`wannier90`: User Guide

Version 2.0

14th October 2013

Contents

Part I

Introduction

Introduction

Getting Help

The latest version of `wannier90` and documentation can always be found at `http://www.wannier.org`.

There is a `wannier90` mailing list for discussing issues in the development, theory, coding and algorithms pertinent to MLWF. You can register for this mailing list by following the links at `http://www.wannier.org/forum.html`

Finally, many frequently asked questions are answered in Appendix B.

Citation

We ask that you acknowledge the use of `wannier90` in any publications arising from the use of this code through the following reference

> [ref] A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt and N. Marzari,
> `wannier90`: A Tool for Obtaining Maximally-Localised Wannier Functions,
> *Comput. Phys. Commun.* **178**, 685 (2008)

It would also be appropriate to cite the original articles:

Maximally localized generalized Wannier functions for composite energy bands,
N. Marzari and D. Vanderbilt, *Phys. Rev. B* **56**, 12847 (1997)

Maximally localized Wannier functions for entangled energy bands,
I. Souza, N. Marzari and D. Vanderbilt, *Phys. Rev. B* **65**, 035109 (2001)

Credits

The present release of `wannier90` was written by Arash A. Mostofi (Imperial College London, UK), Giovanni Pizzi (EPFL, Switzerland), Ivo Souza (Universidad del Pais Vasco, Spain) and Jonathan R. Yates (University of Oxford, UK). Contributors to the code include Young-Su Lee (KIST, S. Korea), Matthew Shelley (Imperial College London, UK) and Nicolas Poilvert (Harvard University, USA). `wannier90` is based on the Fortran 77 codes written for isolated bands by Nicola Marzari and David Vanderbilt, for entangled bands by Ivo Souza, Nicola Marzari, and David Vanderbilt, and for quantum transport by Marco Nardelli.

Licence

Part II

wannier90.x

Chapter 1

Methodology

`wannier90` computes maximally-localised Wannier functions (MLWF) following the method of Marzari and Vanderbilt (MV) [1]. For entangled energy bands, the method of Souza, Marzari and Vanderbilt (SMV) [2] is used. We introduce briefly the methods and key definitions here, but full details can be found in the original papers and in Ref. [3].

First-principles codes typically solve the electronic structure of periodic materials in terms of Bloch states, $\psi_{n\mathbf{k}}$. These extended states are characterised by a band index n and crystal momentum $\mathbf{k}$. An alternative representation can be given in terms of spatially localised functions known as Wannier functions (WF). The WF centred on a lattice site $\mathbf{R}$, $w_{n\mathbf{R}}(\mathbf{r})$, is written in terms of the set of Bloch states as

$$w_{n\mathbf{R}}(\mathbf{r}) = \frac{V}{(2\pi)^3} \int_{\mathrm{BZ}} \left[\sum_m U_{mn}^{(\mathbf{k})} \psi_{m\mathbf{k}}(\mathbf{r}) \right] e^{-i\mathbf{k}.\mathbf{R}} \, d\mathbf{k} \ , \tag{1.1}$$

where V is the unit cell volume, the integral is over the Brillouin zone (BZ), and $\mathbf{U}^{(\mathbf{k})}$ is a unitary matrix that mixes the Bloch states at each $\mathbf{k}$. $\mathbf{U}^{(\mathbf{k})}$ is not uniquely defined and different choices will lead to WF with varying spatial localisations. We define the spread Ω of the WF as

$$\Omega = \sum_n \left[\langle w_{n\mathbf{0}}(\mathbf{r})|r^2|w_{n\mathbf{0}}(\mathbf{r})\rangle - |\langle w_{n\mathbf{0}}(\mathbf{r})|\mathbf{r}|w_{n\mathbf{0}}(\mathbf{r})\rangle|^2 \right] . \tag{1.2}$$

The total spread can be decomposed into a gauge invariant term Ω_{I} plus a term $\tilde{\Omega}$ that is dependant on the gauge choice $\mathbf{U}^{(\mathbf{k})}$. $\tilde{\Omega}$ can be further divided into terms diagonal and off-diagonal in the WF basis, Ω_{D} and Ω_{OD},

$$\Omega = \Omega_{\mathrm{I}} + \tilde{\Omega} = \Omega_{\mathrm{I}} + \Omega_{\mathrm{D}} + \Omega_{\mathrm{OD}} \tag{1.3}$$

where

$$\Omega_{\mathrm{I}} = \sum_n \left[\langle w_{n\mathbf{0}}(\mathbf{r})|r^2|w_{n\mathbf{0}}(\mathbf{r})\rangle - \sum_{\mathbf{R}m} |\langle w_{n\mathbf{R}}(\mathbf{r})|\mathbf{r}|w_{n\mathbf{0}}(\mathbf{r})\rangle|^2 \right] \tag{1.4}$$

$$\Omega_{\mathrm{D}} = \sum_n \sum_{\mathbf{R}\neq\mathbf{0}} |\langle w_{n\mathbf{R}}(\mathbf{r})|\mathbf{r}|w_{n\mathbf{0}}(\mathbf{r})\rangle|^2 \tag{1.5}$$

$$\Omega_{\mathrm{OD}} = \sum_{m\neq n} \sum_{\mathbf{R}} |\langle w_{m\mathbf{R}}(\mathbf{r})|\mathbf{r}|w_{n\mathbf{0}}(\mathbf{r})\rangle|^2 \tag{1.6}$$

The MV method minimises the gauge dependent spread $\tilde{\Omega}$ with respect the set of $\mathbf{U}^{(\mathbf{k})}$ to obtain MLWF.

`wannier90` requires two ingredients from an initial electronic structure calculation.

1. The overlaps between the cell periodic part of the Bloch states $|u_{n\mathbf{k}}\rangle$

$$M_{mn}^{(\mathbf{k},\mathbf{b})} = \langle u_{m\mathbf{k}}|u_{n\mathbf{k}+\mathbf{b}}\rangle, \tag{1.7}$$

where the vectors $\mathbf{b}$, which connect a given k-point with its neighbours, are determined by `wannier90` according to the prescription outlined in Ref. [1].

2. As a starting guess the projection of the Bloch states $|\psi_{n\mathbf{k}}\rangle$ onto trial localised orbitals $|g_n\rangle$

$$A_{mn}^{(\mathbf{k})} = \langle \psi_{m\mathbf{k}}|g_n\rangle, \tag{1.8}$$

Note that $\mathbf{M}^{(\mathbf{k},\mathbf{b})}$, $\mathbf{A}^{(\mathbf{k})}$ and $\mathbf{U}^{(\mathbf{k})}$ are all small, $N \times N$ matrices[1] that are independent of the basis set used to obtain the original Bloch states.

To date, `wannier90` has been used in combination with electronic codes based on plane-waves and pseudopotentials (norm-conserving and ultrasoft [4]) as well as mixed basis set techniques such as FLAPW [5].

1.1   Entangled Energy Bands

The above description is sufficient to obtain MLWF for an isolated set of bands, such as the valence states in an insulator. In order to obtain MLWF for entangled energy bands we use the "disentanglement" procedure introduced in Ref. [2].

