

## Hints how to use the CFP manual

P. Novák

*Institute of Physics of ASCR, Cukrovarnická 10, 162 53 Prague 6, Czech Republic*

(Dated: December 23, 2016)

PACS numbers:

Keywords:

The hints given below are by no means obligatory and every user is free to modify them or to use different way.

We recommend to try first one or both of the examples. To this end after downloading

*CFP\_example1.tar.gz*, *CFP\_example2.tar.gz*

for the first example:

```
gunzip CFP_example1.tar.gz
```

```
tar -xvf CFP_example1.tar
```

```
cd CFP_example1/1st_step
```

```
cp -r dyalo3 CFP_manual/1st_step
```

Then go to directory *CFP\_manual/1st\_step/dyalo3* This directory contains script *jstep1*, which run the calculation described in *CFP\_manual/1st\_step*. The script can be modified according to your needs and the computer requirements.

Repeat this for remaining steps.

Both step 1 and step 2 can be run *k*-parallelized. Remaining steps are non-parallelized.

Step 3, however, can use multiple *vector* and *energy* files created by step 2 and you have to run *jstep3* in the same directory as the 2nd step or you have to copy *vector* and *energy* files to *CFP\_manual/3rd\_step/dyalo3*. Do not forget that in *jstep3* you have to insert the correct way to *wannier90* package. Then run

```
./jstep3 dyalo3
```

```
cd ../../4th_step/dyalo3
```

```
./jstep4 dyalo3
```

```
cd ../../5th_step/dyalo3
```

```
./jstep5 dyalo3
```

Most complicated is the 6th\_step. We usually test the sensitivity of results to the value of the hybridization parameter  $\Delta$ . For this reason in the 6<sub>th</sub> step the subdirectory *m06* is created which indicates that the calculations were performed for  $\Delta = -0.6$  Ry. *m06* contains several subdirectories names of which indicate direction of external field.

In subdirectory *a* are thus results for  $\vec{B} \parallel a$ , subdirectory *ab* contains results for  $\vec{B}$  rotated in the (*ab*) plane. The directory 6th\_step/dyalo3 contains two scripts: *jmag* calculates the dependence of eigenenergies on external magnetic field, *jang* dependence of eigenenergies on direction of external magnetic field in selected plane. Example for execution of *jmag* (from directory *CFP\_manual/4th\_step/dyalo3/*) to get results in subdirectory *m06/a* is

```
jmag m06 a 11
```

where 11 means number of steps. Note, however, that before the execution of *jmag*

```
cp CFP_manual/4th_step/dyalo3/dyalo3.cfp m06/a/fort.8
```

```
cp CFP_manual/5th_step/REparam/dy.inp m06/a/fort.7
```

If the starting value of magnetic field is nonzero, fort.7 must be modified accordingly.