Manual:
wannier-proj

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1 Introduction

`wannier-proj` is an implementation to calculate projectors from bloch used in wien2k to wannier states as described in [1].

The latest version can be found in
`http://itp.uni-frankfurt.de/~jdiehl/download/wannier-proj/`.

2 Installation and compilation

- `wannier-proj` uses the Eigen library for linear algebra arithmetics. You can get it from
  `http://eigen.tuxfamily.org/`
- unzip where you want, for example your home
- add the following to your `~/.bashrc`

  ```
  export CPLUS_INCLUDE_PATH=~/eigen-3.1.3
  ```

- run from bash

  ```
  source ~/.bashrc
  ```

- now the Eigen library should be available for the linker from this terminal without reboot. If not try rebooting.
- unzip the `wannier-proj` files you downloaded
- run change to wannier-proj directory and run `make`
- now `wannier-proj` should be compiled, check subdirectory `wannier-proj/bin` for existing executables

3 Preparation

- You need a fully converged `wien2k` calculation
- change the `TOT` switch in the `case.in2` in your wien2k project directory to `ALM`
- this will produce the `case.almblm` file when running `x lapw2`
- use not the original `lapw2` (this will produce a really huge file), instead the modified one in `wannier-proj/wien2k/`
- create or use the `case.inproj` file in your wien2k project directory, rename it to your case

```
1 #  number of atoms
2  1  2 #  atom index, No. of orbitals, l
-5.5 3.0 #  Energy window
45.0 0.0 0.0 1 #  Euler angles (zyz convention), rad/degree
```

- If you want for example project out the Fe3d orbitals, then you set the first line to `1` for one (irreducible) iron atom, the second line to `2 1 2` referring with the first number to the iron atoms (index in `case.struct`, second number one orbital shell in total you project out, third number meaning you chose the $l = 2$, i.e. d orbitals, to be projected. In the third line you select an energy window. Bigger is better, but try to narrow down. It is very sensitve to this window. At first do not care about the last line ;)
- this file acts as an input file for the modified `lapw2`, selecting only certain orbitals in a defined energy window
- it also acts as an input file later for the `wannier-proj`, so if you play around with different orbitals and energy windows, select first a bigger range and run `lapw2`, later you can narrow down without reproducing the `case.almblm` file again, if you select in the later steps a subset of orbitals/energies you have written to this file
- run `x lapw2`

- copy `case.indm` from the wien2k `SRC_templates` folder to your wien2k project directory
- this file is not important for the modified `lapwdm` from the `wannier-proj/wien2k` directory, but needs to be there. so no changes needed.
- run `x lapwdm`
- this procedure should have at least produced the following files

  ```
  case.almblm
  case.rot
  case.symm
  ```

- additionally you should also have at least the following files from scf-cycle:

  ```
  case.struct
  case.energy
  case.scf
  ```

4 Running `wannier-proj`

- all the following executables can be found in `wannier-proj/bin`
- run `init_smat` in your wien2k project folder to produce the `case.smat` file, which contains the connection between spherical and cubic harmonics meaning conversion to irreducible representation of orbitals (yet only s, p, d, no f orbitals)
- now you could - if you want - narrow down the seletion of orbitals or energies in the `case.inproj` file
- running now `run_proj` will produce the projectors, and the following output files

  ```
  case.projtilde
  case.overtilde
  case.proj
  case.over
  case.outputproj
  ```

- `case.projtilde` the auxiliary projectors no orthonormalized, `case.overtilde` the corresponding overlap matrix, `case.proj` the orthogonalized/-normalized projectors, and to check this `case.over` their overlap matrix - which should always be a unitary matrix for each kpoint.
- `case.outputproj` summarizes which orbitals where projected out, the first rows (also in this order) name the columns of the projector files. The later energy lines, give the energy index from the `case.energy` file which corresponds to the rows in the projector files.

5 Literatur

[1] Phys Rev B 80, 085101 (2009)