{g}}{2Mc r} \vec{\sigma} \vec{l} \right) Y_{lm} \chi_s \quad (26)$$

Functions $\tilde{\Psi}$ are not eigenfunctions of the Dirac Hamiltonian (1) and their deviation from eigenfunction is used to define the spin-orbit Hamiltonian H_{so} :

$$H \tilde{\psi} = \varepsilon \tilde{\psi} + H_{so} \tilde{\psi} \quad (27)$$

In the basis of functions (23) H_{so} has the form:

$$H_{so} = \frac{\hbar}{2Mc^2} \frac{1}{r} \frac{dV}{dr} \begin{pmatrix} \vec{\sigma} \vec{l} & 0 \\ 0 & 0 \end{pmatrix} \quad (28)$$

Note that H_{so} defined in this way acts on the large component of the wave function only.

3 Second variational treatment of spin-orbit coupling

The WIEN package provides the possibility to perform both non-relativistic and relativistic calculations. When running the relativistic calculations, the way in which relativity is included differs for core and valence states. The core states are assumed to be fully occupied and fully relativistic calculation is possible. The following discussion concerns therefore the valence (and/or local) orbitals only. These orbitals are - within the atomic spheres - treated in the scalar relativistic approximation. To obtain the basis set for the LAPW calculation, coupled equations (22, 23) are first solved. Spin is good quantum number, therefore spin up and spin down states are considered separately:

$$\phi_{lm}^\uparrow = \begin{pmatrix} \tilde{g}_l^\uparrow Y_{lm} \\ -i\tilde{f}_l^\uparrow Y_{lm} \end{pmatrix} \chi_\uparrow; \quad \phi_{lm}^\downarrow = \begin{pmatrix} \tilde{g}_l^\downarrow Y_{lm} \\ -i\tilde{f}_l^\downarrow Y_{lm} \end{pmatrix} \chi_\downarrow; \quad \chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad \chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (29)$$

By combining ϕ_{lm}^\uparrow (ϕ_{lm}^\downarrow) the LAPW basis set for spin up (spin down) within the atomic spheres is constructed.

As the spin-orbit coupling has nonzero matrix elements between spin up and spin down basis functions, an obvious way to include H_{so} would be to double the dimension of the eigenvalue problem. For large systems this may be difficult. Fortunately there exists more efficient way (called second variational method) to achieve the same goal. First the eigenvalue problem is solved in the usual way i.e. separately for spin up and spin down states for Hamiltonian not containing H_{so} . Resulting eigenvalues and eigenfunctions are (we omit the index k distinguishing different \vec{k} in the Brillouin zone):

$$\psi_n^\uparrow, E_n^\uparrow \quad \psi_n^\downarrow, E_n^\downarrow \quad (30)$$

In the second step new eigenvalue problem is considered for total Hamiltonian (including H_{so}) with basis functions (30). Calculation of matrix elements requires only modest effort - scalar relativistic Hamiltonian contributes only to the diagonal matrix elements by $E_n^\uparrow, E_n^\downarrow$, which were already calculated, and calculation of H_{so} matrix elements is straightforward. The number of $\psi_n^\uparrow, \psi_n^\downarrow$ is usually much smaller than the number of functions in original basis set, which results in an eigenvalue problem of smaller dimension. The second variational method has an additional advantage of increasing the flexibility of the calculation - in many cases H_{so} is relatively small. The second variational method then allows to neglect matrix elements of H_{so} between states differing by more than a prescribed energy. Another possibility is to choose a subset of levels from (30) and consider effect of H_{so} within this subset only.

4 Implementation of spin-orbit coupling in WIEN

Present implementation of the s-o coupling in WIEN97 is contained in the package LAPWSO. It allows inclusion of the spin-orbit coupling for non spin-polarized as well as spin-polarized calculations. The spin-orbit coupling may be included selfconsistently or non-selfconsistently.

