Hilbert++ Manual

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Abstract

We present here an installation guide, a hand-on mini-tutorial through examples, and the theoretical foundations of the Hilbert++ code.

1 INSTALLATION

The code is provided in both source and binary forms. The binaries are meant to run under the Linux-i386 system. The distribution package is composed of two archives. The first one (let’s call it installation archive) which provides all the necessary libraries that Hilbert++ needs, and a second one, Hilbert++ itself, which comprises sources, binaries, and examples.

Hilbert++ loads dynamically the libraries of the installation archive and does not depend on which Linux-packages are installed on your system with the exception of libc and libX11. As these libraries are quite stable one should be able to run Hilbert++ on any Linux system without recompiling it.

The current installation archive and the Hilbert++ packages can be retrieved from these addresses: [http://ftp.esrf.fr/pub/scisoft/ESRF_sw/scisoft_ESRF_sw_linuxi386_03.tar.gz](http://ftp.esrf.fr/pub/scisoft/ESRF_sw/scisoft_ESRF_sw_linuxi386_03.tar.gz) and [http://ftp.esrf.fr/pub/scisoft/ESRF_sw/linux_i386_03/hilbertxx.tar.gz](http://ftp.esrf.fr/pub/scisoft/ESRF_sw/linux_i386_03/hilbertxx.tar.gz) respectively.

The installation archive must be untarred using the following commands

```
cd /
tar -xzvf yourdownloaddirectory/scisoft_ESRF_sw_linuxi386_03.tar.gz
```
this creates the directory /scisoft/ESRF_sw/linux_i386_03/.

The hilbertxx directory can be untarred from any directory with the command:

```
cd <whereeever>
tar -xzvf yourdownloaddirectory/hilbertxx.tar.gz
```

2 Hand on mini-tutorial by examples

To launch the program you go to hilbertxx/examples/exa_class, where class corresponds to an example class. The example classes provided so far are:
Ex. a) \textit{class}=2p3d for L2-L3 spectroscopy

Ex. b) \textit{class}=rixs for 1s-3p RIXS spectroscopy, with a 3d resonant intermediate state, in transition metal oxides.

Ex. c) \textit{class}=df for dipolar $d$ to $f$ transitions.

You choose an example system by moving to one of the subdirectories. For instance

\texttt{cd hilbertxx/examples/exa_2p3d/Mn3+/

Once you are in the exa\texttt{class/system} directory you start the application by running the Python script:

\texttt{../runthisscript}

You get a command line prompt:

\texttt{>>>}

and you can get some help by typing

\texttt{>>>help()}

The help function prints some brief instructions for every Hilbert++-command (hxx-command). A hxx-command is always one line long and writing it does not require any knowledge of Python. The advanced user can write Python scripts. We explain for each example the available commands

\subsection{The 2p3d examples class}

\subsubsection{Mn3+}

\texttt{cd} to the appropriate directory

\texttt{cd hilbertxx/examples/exa_2p3d/Mn3+/

and start the script

\texttt{../runthisscript}

You get now a Python prompt. You can type several commands. In this manual we are going to explain all the commands. The command \texttt{help()} which produces the following list of available commands:

\begin{verbatim}
AVAILABLE HXX-COMMANDS ( examples of )
set(system)  # or use directly python syntax to change the attributes of object system.
# When using the set(system) function you can also give a filename of a previously saved ( and edited ) file
save(system)  # You are asked a filename and you have to quote it like "filename"
scriviFiles(5, prefix="datas", nhopped=0)  # To generate matrices files. This command creates the Hilbert space
# and writes the terms composing the Hamiltonian into (sub)directory "datas" which must exist.
# The above example generates a Hilbert space where 5 electrons are distributed in the 3d
\end{verbatim}
# shell in all possible combinations.  
# Giving nhopped=n as argument, besides the configurations with 5 electrons on 3d also the configurations  
# with 5+i electrons on 3d and 10-i on Ligands orbitals are considered ( 0<=i<=nhopped )

system.case="datas"  # This chooses the system that you have expanded with scriverFiles command.    
# You can access this property also with the set(system) command

res=system.GetSpectrum()  # to calculate a spectrum. res is a list. res[0] is an array of floats : the energies.  
# res[i>=1] are the resonances ( real and imaginary part). Dipolar transitions are calculated as  
# res[1], where i=1,2,3 and Mz= -1,0,1

res=system.GetSpectrum([ fm1,f0,f1 ])  # Absorption (it is res[1].imag) for a definite polarisation.  
# fm1,f0,f1 are three coefficients.  
# They can be complex. So you can define any polarisation :  
# For Z polarisation [ fm1,f0,f1 ] = [ 0, 1, 0]  
# For X polarisation [ fm1,f0,f1 ] = [ -1/sqrt(2.0) , 0 ,1/sqrt(2.0)]  
# For Y polarisation [ fm1,f0,f1 ] = [ 1.0j /sqrt(2.0) , 0 ,1.0j/sqrt(2.0)]  
# ..... and so on

write(res,filename)  # To save res on a file  
# and the file will have several columns ( 1 for energies and two (real, imag) for each polarisation)