We define an energy window (the "outer window"). At a given k-point $\mathbf{k}$, $N_{\text{win}}^{(\mathbf{k})}$ states lie within this energy window. We obtain a set of N Bloch states by performing a unitary transformation amongst the Bloch states which fall within the energy window at each k-point:

$$|u_{n\mathbf{k}}^{\text{opt}}\rangle = \sum_{m \in N_{\text{win}}^{(\mathbf{k})}} U_{mn}^{\text{dis}(\mathbf{k})}|u_{m\mathbf{k}}\rangle \tag{1.9}$$

where $\mathbf{U}^{\text{dis}(\mathbf{k})}$ is a rectangular $N \times N_{\text{win}}^{(\mathbf{k})}$ matrix[2]. The set of $\mathbf{U}^{\text{dis}(\mathbf{k})}$ are obtained by minimising the gauge invariant spread Ω_{I} within the outer energy window. The MV procedure can then be used to minimise $\tilde{\Omega}$ and hence obtain MLWF for this optimal subspace.

It should be noted that the energy bands of this optimal subspace may not correspond to any of the original energy bands (due to mixing between states). In order to preserve exactly the properties of a system in a given energy range (e.g., around the Fermi level) we introduce a second energy window. States lying within this inner, or "frozen", energy window are included unchanged in the optimal subspace.

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[1]Technically, this is true for the case of an isolated group of N bands from which we obtain N MLWF. When using the disentanglement procedure of Ref. [2], $\mathbf{A}^{(\mathbf{k})}$, for example, is a rectangular matrix. See Section 1.1.

[2]As $\mathbf{U}^{\text{dis}(\mathbf{k})}$ is a rectangular matrix this is a unitary operation in the sense that $(\mathbf{U}^{\text{dis}(\mathbf{k})})^{\dagger}\mathbf{U}^{\text{dis}(\mathbf{k})} = \mathbf{1}$.

Chapter 2

Parameters

2.1 Usage

```
wannier90.x [-pp] [seedname]
```

- **seedname**: If a seedname string is given the code will read its input from a file `seedname.win`. The default value is `wannier`. One can also equivalently provide the string `seedname.win` instead of `seedname`.

- **-pp**: This optional flag tells the code to generate a list of the required overlaps and then exit. This information is written to the file `seedname.nnkp`.

2.2 `seedname.win` File

The `wannier90` input file `seedname.win` has a flexible free-form structure.

The ordering of the keywords is not significant. Case is ignored (so `num_bands` is the same as `Num_Bands`). Characters after !, or # are treated as comments. Most keywords have a default value that is used unless the keyword is given in `seedname.win`. Keywords can be set in any of the following ways

```
num_wann 4
num_wann = 4
num_wann :  4
```

A logical keyword can be set to `true` using any of the following strings: `T`, `true`, `.true.`.

For further examples see Section 9.1 and the the `wannier90` Tutorial.

2.3 Keyword List

Keyword	Type	Description
System Parameters		
NUM_WANN	I	Number of WF
NUM_BANDS	I	Number of bands passed to the code
UNIT_CELL_CART	P	Unit cell vectors in Cartesian coordinates
ATOMS_CART *	P	Positions of atoms in Cartesian coordinates
ATOMS_FRAC *	R	Positions of atoms in fractional coordinates with respect to the lattice vectors
MP_GRID	I	Dimensions of the Monkhorst-Pack grid of k-points
KPOINTS	R	List of k-points in the Monkhorst-Pack grid
GAMMA_ONLY	L	Wavefunctions from underlying ab initio calculation are manifestly real
SPINORS	L	WF are spinors
SHELL_LIST	I	Which shells to use in finite difference formula
SEARCH_SHELLS	I	The number of shells to search when determining finite difference formula
KMESH_TOL	R	The tolerance to control if two kpoint belong to the same shell

Table 2.1: `seedname.win` file keywords defining the system. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.
* ATOMS_CART and ATOMS_FRAC may not both be defined in the same input file.

Keyword	Type	Description
Job Control		
POSTPROC_SETUP	L	To output the `seedname.nnkp` file
EXCLUDE_BANDS	I	List of bands to exclude from the calculation
RESTART	S	Restart from checkpoint file
IPRINT	I	Output verbosity level
LENGTH_UNIT	S	System of units to output lengths
WVFN_FORMATTED	L	Read the wavefunctions from a (un)formatted file
SPIN	S	Which spin channel to read
DEVEL_FLAG	S	Flag for development use
TIMING_LEVEL	I	Determines amount of timing information written to output
OPTIMISATION	I	Optimisation level
TRANSLATE_HOME_CELL	L	To translate final Wannier centres to home unit cell when writing xyz file
WRITE_XYZ	L	To write atomic positions and final centres in xyz file format
WRITE_VDW_DATA	L	To write data for futher processing by w90vdw utility
WRITE_HR_DIAG	L	To write the diagonal elements of the Hamiltonian in the Wannier basis to seedname.wout (in eV)

Table 2.2: `seedname.win` file keywords defining job control. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string. TRANSLATE_HOME_CELL only relevant if WRITE_XYZ is `.true.`

Keyword	Type	Description
Disentanglement Parameters		
DIS_WIN_MIN	P	Bottom of the outer energy window
DIS_WIN_MAX	P	Top of the outer energy window
DIS_FROZ_MIN	P	Bottom of the inner (frozen) energy window
DIS_FROZ_MAX	P	Top of the inner (frozen) energy window
DIS_NUM_ITER	I	Number of iterations for the minimisation of Ω_I
DIS_MIX_RATIO	R	Mixing ratio during the minimisation of Ω_I
DIS_CONV_TOL	R	The convergence tolerance for finding Ω_I
DIS_CONV_WINDOW	I	The number of iterations over which convergence of Ω_I is assessed.
DIS_SPHERES_NUM	I	Number of spheres in k-space where disentaglement is performed
DIS_SPHERES_FIRST_WANN	I	Index of the first band to be considered a Wannier function
DIS_SPHERES	R	List of centers and radii, for disentanglement only in spheres

Table 2.3: `seedname.win` file keywords controlling the disentanglement. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

Keyword	Type	Description
Wannierise Parameters		
NUM_ITER	I	Number of iterations for the minimisation of Ω
NUM_CG_STEPS	I	During the minimisation of Ω the number of Conjugate Gradient steps before resetting to Steepest Descents
CONV_WINDOW	I	The number of iterations over which convergence of Ω is assessed
CONV_TOL	P	The convergence tolerance for finding Ω
CONV_NOISE_AMP	R	The amplitude of random noise applied towards end of minimisation procedure
CONV_NOISE_NUM	I	The number of times random noise is applied
NUM_DUMP_CYCLES	I	Control frequency of check-pointing
NUM_PRINT_CYCLES	I	Control frequency of printing
WRITE_R2MN	L	Write matrix elements of r^2 between WF to file
GUIDING_CENTRES	L	Use guiding centres
NUM_GUIDE_CYCLES	I	Frequency of guiding centres
NUM_NO_GUIDE_ITER	I	The number of iterations after which guiding centres are used
TRIAL_STEP *	R	The trial step length for the parabolic line search during the minimisation of Ω
FIXED_STEP *	R	The fixed step length to take during the minimisation of Ω, instead of doing a parabolic line search
USE_BLOCH_PHASES **	L	To use phases for initial projections

Table 2.4: `seedname.win` file keywords controlling the wannierisation. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string. * FIXED_STEP and TRIAL_STEP may not both be defined in the same input file. **Cannot be used in conjunction with disentanglement.