4.1 Files needed by LAPWSO

Definition file with explanation of the meaning of files for case=ni:

number , 'name', 'status', 'formatted/unformatted'

- 5 , 'ni.inso', 'old', 'formatted', 0
input: input of data

- 6 , 'ni.outputso', 'unknown', 'formatted', 0
output: complete output

- 8 , 'ni.scfso', 'unknown', 'formatted', 0
output: spin-orbit part of the scf file

- 9 , 'ni.vectordn', 'old', 'unformatted', 0
input: eigenvectors from spin down LAPW1 calculation or
in nonmagnetic calculation LAPW1 eigenvectors

- 10 , 'ni.vectorup', 'unknown', 'unformatted', 0
input: eigenvectors from spin up LAPW1 calculation or
in nonmagnetic calculation dummy

- 18, 'ni.vspdn', 'old', 'formatted', 0
input: spin down spherical potential or
in nonmagnetic calculation spherical potential

- 19, 'ni.vspup', 'unknown', 'formatted', 0
input: spin up spherical potential
in nonmagnetic calculation dummy

- 20 , 'ni.struct', 'old', 'formatted', 0
input: basic structure file

- 41, 'ni.vectsodn', 'unknown', 'unformatted', 0
output: spin down part of the s-o eigenvectors in the same basis
as eigenvectors of LAPW1 (ni.vectordn), to be used in LAPW2.

- 42, 'ni.vectsoup', 'unknown', 'unformatted', 0
output: spin up part of the s-o eigenvectors in the same basis
as eigenvectors of LAPW1 (ni.vectordn), to be used in LAPW2.

- 43, 'ni.vectdum', 'unknown', 'unformatted', 0
output: auxiliary 'eigenvector' file to be used in LAPW2 as file 9.
Structure of this file is the same as 41, 42, but vectors are short
to save the memory, eigenvalues are larger than any s-o eigenvalue,
so that the states are never populated.

- 44,'ni.vect1', 'unknown','unformatted',0
 output: spin-orbit eigenvectors in the basis of eigenvectors of LAPW1
 this file is used when calculating average value of an operator X
 (package AVERX)
- 45,'ni.normdn', 'unknown','formatted',0
 output: norms of spin down parts of the s-o eigenvectors (to be used in
 s-o version of LAPW2)
- 46,'ni.normup', 'unknown','formatted',0
 output: norms of spin up parts of the s-o eigenvectors (to be used in
 s-o version of LAPW2)
- 47,'ni.norm', 'unknown','formatted',0
 output: norms of spin up and spin down parts as well as complete norms
 of the s-o eigenvectors

4.2 Description of input data for LAPWSO

The input data (case.inso) are:

WFFIL			FORMAT(A5)	mode of calculation
4 0 0 0			FORMAT(4I3)	LLMAX, icmplx, ipr, kpot
-10.0000	10.0000	2.0000	FORMAT(3F10.3)	EMM(1),EMM(2),EMM(3)
90.	0.		FORMAT(2F10.3)	theta, phi

- 1st line

mode of calculation, if equal to WFFIL s-o eigenvectors are calculated else only eigenvalues

- 2nd line

LLMAX - maximum L for wavefunctions in atomic spheres
 icmplx if =1 eigenvectors on input (files .vector) are complex
 else eigenvectors on input are real}
 ipr print parameter: the larger ipr, the longer output.
 kpot - if=0 potential is not averaged when calculating dV/dr
 =1 potential is averaged (see also below).

- 3rd line

EMM(1) minimum energy for which the eigenvectors on input will
 be considered (Ry)
 EMM(2) maximum energy for which the eigenvectors on input will
 be considered (Ry)
 EMM(3) s-o matrix elements will be calculated for states, energy

of which differ by less than EMM(3).

- 4th line

theta azimuthal angle of magnetization
phi polar angle of magnetization

4th line is relevant only if the calculation is spin-polarized

When calculating dV/dr (necessary for s-o) V_{\downarrow} potential was used for $\langle \downarrow |V| \downarrow \rangle$ elements, V_{\uparrow} for $\langle \uparrow |V| \uparrow \rangle$ and $[V_{\downarrow} + V_{\uparrow}]/2$ for $\langle \uparrow |V| \downarrow \rangle$. This is difficult to justify. Therefore LAPWSO was modified - switch KPOT makes possible to calculate these elements with averaged potential (KPOT=1, if KPOT=0 potential is not averaged). For YCo₅ KPOT=1 and KPOT=0 give virtually identical results, however.

4.3 Parameters in LAPWSO

LMAX is maximum value of the orbital momentum in atomic spheres. LABC gives maximum L for wave functions in atomic spheres used when calculating the spin-orbit coupling. LABC must be greater or equal LMMAX read in data (LABC.ge.LMMAX is controlled in INIT).