Plot(Curve(res[0], res[n>=1].imag, Pen(Red), "legend"))  # To plot. Change n to select the polarisation that you want  
# The plotting feature uses qt, iqt and qwt. If you run a long job in the background you must  
# desactivate this graphics feature by commenting out, in the file init.py, the lines where such packages  
# are imported

Es, S2s, L2s, SL2, occPs , Szs, Lzs= system.GetESLcounters()  # to get statistics: a list of E, the list of 3d L2 ,  
# the list of 3d S2, the list of 3d SL, a list of ligand expected occupation, a list of 3d Sz expectation

The system is represented by the Python variable system. Such a variable is an object and its properties are the parameters. There are several ways to change such properties. One is to use the set(system) command. This command prints the list of parameters :

```python
d>>> set(system)
-- BASE HAMILTONIAN --
1) base_couche1_F0 : 5.0
2) base_couche1_F2 : 12.456828106
3) base_couche1_F4 : 7.81967819912
4) base_couche0_1_F0 : 5.5
5) base_couche0_1_F2 : 6.86721502072
6) base_couche0_1_G1 : 5.02109490016
7) base_couche0_1_G3 : 2.65321756768
8) base_SO_0 : 6.568603656
9) base_SO_1 : 0.05238772
10) base_Sop_Zero : 0.0
11) base_Sop_Minus : 0.0
12) base_Sop_Plus : 0.0
13) base_counterDL : -4
-- EXCITED HAMILTONIAN --
14) exci_couche1_F0 : 5.0
15) exci_couche1_F2 : 13.1769752072
16) exci_couche1_F4 : 8.299507532
17) exci_couche0_1_F0 : 5.5
18) exci_couche0_1_F2 : 7.6574518
19) exci_couche0_1_G1 : 5.77390099368
20) exci_couche0_1_G3 : 3.28715525784
21) exci_SO_0 : 6.845918392
22) exci_SO_1 : 0.066403136
23) exci_Sop_Zero : 0.0
24) exci_Sop_Minus : 0.0
25) exci_Sop_Plus : 0.0
26) exci_counterDL : -4
-- CALCULATION PARAMETERS --
```
To change a parameter, one enters the corresponding number and then the new value. If, instead of a number, one enters a file-name like "paramfile" of a previously saved parameter file (the quotes are important), then that file will be loaded. Such a file can be edited with any text editor.

All energies are given in eV and all distances in Angstrom. The parameters can be divided in three blocks. The first two are atomic Hamiltonian parameters for the base and excited configurations respectively. The first seven atomic parameters are Slater integrals: three (F0,F2,F4) for the d-d interaction (couch1), and four for the interaction between the 2p shell and the 3d one (couch0_1). The parameter SO_n is the spin-orbit interaction for the n^{th} shell (in this example 0 is 2p and 1 means 3d). The one-particle energy of the orbitals is not given in input. Therefore the absolute energy scale of the spectra is arbitrary.

The parameters Sop_Zero, Sop_Minus, Sop_Plus are the three components of an external exchange field acting on the 3d shell. They multiply the three components of the 3d spin operator S_z, S_{-1}, S_{+1}. These factors can be real or complex. Finally the parameter counterDL is an energy which multiplies the number of electrons on the Oxygen orbitals.

The block called CALCULATION PARAMETERS contains other interesting parameters. We start discussing the last ten: Vs, Vp, VC0, VC1, DREF, ALPHAVC, ALPHAVSP, BONDS, factorhopexci, facts_hop. These parameters are relevant for the Hamiltonian. They describe hybridisation and crystal field.