Keyword	Type	Description
Plot Parameters		
WANNIER_PLOT	L	Plot the WF
WANNIER_PLOT_LIST	I	List of WF to plot
WANNIER_PLOT_SUPERCELL	I	Size of the supercell for plotting the WF
WANNIER_PLOT_FORMAT	S	File format in which to plot the WF
WANNIER_PLOT_MODE	S	Mode in which to plot the WF, molecule or crystal
WANNIER_PLOT_RADIUS	R	Cut-off radius of WF*
BANDS_PLOT	L	Plot interpolated band structure
KPOINT_PATH	P	K-point path for the interpolated band structure
BANDS_NUM_POINTS	I	Number of points along the first section of the k-point path
BANDS_PLOT_FORMAT	S	File format in which to plot the interpolated bands
BANDS_PLOT_PROJECT	I	WF to project the band structure onto
BANDS_PLOT_MODE	S	Slater-Koster type interpolation or Hamiltonian cut-off
BANDS_PLOT_DIM	I	Dimension of the system
FERMI_SURFACE_PLOT	L	Plot the Fermi surface
FERMI_SURFACE_NUM_POINTS	I	Number of points in the Fermi surface plot
FERMI_ENERGY	P	The Fermi energy
FERMI_ENERGY_MIN	P	Lower limit of the Fermi energy range
FERMI_ENERGY_MAX	P	Upper limit of the Fermi energy range
FERMI_ENERGY_STEP	R	Step for increasing the Fermi energy in the specified range
FERMI_SURFACE_PLOT_FORMAT	S	File format for the Fermi surface plot
HR_PLOT	L	Write the Hamiltonian in the WF basis
HR_CUTOFF	P	Cut-off for the absolute value of the Hamiltonian
DIST_CUTOFF	P	Cut-off for the distance between WF
DIST_CUTOFF_MODE	S	Dimension in which the distance between WF is calculated
TRANSLATION_CENTRE_FRAC	R	Centre of the unit cell to which final WF are translated

Table 2.5: `seedname.win` file keywords controlling the plotting. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string. * Only applies when WANNIER_PLOT_FORMAT is `cube`.

Keyword	Type	Description
Transport Parameters		
TRANSPORT	L	Calculate quantum conductance and density of states
TRANSPORT_MODE	S	Bulk or left-lead_conductor_right-lead calculation
TRAN_WIN_MIN	P	Bottom of the energy window for transport calculation
TRAN_WIN_MAX	P	Top of the energy window for transport calculation
TRAN_ENERGY_STEP	R	Sampling interval of the energy values
FERMI_ENERGY	R	The Fermi energy
TRAN_NUM_BB	I	Size of a bulk Hamiltonian
TRAN_NUM_LL	I	Size of a left-lead Hamiltonian
TRAN_NUM_RR	I	Size of a right-lead Hamiltonian
TRAN_NUM_CC	I	Size of a conductor Hamiltonian
TRAN_NUM_LC	I	Number of columns in a left-lead_conductor Hamiltonian
TRAN_NUM_CR	I	Number of rows in a conductor_right-lead Hamiltonian
TRAN_NUM_CELL_LL	I	Number of unit cells in PL of left lead
TRAN_NUM_CELL_RR	I	Number of unit cells in PL of right lead
TRAN_NUM_BANDC	I	Half-bandwidth+1 of a band-diagonal conductor Hamiltonian
TRAN_WRITE_HT	L	Write the Hamiltonian for transport calculation
TRAN_READ_HT	L	Read the Hamiltonian for transport calculation
TRAN_USE_SAME_LEAD	L	Left and right leads are the same
TRAN_GROUP_THRESHOLD	R	Distance that determines the grouping of WFs
HR_CUTOFF	P	Cut-off for the absolute value of the Hamiltonian
DIST_CUTOFF	P	Cut-off for the distance between WF
DIST_CUTOFF_MODE	S	Dimension in which the distance between WF is calculated
ONE_DIM_AXIS	S	Extended direction for a one-dimensional system
TRANSLATION_CENTRE_FRAC	R	Centre of the unit cell to which final WF are translated

Table 2.6: `seedname.win` file keywords controlling transport. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

2.4   System

2.4.1   integer :: num_wann

Number of WF to be found.

No default.

2.4.2   integer :: num_bands

Total number of bands passed to the code in the `seedname.mmn` file.

Default `num_bands=num_wann`

2.4.3   Cell Lattice Vectors

The cell lattice vectors should be specified in Cartesian coordinates.

```
begin unit_cell_cart
[units]
```

$$
\begin{array}{ccc}
A_{1x} & A_{1y} & A_{1z} \\
A_{2x} & A_{2y} & A_{2z} \\
A_{3x} & A_{3y} & A_{3z}
\end{array}
$$

```
end unit_cell_cart
```

Here A_{1x} is the x-component of the first lattice vector $\mathbf{A}_1$, A_{2y} is the y-component of the second lattice vector $\mathbf{A}_2$, etc.

`[units]` specifies the units in which the lattice vectors are defined: either `Bohr` or `Ang`.

The default value is `Ang`.

2.4.4   Ionic Positions

The ionic positions may be specified in fractional coordinates relative to the lattice vectors of the unit cell, or in absolute Cartesian coordinates. Only one of `atoms_cart` and `atoms_frac` may be given in the input file.

Cartesian coordinates

```
begin atoms_cart
[units]
```

$$
\begin{array}{cccc}
P & R_x^P & R_y^P & R_z^P \\
Q & R_x^Q & R_y^Q & R_z^Q \\
& \vdots
\end{array}
$$

```
end atoms_cart
```

The first entry on a line is the atomic symbol. The next three entries are the atom's position $\mathbf{R} = (R_x, R_y, R_z)$ in Cartesian coordinates. The first line of the block, [units], specifies the units in which the coordinates are given and can be either bohr or ang. If not present, the default is ang.

Fractional coordinates

begin atoms_frac

$$
\begin{array}{cccc}
P & F_1^P & F_2^P & F_3^P \\
Q & F_1^Q & F_2^Q & F_3^Q \\
& \vdots &
\end{array}
$$

end atoms_frac

The first entry on a line is the atomic symbol. The next three entries are the atom's position in fractional coordinates $\mathbf{F} = F_1\mathbf{A}_1 + F_2\mathbf{A}_2 + F_3\mathbf{A}_3$ relative to the cell lattice vectors $\mathbf{A}_i$, $i \in [1, 3]$.

2.4.5   integer, dimension ::   mp_grid(3)

Dimensions of the regular (Monkhorst-Pack) k-point mesh. For example, for a $2 \times 2 \times 2$ grid:

mp_grid : 2 2 2

No default.

2.4.6   K-points

Each line gives the coordinate $\mathbf{K} = K_1\mathbf{B}_1 + K_2\mathbf{B}_2 + K_3\mathbf{B}_3$ of a k-point in relative (crystallographic) units, i.e., in fractional units with respect to the primitive reciprocal lattice vectors $\mathbf{B}_i$, $i \in [1, 3]$. The position of each k-point in this list assigns its numbering; the first k-point is k-point 1, the second is k-point 2, and so on.

begin kpoints

$$
\begin{array}{ccc}
K_1^1 & K_2^1 & K_3^1 \\
K_1^2 & K_2^2 & K_3^2 \\
& \vdots &
\end{array}
$$

end kpoints

There is no default.