Otherwise meaning of the parameters is the same as in LAPW1, LAPW2

```
c
c   Constant parameter definition
c
      INTEGER      LMAX,  NATO, NDIF, NUME,  NMAT,  NRAD
      INTEGER      LOMAX, FLMAX, LABC,  LABC2
      INTEGER      LMX,   MMAX, NUME2
c
      PARAMETER (LMAX=   12)
      PARAMETER      (NATO=   6)
      PARAMETER      (NDIF=  12)
      PARAMETER      (NUME= 124)
      PARAMETER      (NMAT= 792)
      PARAMETER (NRAD=  881)
c LOMAX must be = LOMAX in LAPW1 otherwise conflict in INIT
      PARAMETER (LOMAX=   2)
      PARAMETER (FLMAX=   3)
c LMX (not LMAX!) must be = LMAX in LAPW1 otherwise conflict in INIT
      PARAMETER (LMX=   LMAX+1)
      PARAMETER (LABC =    4)
      PARAMETER (LABC2= (LABC+1)*(LABC+1))
      PARAMETER (MMAX= 2*LMAX+1)
      PARAMETER (NUME2= 2*NUME)
      PARAMETER (NUM2= NUME2*(NUME2+1)/2)
```


4.4 Using LAPWSO

In non-magnetic systems the inclusion of the spin-orbit coupling does not lead to lowering of the symmetry. Using LAPWSO is then simple, the only complication being that s-o eigenvectors are in general complex. This must be taken into account when calculating the density (LAPW2c, not LAPW2 must be used).

In magnetic systems the inclusion of s-o coupling generally leads to the lowering of symmetry. If $\vec{M} \parallel \vec{\zeta}$ then the symmetry group \mathcal{G}_{so} of the system with s-o coupling is given by:

$$\mathcal{G}_{so} = \mathcal{G} \cap D_{\infty}(\vec{\zeta}) \quad (31)$$

where \mathcal{G} is the group without the s-o coupling. In special cases (hexagonal or tetragonal symmetry, $\vec{M} \parallel c$) $\mathcal{G} \equiv \mathcal{G}_{so}$. In most cases, however, simultaneous presence of \vec{m} and spin-orbit coupling reduces the symmetry. The reduction has the following consequences:

- number of the symmetry operations is reduced (change of case.struct file).
- Irreducible wedge of the Brillouin zone must be enlarged (files case.klist, case.kgen have to be changed).
- The atoms which were equivalent in nonmagnetic system may become nonequivalent, their local co-ordination system may be changed (change of case.struct and inputs to LSTART, LAPW1, LAPW2, LCORE).
- Reduction of the local symmetry results in increase of the components of non-spherical potential (change of input to LAPW2).

In order to ease writing the structure and input files, the following way, which imitates the effect of the symmetry lowering caused by simultaneous presence of the s-o coupling and \vec{M} may be used:

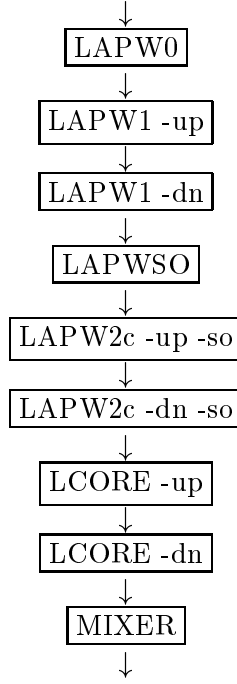
1. From each atom in the struct file make a dumbbell. Axis of the dumbbell is along $\vec{\zeta} \parallel \vec{M}$ and its center lies in the original position of the atom (to do it the atom multiplicity must be doubled).
2. Run the NN program and use the structure file, which this program creates.
3. Create the input files in a normal way by running SYMMETRY, LSTART and KGEN.
4. Reverse step 1/ (from the dumbbels created in the first step make the atoms).

Still easier way exists if s-o coupling is not taken into account selfconsistently (in many cases this may be a good approximation because of relative smallness of H_{so} and because of the force theorem). Then:

1. perform normal selfconsistent calculation without s-o coupling with original (high symmetry) structure file.

2. Prepare klist and kgen files corresponding to situation when the symmetry is lowered by combined presence of the s-o and \vec{M} as described above.
3. Run LAPW1, LAPW2, LAPWSO, LAPW2c with the new klist, kgen files and original (symmetrical) struct file.

A block scheme of the WIEN iteration (spin-polarized calculation) with LAPWSO included looks as follows:



In the non spin-polarized calculations LAPW1, LAPW2c and LCORE are run - as usual - only once.