The hybridisation of the 3d shell with the Oxygen 2p orbitals is described by the Slater-Koster parameters Vs and Vp for \( \sigma = 3z^2 - r^2 \) and \( \pi = \tilde{x}\tilde{z}, \tilde{y}\tilde{z} \) orbitals, where \( \tilde{z} \) is aligned along the bond direction. The hybridisation term
is summed over all the bonds given by the \textit{BONDS} variable. The Slater-Koster parameters are rescaled as \((R_{bond}/DREF)^{ALPHA_{AV}SP}\) where \(R_{bond}\) is the bond length.

The parameters \(VC0\) and \(VC1\) work in a similar way and describe the crystal field. They are the energy shifts for \(\sigma\) and \(\pi\) orbitals, respectively, assuming that \(\tilde{z}\) is aligned along the bond direction. The scaling factor is \((R_{bond}/DREF)^{ALPHA_{AVC}}\).

The other parameters are described here:

P) \textit{case} : the directory where the Hilbert space has been generated by the \textit{scriviFiles} command.

P) \textit{reduc}_{1} : the usual Slater integral reduction factor for \(3d\) shell

P) \textit{reduc}_{0,1} : reduction factor for \(2p - 3d\) Slater integrals.

P) \textit{all1} : Lorentzian broadening before \textit{El2l3}

P) \textit{El2l3} : an energy between \textit{L2} and \textit{L3}.

P) \textit{all2} : broadening after \textit{El2l3}

P) \textit{shift} : an energy shift.

P) \textit{npunti} : number of points in the spectrum.

P) \textit{dxleft} : the spectrum is calculated from \textit{dxleft}.

P) \textit{dxright} : .... to \textit{dxright}

P) \textit{temp} : when several ground state eigenvectors are calculated they are Boltzmann averaged with a Temperature=\textit{temp}.

P) \textit{erange} : the lowest energy ground-states are calculated which are within an energy range= \textit{erange}. The smaller the \textit{erange}, the faster will be the calculation since less ground states are considered.

P) \textit{tolefact} : The ground states having Boltzmanian weight less than \textit{tolefact} are neglected

P) \textit{shift}_{\text{~invert}} : not used.

P) \textit{nsearchedeigen} : The Lanczos diagonalisation of the ground state Hamiltonian searches for \textit{nsearchedeigen} eigenvectors. (the smaller this number the faster the calculation)

P) \textit{NstepsTridiag} : dimension of the tridiagonalised matrix used for calculating the spectra.
When the program is started, the system parameters are initialised with default values. If two files named `out36_base` and `out36_exci` are found in the working directory, the Slater integrals and the spin-orbit-coupling are searched for in such files. These files are not mandatory. If they are not there you will have to input the entries by hand.

The `out36` files are the output as from the Cowan’s Rcn program. Hilbertxx comes with a GUI which allows to run Rcn and generate the `out36` file. To run the GUI, from the working directory:

```bash
hilbertxx_directory/cowan/cowan in36
```

There is a short help for every RCN parameter. You can play with the parameters and create the `out36` files that you need.

The examples are already provided with the related `out36` files, so you need to run RCN only for the cases you want to study.

To run a simulation you must first create a directory with the Hamiltonian components in the Hilbert space. Let’s call it HCD (hamiltonian components directory). You obtain this by the command `scriviFiles`. When you run `../runthisscript`, and your working directory has subdirectory name `datas`, write the command:

```python
scriviFiles(4,prefix="datas", nhopped=2)
```

the first argument is the minimum occupation number for the 3d shell. Such command creates a Hilbert space for the base system and another for the excited system. The base space spans all the configurations having 4, 5 and 6 electrons on the 3d shell. The excited space spans those having 5, 6 and 7 electrons on 3d and 5 on the Mn 2p shell. The number of electrons on the Oxygen 2p orbitals can be either 10 or 9 or 8 and the total number of electrons is conserved.

The program considers only those Oxygen orbitals that are obtained projecting the 3d orbitals through the hopping operator.

When the HCD has been populated with files created by the above command, you are ready to calculate a spectrum. The HCD needs to be created only once, and then you can play with parameters.

In the example directory there is already a file with parameters which correspond to a case with strong hybridisation. Such a file is named `paramn` and can be loaded using the `set(system)` command.

To calculate a spectrum:

```python
res=system.GetSpectrum()
```

and to plot the isotropic absorption

```python
Plot(Curve(res[0], (res[1]+res[2]+res[3]).imag, Pen(Red), "legend"))
```

Several expectation values can be calculated with the following commands

```python
Es, S2s, L2s, SL2, occPs, Szs, Lzs= system.GetESLcounters()
```
Each variable $E_s, S_2 s, L_2 s, \text{occPs }, S_z s, L_z s$ is a list of expectation values of a given operator. There is an expectation value for each calculated ground eigenvector. The operators are energy, $S.S, L.L, 2S.L$, the occupation of the ligand orbitals, $S_z, L_z$. The angular operators are restricted to the 3d shell.