Note: There is an utility provided with `wannier90`, called kmesh.pl, which helps to generate the explicit list of k points required by `wannier90`. See Sec. A.1.

2.4.7   logical ::   gamma_only

If gamma_only=true, then `wannier90` uses a branch of algorithms for disentanglement and localisation that exploit the fact that the Bloch eigenstates obtained from the underlying ab initio calculation are manifestly real. This can be the case when only the Γ-point is used to sample the Brillouin zone. The localisation procedure that is used in the Γ-only branch is based on the method of Ref. [6].

The default value is `false`.

2.4.8 logical :: spinors

If `spinors=true`, then `wannier90` assumes that the WF correspond to singularly occupied spinor states and `num_elec_per_state=1`.

The default value is `false`.

2.4.9 Shells

The MV scheme requires a finite difference expression for $\nabla_{\mathbf{k}}$ defined on a uniform Monkhorst-Pack mesh of k-points. The vectors $\{\mathbf{b}\}$ connect each mesh-point $\mathbf{k}$ to its nearest neighbours. $N_{\rm sh}$ shells of neighbours are included in the finite-difference formula, with M_s vectors in the $s^{\rm th}$ shell. For $\nabla_{\mathbf{k}}$ to be correct to linear order, we require that the following equation is satisfied (Eq. B1 of Ref. [1]):

$$\sum_s^{N_{\rm sh}} w_s \sum_i^{M_{\rm s}} b_\alpha^{i,s} b_\beta^{i,s} = \delta_{\alpha\beta} \; , \tag{2.1}$$

where $\mathbf{b}^{i,s}$, $i \in [1, M_s]$, is the $i^{\rm th}$ vector belonging to the $s^{\rm th}$ shell with associated weight w_s, and α and β run over the three Cartesian indices.

2.4.10 integer :: shell_list(:)

`shell_list` is vector listing the shells to include in the finite difference expression. If this keyword is absent, the shells are chosen automatically.

2.4.11 integer :: search_shells

Specifies the number of shells of neighbours over which to search in attempting to determine an automatic solution to the B1 condition Eq. 2.1. Larger values than the default may be required in special cases e.g. for very long thin unit cells.

The default value is 12.

2.4.12 real(kind=dp) :: kmesh_tol

Two kpoints belong to the same shell if the distance between them is less than `kmesh_tol`. Units are Ang.

The default value is 0.000001 Ang.

2.5 Projection

The projections block defines a set of localised functions used to generate an initial guess for the unitary transformations. This data will be written in the `seedname.nnkp` file to be used by a first-principles code.

```
begin projections
.
.
end projections
```

If `guiding_centres`=`true`, then the projection centres are used as the guiding centres in the Wannierisation routine.

For details see Section 3.1.

2.6   Job Control

2.6.1   `logical :: postproc_setup`

If `postproc_setup`=`true`, then the wannier code will write `seedname.nnkp` file and exit. If `wannier90` is called with the option `-pp`, then `postproc_setup` is set to `true`, over-riding its value in the `seedname.win` file.

The default value is `false`.

2.6.2   `integer :: iprint`

This indicates the level of verbosity of the output from 0, the bare minimum, to 3, which corresponds to full debugging output.

The default value is 1.

2.6.3   `integer :: optimisation`

This indicates the level of optimisation used in the code. This is a trade between speed and memory. A positive number indicates fastest execution time at the cost of more memory. Zero or negative numbers indicates a smaller memory footprint - at increased execution time.

At the moment the only values that have an effect are `optimisation<=0` (low memory) and `optimisation>0` (fast)

The default value is 3.

2.6.4   `character(len=20) :: length_unit`

The length unit to be used for writing quantities in the output file `seedname.wout`.

The valid options for this parameter are:

   – `Ang` (default)

   – `Bohr`

2.6.5 character(len=50) :: devel_flag

Not a regular keyword. Its purpose is to allow a developer to pass a string into the code to be used inside a new routine as it is developed.

No default.

2.6.6 integer :: exclude_bands(:)

A k-point independent list of states to excluded from the calculation of the overlap matrices; for example to select only valence states, or ignore semi-core states. This keyword is passed to the first-principles code via the `seedname.nnkp` file. For example, to exclude bands 2, 6, 7, 8 and 12:

exclude_bands : 2, 6-8, 12

2.6.7 character(len=20) :: restart

If `restart` is present the code will attempt to restart the calculation from the `seedname.chk` file. The value of the parameter determines the position of the restart

The valid options for this parameter are:

  – `default`. Restart from the point at which the check file `seedname.chk` was written

  – `wannierise`. Restart from the beginning of the wannierise routine

  – `plot`. Go directly to the plotting phase

  – `transport`. Go directly to the transport routines

2.6.8 character(len=20) :: wvfn_formatted

If `wvfn_formatted`=`true`, then the wavefunctions will be read from disk as formatted (ie ASCII) files; otherwise they will be read as unformatted files. Unformatted is generally preferable as the files will take less disk space and I/O is significantly faster. However such files will not be transferable between all machine architectures and formatted files should be used if transferability is required (i.e., for test cases).

The default value of this parameter is `false`.

2.6.9 character(len=20) :: spin

For bands from a spin polarised calculation `spin` determines which set of bands to read in, either `up` or `down`.

The default value of this parameter is `up`.

2.6.10   integer :: timing_level

Determines the amount of timing information regarding the calculation that will be written to the output file. A value of 1 produces the least information.

The default value is 1.

2.6.11   logical :: translate_home_cell

Determines whether to translate the final Wannier centres to the home unit cell at the end of the calculation. Mainly useful for molecular systems in which the molecule resides entirely within the home unit cell and user wants to write an xyz file (`write_xyz=.true.`) for the WF centres to compare with the structure.

The default value is `false`.

2.6.12   logical :: write_xyz

Determines whether to write the atomic positions and final Wannier centres to an xyzfile, `seedname_centres.xyz`, for subsequent visualisation.

The default value is `false`.

2.6.13   logical :: write_vdw_data

Determines whether to write `seedname.vdw` for subsequent post-processing by the `w90vdw` utility (in the `utility/w90vdw/` directory of the distribution) for calculating van der Waals energies. Brillouin zone sampling must be at the Gamma-point only.

The default value is `false`.

2.7   Disentanglement

These keywords control the disentanglement routine of Ref. [2], i.e., the iterative minimisation of Ω_I. This routine will be activated if `num_wann` < `num_bands`.

2.7.1   real(kind=dp) :: dis_win_min

The lower bound of the outer energy window for the disentanglement procedure. Units are eV.

The default is the lowest eigenvalue in the system.

2.7.2   real(kind=dp) :: dis_win_max

The upper bound of the outer energy window for the disentanglement procedure. Units are eV.

The default is the highest eigenvalue in the given states (i.e., all states are included in the disentanglement procedure).

2.7.3 real(kind=dp) :: dis_froz_min

The lower bound of the inner energy window for the disentanglement procedure. Units are eV.

If dis_froz_max is given, then the default for dis_froz_min is dis_win_min.