5 Calculation of average values

Often we are interested in an average value of an operator \hat{X} taken in space of $H = H_D + H_{so}$ eigenfunctions, where \hat{X} is - similarly as H_{so} - zero in the interstitial and it can be expressed as a product:

$$\hat{X} = \hat{X}_r(r)\hat{X}_{ls}(\vec{l}, \vec{s}) \quad (32)$$

Average value of \hat{X} may be expressed as a weighted sum over irreducible k points \vec{k}_j :

$$\langle \hat{X} \rangle = \sum_{j,n} X_n(\vec{k}_j)w_{n,j} \quad (33)$$

where

$$X_n(\vec{k}_j) = \langle \psi_{n,j}^{so} | \hat{X} | \psi_{n,j}^{so} \rangle \quad (34)$$

$\psi_{n,j}^{so}$ being the eigenfunctions calculated in LAPWSO. The weights $w_{n,j}$ are produced in LAPW2, $w_{n,j} = 0$ for $E_{n,j} > E_F$. The calculation of $\langle \hat{X} \rangle$ is performed by the package AVERX which is very similar to LAPWSO. In particular the parameters needed by AVERX are the same as those needed by LAPWSO. Of course the form of $\hat{X}_r(r)\hat{X}_{ls}(\vec{l}, \vec{s})$ must be specified. This is done in the data file:

```

WFFIL                                FORMAT(A5)   mode of calculation
4  0  1  3                            FORMAT(4I3) LLMAX, icmplx, RINDEX,LSINDEX
-10.0000   10.0000   2.0000  FORMAT(3F10.3) EMM(1),EMM(2),EMM(3)
90.         0.         FORMAT(2F10.3) theta, phi

```

where first, third and fourth lines are the same as for LAPWSO, RINDEX and LSINDEX in the second line determine the form of $\hat{X}_r(r)$ and $\hat{X}_{ls}(\vec{l}, \vec{s})$, respectively, in the following way:

- RINDEX=1 LSINDEX=1: $\langle X \rangle$ is number of electrons inside the atomic sphere (for test)
- RINDEX=2 LSINDEX=1: $\langle X \rangle$ is the $\langle 1/r^3 \rangle$ expectation value inside the atomic sphere
- RINDEX=1 LSINDEX=2: $\langle X \rangle$ is the projection of the spin moment inside the atomic sphere
- RINDEX=1 LSINDEX=3: $\langle X \rangle$ is the projection of the orbital moment inside the atomic sphere
- RINDEX=3 LSINDEX=3: $\langle X \rangle$ is the orbital part of the hyperfine field at the nucleus
- RINDEX=3 LSINDEX=5: $\langle X \rangle$ is the spin dipolar part of the hyperfine field at the nucleus

The files needed by AVERX are:

```

5 , 'ni.inaverx', 'old', 'formatted', 0
6 , 'ni.outputaverx', 'unknown', 'formatted', 0
8 , 'ni.scfaverx', 'unknown', 'formatted', 0
9 , 'ni.vectordn', 'old', 'unformatted', 9000
10 , 'ni.vectorup', 'old', 'unformatted', 9000
16 , 'ni.weightaversoup', 'old', 'formatted', 0
18 , 'ni.vspdn', 'old', 'formatted', 0
19 , 'ni.vspup', 'old', 'formatted', 0
20 , 'ni.struct', 'old', 'formatted', 0
26 , 'ni.weightaverdn', 'unknown', 'formatted', 0
27 , 'ni.weightaverup', 'unknown', 'formatted', 0
41 , 'ni.vectorsodn', 'unknown', 'unformatted', 9000
42 , 'ni.vectorsoup', 'unknown', 'unformatted', 9000
43 , 'ni.vectordum', 'unknown', 'unformatted', 9000
44 , 'ni.vect1', 'unknown', 'unformatted', 9000

```

File 16 contains the weights of spin-orbit eigenstates needed for the calculation of $\langle \hat{X} \rangle$ (33). Files 26, 27 contains analogous weights for down and up spin eigenstates without the spin-orbit. Depending on whether files 26, 27 are present AVERX calculates (or does not calculate) $\langle \hat{X} \rangle$ also without the spin-orbit coupling included. Other files have the same or analogous meaning as for the LAPWSO package.