2.2 The RIXS examples class

The directory `hilbertxx/examples/extra/rixs/` contains the code to calculate the 1s-3p RIXS.

2.2.1 Mn3+

As in the previous example, you run the command

```
../runthisscript
```

from the example directory `hilbertxx/examples/extra/rixs/Mn3+`. You get a summary of the available commands by entering `help()`. You can calculate 1s-3d absorption spectra, as in the previous example, and RIXS. The absorption can be calculated either for the quadrupolar or for the dipolar interaction. The dipolar absorption can be calculated for centrosymmetric systems. To do this the program calculates a dipolar transition to a virtual 4p state which is projected through an hybridisation operator onto the Oxygen orbitals. The command to get the dipolar absorption is the same as for the previous example:

```
res=system.GetSpectrum()
```

The quadrupolar absorption can be calculated for a defined polarisation. You define the polarisation giving its 5 components on a L=2 basis.

```
res=system.GetSpectrum([-fm2, fm1,f0,f1, fp2 ])
```

where fm2, fm1,f0,f1, fp2 are the five polarisation coefficients in the angular momentum representation. For example for xy polarisation $[-fm2, fm1,f0,f1, fp2 ] = [1,0,0,0,-1]$ while for calculating x2y2 $[-fm2, fm1,f0,f1, fp2 ] = [1,0,0,0,1]$.

The `scriviFiles` command has one more argument `spinfixed`. It defaults to zero (no spin constraint). If it is set to one, the Hilbert space is generated under the constraint of a fixed total spin $S_z$. This has in general little effect on the absorption spectrum because the spin-orbit coupling is small in the 3d shell and the calculation is faster.

The use of the `set(system)` command is the same as in the previous example. The difference is that there are some more parameters for the final state (for RIXS) and some more for the 4p-Oxygen hybridisation which is used to calculate the dipolar 1s-3d transition. The latter parameters are `Dips`, `Dipp`, which are the Slater-Koster $\sigma$ and $\pi$ parameters for 4p-2p hybridisation, and `ALPHADIPO`, which is the analogous of `ALPHAVSP`. 

7
A parameter file is provided for the study case of Mn: “paramnH”. The calculation must be run in the Hilbert space created with the following command:

```
scriviFiles(4, prefix="datas", nhopped=2, spinfixed=1)
```

The studied ion is in a non-centrosymmetric position and we can calculate both quadrupolar and dipolar absorption. The following commands:

```python
resx2y2 = system.GetSpectrum([ 1.0 , 0.0 , 0 , 0 , 1.0 ])
resyz = system.GetSpectrum([ 0.0 , 1.0 , 0 , 1.0 , 0 ])
resdip = system.GetSpectrum()
```

allow to compute the absorption spectra for $x^2 - y^2$, $yz$ and dipolar polarisation respectively.

You can compare the polarisation dependence of the quadrupolar absorption:

```python
Plot(Curve(resx2y2[0], resx2y2[1].imag, Pen(Red), "x2y2"),
     Curve(resyz[0], resyz[1].imag, Pen(), "yz"))
```

and you can plot a dipolar isotropic spectrum:

```python
Plot(Curve(resdip[0], (resdip[1]+resdip[2]+resdip[3]).imag, Pen(Red), "dipole"))
```

Now you can calculate a RIXS spectrum:

```
res = system.GetRIXS( polarisationIn=[0.0, 1.0,0.0, 1.0,0.0] , polarisationOut=[1.0,0.0],
                      ein=26.43, eout1=630, eout2=790, dout=0.1, gammain=0.2,
                      gammaout= [ 0.5 , 20 , 1.0 ])
```

where the energy is tuned to the first absorption peak. The RIXS calculation is performed considering only one ground state, the lowest one regardless of the temperature and erange parameter.

### 2.3 The df examples class

The directory hilbertxx/examples/exa_df/ contains the code to calculate dipolar $d$ to $f$ transitions. This example considers a crystal field on the f shell but not hybridisation.

#### 2.3.1 Ho

This example is very similar to the pd case. The only difference is that there are three parameters for the crystal field and no hybridisation.
3 Description of the code

The low level objects are coded in C++ and wrapped in Python. The description of the system and the manipulation of basic objects are done in Python.