2.7.4 real(kind=dp) :: dis_froz_max

The upper bound of the inner (frozen) energy window for the disentanglement procedure. If dis_froz_max is not specified, then there are no frozen states. Units are eV.

No default.

2.7.5 integer :: dis_num_iter

In the disentanglement procedure, the number of iterations used to extract the most connected subspace.

The default value is 200.

2.7.6 real(kind=dp) :: dis_mix_ratio

In the disentanglement procedure, the mixing parameter to use for convergence (see pages 4-5 of Ref. [2]). A value of 0.5 is a 'safe' choice. Using 1.0 (i.e., no mixing) often gives faster convergence, but may cause the minimisation of Ω_I to be unstable in some cases.

Restriction: $0.0 < $ dis_mix_ratio ≤ 1.0

The default value is 0.5

2.7.7 real(kind=dp) :: dis_conv_tol

In the disentanglement procedure, the minimisation of Ω_I is said to be converged if the fractional change in the gauge-invariant spread between successive iterations is less than dis_conv_tol for dis_conv_window iterations. Units are Å^2.

The default value is 1.0E-10

2.7.8 integer :: dis_conv_window

In the disentanglement procedure, the minimisation is said to be converged if the fractional change in the spread between successive iterations is less than dis_conv_tol for dis_conv_window iterations.

The default value of this parameter is 3.

2.7.9 integer :: dis_spheres_num

Number of spheres in reciprocal space where the k-dependent disentanglement is performed. No disentanglement is performed for those k-points that are not included in any of the spheres.

The default is 0, which means disentangle at every k-point in the full BZ (the standard mode in Wannier90).

2.7.10 integer :: dis_spheres_first_wann

Index of the first band that has to be considered as a Wannier function. Used only if `dis_spheres_num` is greater than zero. At k-points where disentanglement is not performed the bands from `dis_first_wann` to `dis_first_wann+num_wann` are used to wannierise. The bands excluded using `exclude_bands` should not be counted.

The default is 1, the band at the lowest energy.

2.7.11 dis_spheres

Each line gives the coordinate $\mathbf{K} = K_1\mathbf{B}_1 + K_2\mathbf{B}_2 + K_3\mathbf{B}_3$ of a k-point representing the center of one of the spheres used for k-dependent disentanglement. The same crystallographic units as for `kpoints` are used here. Each k-point coordinate $\mathbf{K}^i$ must the followed by the respectice sphere radius r_i in inverse angstrom (on the same line).

The number of lines must be equal to `dis_spheres_num`.

`begin dis_spheres`

$$
\begin{array}{cccc}
K_1^1 & K_2^1 & K_3^1 & r_1 \\
K_1^2 & K_2^2 & K_3^2 & r_2 \\
& \vdots &
\end{array}
$$

`end dis_spheres`

There is no default.

2.8 Wannierise

Iterative minimisation of $\widetilde{\Omega}$, the non-gauge-invariant part of the spread functional.

2.8.1 integer :: num_iter

Total number of iterations in the minimisation procedure. Set `num_iter=0` if you wish to generate projected WFs rather than maximally-localized WFs (see Example 8 in the Tutorial).

The default value is 100

2.8.2 integer :: num_cg_steps

Number of conjugate gradient steps to take before resetting to steepest descents.

The default value is 5

2.8.3 `integer :: conv_window`

If `conv_window` > 1, then the minimisation is said to be converged if the change in Ω over `conv_window` successive iterations is less than `conv_tol`. Otherwise, the minimisation proceeds for num_iter iterations (default).

The default value is -1

2.8.4 `real(kind=dp) :: conv_tol`

If `conv_window` > 1, then this is the convergence tolerance on Ω, otherwise not used. Units are Å^2.

The default value is 1.0E-10

2.8.5 `real(kind=dp) :: conv_noise_amp`

If `conv_noise_amp` > 0, once convergence (as defined above) is achieved, some random noise f is added to the search direction, and the minimisation is continued until convergence is achieved once more. If the same value of Ω as before is arrived at, then the calculation is considered to be converged. If not, then random noise is added again and the procedure repeated up to a maximum of `conv_noise_num` times. `conv_noise_amp` is the amplitude of the random noise f that is added to the search direction: $0 < |f| < $ `conv_noise_amp`. This functionality requires `conv_window` > 1. If `conv_window` is not specified, it is set to the value 5 by default.

If `conv_noise_amp` $\leq$ 0, then no noise is added (default).

The default value is -1.0

2.8.6 `integer :: conv_noise_num`

If `conv_noise_amp` > 0, then this is the number of times in the minimisation that random noise is added.

The default value is 3

2.8.7 `integer :: num_dump_cycles`

Write sufficient information to do a restart every `num_dump_cycles` iterations.

The default is 100

2.8.8 `integer :: num_print_cycles`

Write data to the master output file `seedname.wout` every `num_print_cycles` iterations.

The default is 1

2.8.9 logical :: write_r2mn

If `write_r2mn = true`, then the matrix elements $\langle m|r^2|n \rangle$ (where m and n refer to WF) are written to file `seedname.r2mn` at the end of the Wannierisation procedure.

The default value of this parameter is `false`.

2.8.10 logical :: guiding_centres

Use guiding centres during the minimisation, in order to avoid local minima.

The default value is `false`.

2.8.11 integer :: num_guide_cycles

If `guiding_centres` is set to true, then the guiding centres are used only every `num_guide_cycles`.

The default value is 1.

2.8.12 integer :: num_no_guide_iter

If `guiding_centres` is set to true, then the guiding centres are used only after `num_no_guide_iter` minimisation iterations have been completed.

The default value is 0.

2.8.13 real(kind=dp) :: trial_step

The value of the trial step for the parabolic fit in the line search minimisation used in the minimisation of the spread function. Cannot be used in conjunction with `fixed_step` (see below). If the minimisation procedure doesn't converge, try decreasing the value of `trial_step` to give a more accurate line search.

The default value is 2.0

2.8.14 real(kind=dp) :: fixed_step

If this is given a value in the input file, then a fixed step of length `fixed_step` (instead of a parabolic line search) is used at each iteration of the spread function minimisation. Cannot be used in conjunction with `trial_step`. This can be useful in cases in which minimisation with a line search fails to converge.

There is no default value.

2.8.15 logical :: use_bloch_phases

Determines whether to use the Bloch functions as the initial guess for the projections. Can only be used if `disentanglement = false`.

Th default value is `false`.

2.9   Post-Processing

Capabilities:

- – Plot the WF

- – Plot the interpolated band structure

- – Plot the Fermi surface

- – Output the Hamiltonian in the WF basis

- – Transport calculation (quantum conductance and density of states)

2.9.1   `logical :: wannier_plot`

If `wannier_plot = true`, then the code will write out the Wannier functions in a super-cell whose size is defined by the variable `wannier_plot_supercell`, and in a format specified by `wannier_plot_format`

The default value of this parameter is `false`.

2.9.2   `integer :: wannier_plot_supercell`

Dimension of the 'super-unit-cell' in which the WF are plotted. The super-unit-cell is `wannier_plot_supercell` times the unit cell along all three linear dimensions (the 'home' unit cell is kept approximately in the middle) if `wannier_plot_supercell` is provided as a single integer.