6 Examples

6.1 Nonmagnetic - fcc Au

The lattice constant of Au is 7.67 a.u., radius of Au sphere is taken to be 2.6 a.u., standard input data (created by init_lapw) are used except: RKMAX=9, additional d-local orbital at 0.2 and 1.0 Ry, E-window up to 4.5 Ry, GMAX=16. We used 5000 k-points in the Brillouin zone. The au.scfso file after a convergency with the s-o coupling was achieved is:

```

0.0  0.0 angle (M,z), angle (M,x) deg

      SPIN-ORBIT EIGENVALUES:
K=    0.00000  0.00000  0.00000          1
MATRIX SIZE=  73  WEIGHT= 1.00
EIGENVALUES ARE:
-4.1857424  -4.1857424  -3.1319008  -3.1319008  -3.1319008
-3.1319008  -0.0605514  -0.0605514   0.2945419   0.2945419
 0.2945419   0.2945419   0.3814021   0.3814021   0.4757839
 0.4757839   0.4757839   0.4757839   1.7500980   1.7500980
 2.0096272   2.0096272   2.0693398   2.0693398   2.0693398
 2.0693398   2.4256490   2.4256490   2.7456123   2.7456123
 2.7456123   2.7456123   2.7710097   2.7710097   2.7985568
 2.7985568   3.0175067   3.0175067   3.0175067   3.0175067

      3.4422934   3.4422934   3.4422934   3.4422934   4.0296281
      4.0296281   4.3764583   4.3764583   4.3778301   4.3778301
      4.3778301   4.3778301

*****
NUMBER OF K-POINTS:          165

```

In Table 1 some of the results are listed and compared with an older calculation. Note the splitting between Γ_8 and Γ_7 levels which appears due to the presence of the spin-orbit coupling.

6.2 Magnetic - hcp Co

Calculations were made for lattice parameters $a = 4.7375$ a.u., $c = 7.6893$ a.u., atomic sphere radius 2.12 a.u and the standard WIEN input, with exception of mixing pa-

	no s-o	s-o nonscf	s-o scf	ASW
$\varepsilon(\Gamma_8)$	-357	-409	-410	-418
$\varepsilon(\Gamma_7)$	-357	-322	-323	-323
$\varepsilon(\Gamma'_8)$	-241	-230	-230	-244
$E_{tot} - E_0$	-853	-885	-885	

Table 1: fcc Au. $5d$ eigenvalues at the Γ point with respect to E_F and the total energy E_{tot} ($E_0 = -38095$ Ry). All values are in mRy. The ASW results are taken from : T.Takeda, J.Phys. F: Met. Phys. **10** (1980) 1135.

parameter (co.inm), which was reduced to 0.08. 1000 k points in the Brillouin zone was considered. The calculations are not fully converged.

$\vec{M} \parallel c$ In this case the symmetry is not lowered by spin-orbit coupling. The calculation with s-o may thus directly follow after usual spin-polarized calculation. Some of the results are given in Table 2.

$\vec{M} \parallel a$ Presence of the spin-orbit couplings reduces the number of symmetry operations from 24 to 8. After changing klist and kgen files the non-selfconsistent calculation may be performed. Selfconsistent calculation must be started from the scratch. The results are again given in Table 2. If the calculations were fully converged and the number of k points sufficient, the difference of energies for $\vec{M} \parallel c$ and $\vec{M} \parallel a$ would give (after the simple correction for the lattice contribution) the magnetocrystalline anisotropy. In this test example the number of k -points is by far too small, however, and the calculations are not properly converged.

calc.	$\vec{\zeta}$	spin moment (μ_B)	orb. moment (μ_B)	$E_{tot} - E_0$ (mRy)
no s-o	-	1.679	-	-893.06(2)
s-o non-scf	c	1.679	0.088	-893.81(2)
s-o scf	c	1.712	0.090	-893.86(2)
s-o non-scf	a	1.687	0.080	-893.78(2)
s-o scf	a	1.710	0.081	-893.76(2)
Daalderop*	c	1.61	0.085	?

Table 2: hcp Co. Spin, orbital magnetic moments and the total energy E_{tot} ($E_0 = -5573$ Ry). * G.H.O. Daalderop et al.. Phys. Rev. **B 41** (1990) 11919. 1135.

7 Other spin-orbit - like operators

During the last few years numerous attempts appeared to improve the local spin density functional formalism by adding extra terms to the Hamiltonian - this concerns especially the situation when the electron - electron correlation is important and the valence

electron density is strongly inhomogeneous (e.g. compounds containing actinides or rare-earth elements). The success of these attempts is in many cases spectacular, though the strict justification of the methods is lacking. In at least two cases: 'Orbital polarization' and the 'LDA + U ' methods, the extra terms added have analogous form as the spin-orbit coupling discussed above and they may be treated in a similar way.

We will discuss the orbital polarization, which imitates the 2nd Hund's rule, it may be at least partially justified and corresponding package (LAPWOP) is already available.