There are two levels of use of Hilbert++: the developer level and the user level.

At the user level one uses a command line interface which allows to manipulate the parameters of an already defined system.

At the developer level one can create new systems by doing some scriptic programming in Python.

The Hilbert space is spanned by a set of second quantisation base vectors:

\[ e = c_1^+ c_2^+ \ldots c_l^+ |0\rangle \]

The code represents a base vector by a C++ object eo. This object contains two chains of bits: eo.val and eo.signs. The \( i^{th} \) bit of eo.val is equal to the occupancy of the \( i^{th} \) one-particle state (1 or 0). The eo.sign chain of bits is used to keep track of fermionic statistics and is the integral modulus 2 of eo.val.

If, for example, \( c.val = 00010010 \ldots \) then \( c.signs = 00001110 \ldots \).

The creation and annihilation operators are represented under the form of one particle base vectors: they are represented by a base vector co whose co.val has only one bit set to one: i.e. the bit corresponding to the particle state. A co creation operator acts on a base state in the following way: first the “AND” bitwise operation is applied to co.val and eo.val. When the one particle state is already occupied in the vector eo the “AND” operator gives a non-zero bit string and the result is set to zero. Otherwise the result is a new vector reso multiplicated by a ±1 factor. The vector reso is composed by a reso.val which is obtained by the “OR” bitwise operation on co.val and eo.val. The signs strings reso.signs is the result of the “XOR” operation on co.signs and eo.signs. The multiplicative factor is +1 if \((co.val \text{ AND } eo.signs) = 0\), otherwise it is −1.

Starting from these basic objects (base vectors and creation/annihilation operators), the generic operators and vectors are constructed. An operator is in general a linear combination of creation/annihilation operators or their products. A vector is a linear combination of base vectors.

The generation of a Hilbert space starts from a seed basis, which is a basis formed by one or a few base vectors, and a wanderer, i.e. an operator which, operating on the basis, creates new basis vectors. The wanderer is applied several times on the basis, making it grow until no new base vectors are found.

The ground state space spans all the configurations having 4, 5 and 6 electrons on the 3d shell. The excited state one spans those having 5, 6 and 7 electron on 3d and 5 on the Mn 2p shell. The number of electrons on the Oxygen 2p orbitals varies in order to conserve the total number of electrons.

The number of Oxygen orbitals is in principle \(6N_b\) where \(N_b\) is the number of bonds. As in the above model Hamiltonian the Oxygen orbitals are degenerated, one can arbitrarily chose a rotated basis for the Oxygen one-particle wavefunctions. The basis that we choose is such that the first 10 basis vectors
are obtained projecting the 3d space on the oxygen orbitals through the hopping operator and applying a Gramm-Schmidt orthonormalization. The remaining vectors span a space that is not related to this problem and are neglected.

For an absorption study two Hilbert spaces are expanded, one for the ground configurations, and another for the excited ones. The different components of the Hamiltonian are calculated separately and written in files, in the form of sparse matrices.

This is done writing a Hamiltonian component (kinetic energy, electron-electron interactions, spin-orbit coupling, etc... ) as a generic operator. This operator is subsequently applied to every basis vector \(i\) of the considered Hilbert space. The result is a linear combination of a small number of basis vectors to which the vector \(i\) is connected through the operator.

The sparse matrix, representing the operator, is a sequence of triples \((j, i, c_{ji})\) where \(i\) and \(j\) are two connected basis vector indices and \(c_{ji}\) is the matrix element. The total Hamiltonian is built as a linear combination of its components. The dipolar and quadrupolar operators connecting the Hilbert spaces between each other are represented as space matrices as well.

To calculate absorption and RIXS spectra one needs to compute eigenvectors and the respective eigenvalues:

\[
HX_n = \lambda_n X_n
\]

spectra:

\[
\langle X | \frac{1}{\omega - H + i\gamma} | X \rangle
\]

inversion

\[
\frac{1}{\omega - H + i\gamma} | X \rangle
\]

To do this, one just needs to apply the Lanczos algorithm and the conjugate-gradient method, which are based on the simple multiplication

\[
y = Hx
\]