Otherwise, if three integers are provided, the super-unit-cell is `wannier_plot_supercell(i)` times the unit cell along the $i-$th linear dimension.

The default value is $2 \times 2 \times 2$.

2.9.3   `character(len=20) :: wannier_plot_format`

WF can be plotted in either XCrySDen (xsf) format or Gaussian cube format. The valid options for this parameter are:

- – `xcrysden` (default)

- – `cube`

If `wannier_plot_format=cube`: Most visualisation programs (including XCrySDen) are only able to handle cube files for systems with orthogonal lattice vectors.[1] `wannier90` checks this on reading the `seedname.win` and reports an error if cube format has been selected and the lattice vectors are not mutually orthogonal.

---

[1]It's worth noting that the visualisation program VMD (`http://www.ks.uiuc.edu/Research/vmd`), for example, is able to deal with certain special cases of non-orthogonal lattice vectors. See `http://www.ks.uiuc.edu/Research/vmd/plugins/molfile/cubeplugin.html`. At present `wannier90` only supports orthogonal lattice vectors for cube output.

2.9.4   `integer ::   wannier_plot_list(:)`

A list of WF to plot. The WF numbered as per the `seedname.wout` file after the minimisation of the spread.

The default behaviour is to plot all WF. For example, to plot WF 4, 5, 6 and 10:

`wannier_plot_list : 4-6, 10`

2.9.5   `character(len=20) ::   wannier_plot_mode`

Choose the mode in which to plot the WF, either as a molecule or as a crystal. Only relevant if `wannier_plot_format=xcrysden`.

The valid options for this parameter are:

- `crystal` (default)

- `molecule`

2.9.6   `real(kind=dp) ::   wannier_plot_radius`

If `wannier_plot_format` is `cube`, then `wannier_plot_radius` determines the cut-off radius of the WF for the purpose of plotting. `wannier_plot_radius` must be greater than 0. Units are Å.

The default value is 3.5.

2.9.7   `logical ::   bands_plot`

If `bands_plot = true`, then the code will calculate the band structure, through Wannier interpolation, along the path in k-space defined by `bands_kpath` using `bands_num_points` along the first section of the path and write out an output file in a format specified by `bands_plot_format`.

The default value is `false`.

2.9.8   kpoint_path

Defines the path in k-space along which to calculate the bandstructure. Each line gives the start and end point (with labels) for a section of the path. Values are in fractional coordinates with respect to the primitive reciprocal lattice vectors.

`begin kpoint_path`

$$
\begin{array}{cccccccc}
G & 0.0 & 0.0 & 0.0 & L & 0.0 & 0.0 & 1.0 \\
L & 0.0 & 0.0 & 1.0 & N & 0.0 & 1.0 & 1.0 \\
& \vdots & & & & & &
\end{array}
$$

`end kpoint_path`

There is no default

2.9.9 integer :: bands_num_points

If `bands_plot = true`, then the number of points along the first section of the bandstructure plot given by `kpoint_path`. Other sections will have the same density of k-points.

The default value for `bands_num_points` is 100.

2.9.10 character(len=20) :: bands_plot_format

Format in which to plot the interpolated band structure. The valid options for this parameter are:

– `gnuplot` (default)

– `xmgrace`

Note: it is possible to request output in both formats eg `bands_format = gnuplot xmgrace`

2.9.11 integer :: bands_plot_project(:)

If present `wannier90` will compute the contribution of this set of WF to the states at each point of the interpolated band structure. The WF are numbered according to the seedname.wout file. The result is written in the `seedname_band.dat` file, and a corresponding gnuplot script to `seedname_band_proj.dat`.

For example, to project on to WFs 2, 6, 7, 8 and 12:

`bands_plot_project : 2, 6-8, 12`

2.9.12 character(len=20) :: bands_plot_mode

To interpolate the band structure along the k-point path, either use the Slater-Koster interpolation scheme or truncate the Hamiltonian matrix in the WF basis. Truncation criteria are provided by `hr_cutoff` and `dist_cutoff`.

The valid options for this parameter are:

– `s-k` (default)

– `cut`

2.9.13 integer :: bands_plot_dim

Dimension of the system. If `bands_plot_dim` < 3 and `bands_plot_mode = cut`, lattice vector $\mathbf{R} = N_1\mathbf{A}_1 + N_2\mathbf{A}_2 + N_3\mathbf{A}_3$, where $N_i = 0$ if $\mathbf{A}_i$ is parallel to any of the confined directions specified by `one_dim_axis`, are exclusively used in the band structure interpolation.

The valid options for this parameter are:

– 3 (default)

– 2

– 1

2.9.14 logical :: fermi_surface_plot

If `fermi_surface_plot = true`, then the code will calculate, through Wannier interpolation, the eigenvalues on a regular grid with `fermi_surface_num_points` in each direction. The code will write a file in bxsf format which can be read by XCrySDen in order to plot the Fermi surface.

The default value is `false`.

2.9.15 integer :: fermi_surface_num_points

If `fermi_surface_plot = true`, then the number of divisions in the regular k-point grid used to calculate the Fermi surface.

The default value for `fermi_surface_num_points` is 50.

2.9.16 real(kind=dp) :: fermi_energy

The Fermi energy in eV. This parameter is written into the bxsf file. If `fermi_energy` is specified, `fermi_energy_min`, `fermi_energy_max`, and `fermi_energy_step` should not be specified, and vice-versa.

The default value is 0.0

2.9.17 real(kind=dp) :: fermi_energy_min

Instead of specifying a single Fermi energy, it is possible to scan the Fermi level over a range of values, and recompute certain quantities for each ε_F.[2] This is the minimum value in the range (in eV).

There is no default value.

2.9.18 real(kind=dp) :: fermi_energy_max

The maximum value in the range of Fermi energies. Units are eV.

The default value is `fermi_energy_min`+1.0.

2.9.19 real(kind=dp) :: fermi_energy_step

Difference between consecutive values of the Fermi energy when scanning from `fermi_energy_min` to `fermi_energy_max`. Units are eV.

The default value is 0.01.

---

[2]Scanning the Fermi level is currently supported only by the `postw90` module `berry`, for `berry_task=ahc,morb`. For all other functionalities that require a knowledge of ε_F, use `fermi_energy` instead.

2.9.20   character(len=20) :: fermi_surface_plot_format

Format in which to plot the Fermi surface. The valid options for this parameter are:

 − xcrysden (default)

2.9.21   logical :: hr_plot

If hr_plot = true, then the Hamiltonian matrix in the WF basis will be written to a file seedname_hr.dat.
The default value is false.

2.9.22   logical :: transport

If transport = true, then the code will calculate quantum conductance and density of states of a one-dimensional system. The results will be written to files seedname_qc.dat and seedname_dos.dat, respectively. Since both quantities are a function of energy, they will be evaluated from tran_win_min to tran_win_max with an interval of tran_energy_step.

The default value of this parameter is false.

2.9.23   character(len=20) :: transport_mode

If transport_mode = bulk, quantum conductance and density of states are calculated for a perfectly-periodic one-dimensional system. In this case, the transport part can either use the Hamiltonian matrix in the WF basis generated by wannier90 or a Hamiltonian matrix provided by the external file seedname_htB.dat.

If transport_mode = lcr, quantum conductance and density of states are calculated for a system where semi-infinite, left and right leads are connected through a central conductor region. In this case, the transport part will work independently from the disentanglement and wannierise procedure. Details of the method is described in Ref. [7].

If tran_read_ht = true then the Hamiltonian matrices must be provided by the five external files: seedname_htL.dat, seedname_htLC.dat, seedname_htC.dat, seedname_htCR.dat, seedname_htR.dat. If tran_read_ht = false then the Hamiltonian matrices are found automatically provided the super-cell adheres to conditions outlined in Section 7.3.

The valid options for this parameter are:

 − bulk (default)

 − lcr

2.9.24   real(kind=dp) :: tran_win_min

The lower bound of the energy window for the transport calculation. Units are eV.
The default value is -3.0.

2.9.25 `real(kind=dp) :: tran_win_max`

The upper bound of the energy window for the transport calculation. Units are eV.

The default value is 3.0.

2.9.26 `real(kind=dp) :: tran_energy_step`

Sampling interval of the energy values from `tran_win_min` to `tran_win_max`. Units are eV.

The default value is 0.01.

2.9.27 `real(kind=dp) :: fermi_energy`

The Fermi energy in eV. The energy axis of the quantum conductance and density of states data will be shifted rigidly by this amount.

The default value is 0.0

2.9.28 `integer :: tran_num_bb`

Size of a bulk Hamiltonian matrix. This number is equal to the number of WFs in one principal layer.

A one-dimensional system can be viewed as an array of principal layers which are defined in a way that localized basis functions inside a certain principal layer only interact with those in the nearest neighbor principal layer. In `wannier90` a principal layer will be an integer multiple of a unit cell, and the size is determined by `hr_cutoff` and/or `dist_cutoff`. The criterion is rather arbitrary when WFs are adopted as a localized basis set, and it is up to a user's choice.

The default value is 0.

2.9.29 `integer :: tran_num_ll`

Size of a left-lead Hamiltonian matrix. If `transport_mode = lcr` and `tran_read_ht = false` then `tran_num_ll` is the number of Wannier functions in a principal layer.

The default value is 0.

2.9.30 `integer :: tran_num_rr`

Size of a right-lead Hamiltonian matrix.

The default value is 0.

2.9.31 `integer :: tran_num_cc`

Size of a conductor Hamiltonian matrix.

The default value is 0.

2.9.32 integer :: tran_num_lc

Number of columns in a left-lead_conductor Hamiltonian matrix. Number of rows must be equal to `tran_num_ll`.

The default value is 0.

2.9.33 integer :: tran_num_cr

Number of rows in a conductor_right-lead Hamiltonian matrix. Number of columns must be equal to `tran_num_rr`.

The default value is 0.

2.9.34 integer :: tran_num_cell_ll

Number of unit cells in one principal layer of left lead. Used if `transport_mode = lcr` and `tran_read_ht = false`.

The default value is 0.

2.9.35 integer :: tran_num_cell_rr

Number of unit cells in one principal layer of right lead. Not used at present.

The default value is 0.

2.9.36 integer :: tran_num_bandc

Half-bandwidth+1 of a band-diagonal conductor Hamiltonian matrix.

The Hamiltonian matrix of a central conductor part, which is read from `seedname_htC.dat`, will be diagonally dominant when `tran_num_cc` is very large. `tran_num_bandc` is used to construct a compact matrix which contains the non-zero band-diagonal part of a full conductor Hamiltonian matrix. Setting this parameter is only meaningful when `tran_num_bandc` is greater than `tran_num_lc` and `tran_num_cr`.

The default value is 0.

2.9.37 logical :: tran_write_ht

If `tran_write_ht = true`, then the Hamiltonian matrix formatted for the transport calculation will be written to a file `seedname_htB.dat`.

The default value is `false`.

2.9.38 logical :: tran_read_ht

If `tran_write_ht = true`, then the Hamiltonian matrix formatted for the transport calculation will be read from a set of files described in the parameter `transport_mode`. Set `tran_write_ht = false` to perform automated lcr calculations (see Section 7.3).

The default value is `false`.

2.9.39 logical :: tran_use_same_lead

If `tran_use_same_lead = true`, then the left and the right leads are the same. In this case, `seedname_htR.dat` is not required.

The default value is `true`.

2.9.40 real(kind=dp) :: tran_group_threshold

Used to group and sort Wannier functions according to the positions of their centres. Wannier functions in a group are within `tran_group_threshold` from one another in `x,y` and `z` directions. Units are Å

The default is 0.15

2.9.41 real(kind=dp) :: translation_centre_frac(3)

Centre of the unit cell to which the final Wannier centers are translated. Numbers are in fractional coordinates with respect to the lattice vectors.

The default value is (0.0,0.0,0.0).

2.9.42 real(kind=dp) :: hr_cutoff

The absolute value of the smallest matrix element of the Hamiltonian in the WF basis. If $h_{mn}(\mathbf{R}) >$ `hr_cutoff`, then the matrix element $h_{mn}(\mathbf{R})$ is retained and used in the band structure interpolation (when `bands_plot_mode = cut`) or in the transport calculation. Otherwise it is deemed to be insignificant and is discarded. Units are eV.

The default value is 0.0.

2.9.43 real(kind=dp) :: dist_cutoff

The largest distance between two WFs for which the Hamiltonian matrix element is retained and used in the band interpolation (when `bands_plot_mode = cut`) or in the transport calculation. Units are Å.

The default value is 1000.0.

2.9.44 character(len=20) :: dist_cutoff_mode

Dimension in which the distance between two WFs is calculated. The vector connecting two WFs may be projected to a line (one_dim) or a plane (two_dim). The size of the projected vector is calculated, and dist_cutoff is applied. When one_dim or two_dim is used, one_dim_axis must be given to specify extended or confined direction.

The valid options for this parameter are:

 – three_dim (default)

 – two_dim

 – one_dim

2.9.45 character(len=20) :: one_dim_axis

Extended direction for a one-dimensional system or confined direction for a two-dimensional system. This direction must be parallel to one of the Cartesian axes.

The valid options for this parameter are:

 – x

 – y

 – z

No default.

Chapter 3

Projections

3.1 Specification of projections in `seedname.win`

Here we describe the projection functions used to construct the initial guess $A_{mn}^{(\mathbf{k})}$ for the unitary transformations.

Each projection is associated with a site and an angular momentum state defining the projection function. Optionally, one may define, for each projection, the spatial orientation, the radial part, the diffusivity, and the volume over which real-space overlaps A_{mn} are calculated.

The code is able to

1. project onto s,p,d and f angular momentum states, plus the hybrids sp, sp^2, sp^3, sp^3d, sp^3d^2.

2. control the radial part of the projection functions to allow higher angular momentum states, e.g., both 3s and 4s in silicon.

The atomic orbitals of the hydrogen atom provide a good basis to use for constructing the projection functions: analytical mathematical forms exist in terms of the good quantum numbers n, l and m; hybrid orbitals (sp, sp^2, sp^3, sp^3d etc.) can be constructed by simple linear combination $|\phi\rangle = \sum_{nlm} C_{nlm} |nlm\rangle$ for some coefficients C_{nlm}.