We have implemented the Lanczos algorithm with thick restart from Kesheng Wu & Horst Simon [1]. The absorption is obtained finding first the ground eigenvectors \(X_n\) via the Lanczos method. The vector \(DX_n\), where \(D\) is the dipolar (or quadrupolar) operator is then calculated in the excited Hilbert space. This vector is taken as an initial vector at the zero-th step of the Lanczos tridiagonalisation procedure. A large enough number \(N\) of steps is performed to generate the diagonal \(\alpha_i\) \((0 \leq i \leq N)\) and off diagonal \(\beta_j\) \((1 \leq i \leq N)\) elements. The resonance amplitude is then given by the following continued fraction:

\[
\frac{1}{\omega + i\gamma - \alpha_0 - \frac{\beta_1^2}{\omega + i\gamma - \alpha_1 - \frac{\beta_2^2}{\omega + i\gamma - \alpha_2 - \frac{\beta_3^2}{\omega + i\gamma - \alpha_3 - \cdots}}}}
\]

The imaginary part of the above expression is proportional to the absorption.
The RIXS signal is calculated in a similar way and one takes at the first step of the tridiagonalisation procedure, the vector

$$D_{\text{out}} \frac{1}{\omega_{in} - H + i\gamma} |D_{\text{in}}X_n\rangle$$

where $D_{\text{in}}$ and $D_{\text{out}}$ are the dipolar (or quadrupolar) operators for the incoming and outgoing photons, respectively.

4 Details on the hybridisation components of the Hamiltonian

We consider a metal ion surrounded by Oxygen atoms. The total Hamiltonian is:

$$H = H_{\text{ato}} + \sum_b (t_{\sigma,b} d^+_3 \tilde{z}^2 p_\tilde{z} + t_{\pi,b} (d^+_3 \tilde{z} p_\tilde{z} + d^+_3 \tilde{y} p_\tilde{y}) + C.C.) + \epsilon_p \sum_b (p^+_\tilde{x} p_\tilde{x} + p^+_\tilde{y} p_\tilde{y} + p^+_\tilde{z} p_\tilde{z}) + \sum_b (V_{\sigma,b} d^+_3 \tilde{z}^2 d^+_3 \tilde{z}^2 + V_{\pi,b} (d^+_3 \tilde{z} d^+_3 \tilde{z} + d^+_3 \tilde{y} d^+_3 \tilde{y}))$$

In this expression $H_{\text{ato}}$ is the atomic Hamiltonian. The sum $\sum_b$ runs over the metal-oxygen bonds $b$ and the $\tilde{z}$ axis is aligned along the bond direction. For d metals the hopping is expressed as a function of the Slater-Koster parameters $t_{\sigma}$, $t_{\pi}$ which are rescaled according to the bond length. For the same metals the electrostatic crystal field is described in terms of the parameter $V_{\sigma}$ which is the energy shift of the $3\tilde{z}^2 - \tilde{r}^2$ orbital, and of $V_{\pi}$ which is the energy shift of the $\tilde{x}\tilde{z}$ and $\tilde{y}\tilde{z}$ orbitals. The crystal field parameters are rescaled accordingly. The sum over the spin is omitted in the above formulae for conciseness. As to the df case there is one more the crystal field parameter: in total there are three parameters VC0, for $z^3$, VC1 for $(5z^2 - \tilde{r}^2)x$ and $(5z^2 - \tilde{r}^2)y$, and finally VC2 for $zxy$ and $z(x^2 - y^2)$.

5 Acknowledgement

The author has benefitted from preliminary discussions with Peter Krueger, now at the Universite’ de Dijon, about Lanczos tridiagonalisation. The code, originally written C++, has been wrapped in python with the help of Mickael Profeta.
6 Final comment

The code is provided not only as a binary, ready to use executable, but also with the sources. This because, analogously to what happens in research, the only interesting code is the one that has not yet been written. Having the source will hence allow you to better adapt it to your research topic. The supplied examples can nonetheless be very useful and many things can be learned working with the parameters. Like everybody else, the author does not know what he will be doing in the future: may be expanding the code in some way or doing something completely different. However if you have some interesting subject we can possibly discuss it together. The distribution does not contain yet examples with neighbouring metal ions like in [2]. Future versions will.

References

[1] Kesheng Wu and Horst Simon, Thick-restart Lanczos method for large symmetric eigenvalue problems. SIAM Journal on Matrix Analysis and Applications Vol. 22, No. 2, pp. 602-616, 2001.

[2] Alessandro Mirone, S.S. Dhesi, G. van der Laan, Spectroscopy of $La_{0.5}Sr_{1.5}MnO_4$ orbital ordering: a cluster many-body calculation EPJB 2006, VOL 53; NUMBER 1, pages 23-28