The angular functions that use as a basis for the projections are not the canonical spherical harmonics Y_{lm} of the hydrogenic Schrödinger equation but rather the *real* (in the sense of non-imaginary) states $\Theta_{lm_{\mathrm{r}}}$, obtained by a unitary transformation. For example, the canonical eigenstates associated with $l = 1$, $m = \{-1, 0, 1\}$ are not the real p_x, p_y and p_z that we want. See Section 3.4 for our mathematical conventions regarding projection orbitals for different n, l and m_{r}.

We use the following format to specify projections in `<seedname>.win`:

```
Begin Projections
[units]
site:ang_mtm:zaxis:xaxis:radial:zona
    ⋮
End Projections
```

Notes:

`units`:

Optional. Either `Ang` or `Bohr` to specify whether the projection centres specified in this block (if given in Cartesian co-ordinates) are in units of Angstrom or Bohr, respectively. The default value is `Ang`.

`site`:

`C`, `Al`, etc. applies to all atoms of that type

`f=0,0.50,0` – centre on $(0.0,0.5,0.0)$ in **f**ractional coordinates (crystallographic units) relative to the direct lattice vectors

`c=0.0,0.805,0.0` – centre on $(0.0,0.805,0.0)$ in **C**artesian coordinates in units specified by the optional string `units` in the first line of the projections block (see above).

`ang_mtm`:

Angular momentum states may be specified by `l` and `mr`, or by the appropriate character string. See Tables 3.1 and 3.2. Examples:

`l=2,mr=1` or `dz2` – a single projection with $l = 2$, $m_r = 1$ (i.e., d_{z^2})

`l=2,mr=1,4` or `dz2,dx2-y2` – two functions: d_{z^2} and d_{xz}

`l=-3` or `sp3` – four sp^3 hybrids

Specific hybrid orbitals may be specified as follows:

`l=-3,mr=1,3` or `sp3-1,sp3-3` – two specific sp^3 hybrids

Multiple states may be specified by separating with ';', e.g.,

`sp3;l=0` or `l=-3;l=0` – four sp^3 hybrids and one s orbital

`zaxis` (optional):

`z=1,1,1` – set the z-axis to be in the $(1,1,1)$ direction. Default is `z=0,0,1`

`xaxis` (optional):

`x=1,1,1` – set the x-axis to be in the $(1,1,1)$ direction. Default is `x=1,0,0`

`radial` (optional):

`r=2` – use a radial function with one node (ie second highest pseudostate with that angular momentum). Default is `r=1`. Radial functions associated with different values of `r` should be orthogonal to each other.

`zona` (optional):

`zona=2.0` – the value of $\frac{Z}{a}$ for the radial part of the atomic orbital (controls the diffusivity of the radial function). Units always in reciprocal Angstrom. Default is `zona=1.0`.

Examples

1. CuO, s,p and d on all Cu; sp^3 hybrids on O:

`Cu:l=0;l=1;l=2`

`O:l=-3` or `O:sp3`

2. A single projection onto a p$_z$ orbital orientated in the $(1,1,1)$ direction:

`c=0,0,0:l=1,mr=1:z=1,1,1` or `c=0,0,0:pz:z=1,1,1`

3. Project onto s, p and d (with no radial nodes), and s and p (with one radial node) in silicon:

`Si:l=0;l=1;l=2`

`Si:l=0;l=1:r=2`

3.2 Spinor Projections

When `spinors=.true.` it is possible to select a set of localised functions to project onto 'up' states and a set to project onto 'down' states where, for complete flexibility, it is also possible to set the local spin quantisation axis.

Note, however, that this feature requires a recent version of the interface between the ab-initio code and Wannier90 (i.e., written after the release of the 2.0 version, in October 2013) supporting spinor projections.

```
Begin Projections
[units]
site:ang_mtm:zaxis:xaxis:radial:zona(spin)[quant_dir]
    ⋮
End Projections
```

`spin` (optional):
Choose projection onto 'up' or 'down' states
`u` – project onto 'up' states.
`d` – project onto 'down' states.
Default is `u,d`

`quant_dir` (optional):
`1,0,0` – set the spin quantisation axis to be in the (1,0,0) direction. Default is `0,0,1`

Examples

- 18 projections on an iron site

  `Fe:sp3d2;dxy;dxx;dyz`

- same as above

  `Fe:sp3d2;dxy;dxx;dyz(u,d)`

- same as above

  `Fe:sp3d2;dxy;dxz;dyz(u,d)[0,0,1]`

- same as above but quantisation axis is now x

  `Fe:sp3d2;dxy;dxz;dyz(u,d)[1,0,0]`

- now only 9 projections onto up states

  `Fe:sp3d2;dxy;dxz;dyz(u)`

- 9 projections onto up-states and 3 on down

  `Fe:sp3d2;dxy;dxz;dyz(u)`
  `Fe:dxy;dxz;dyz(d)`

- projections onto alternate spin states for two lattice sites (Cr1, Cr2)

  `Cr1:d(u)`
  `Cr2:d(d)`

3.3 Short-Cuts

3.3.1 Random projections

It is possible to specify the projections, for example, as follows:

```
Begin Projections
random
C:sp3
End Projections
```

in which case `wannier90` uses four sp^3 orbitals centred on each C atom and then chooses the appropriate number of randomly-centred s-type Gaussian functions for the remaining projection functions. If the block only consists of the string `random` and no specific projection centres are given, then all of the projection centres are chosen randomly.

3.3.2 Bloch phases

Setting `use_bloch_phases = true` in the input file absolves the user of the need to specify explicit projections. In this case, the Bloch wave-functions are used as the projection orbitals, namely $A_{mn}^{(\mathbf{k})} = \langle \psi_{m\mathbf{k}} | \psi_{n\mathbf{k}} \rangle = \delta_{mn}$.

3.4 Orbital Definitions

The angular functions $\Theta_{lm_{\mathrm{r}}}(\theta, \varphi)$ associated with particular values of l and m_{r} are given in Tables 3.1 and 3.2.

The radial functions $R_{\mathrm{r}}(r)$ associated with different values of r should be orthogonal. One choice would be to take the set of solutions to the radial part of the hydrogenic Schrödinger equation for $l = 0$, i.e., the radial parts of the 1s, 2s, 3s. . . orbitals, which are given in Table 3.3.

l	$m_{\rm r}$	Name	$\Theta_{lm_{\rm r}}(\theta, \varphi)$
0	1	s	$\frac{1}{\sqrt{4\pi}}$
1	1	pz	$\sqrt{\frac{3}{4\pi}}\cos\theta$
1	2	px	$\sqrt{\frac{3}{4\pi}}\sin\theta\cos\varphi$
1	3	py	$\sqrt{\frac{3}{4\pi}}\sin\theta\sin\varphi$
2	1	dz2	$\sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$
2	2	dxz	$\sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\cos\varphi$
2	3	dyz	$\sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\sin\varphi$
2	4	dx2-y2	$\sqrt{\frac{15}{16\pi}}\sin^2\theta\cos 2\varphi$
2	5	dxy	$\sqrt{\frac{15}{16\pi}}\sin^2\theta\sin 2\varphi$
3	1	fz3	$\frac{\sqrt{7}}{4\sqrt{\pi}}(5\cos^3\theta - 3\cos\theta)$
3	2	fxz2	$\frac{\sqrt{21}}{4\sqrt{2\pi}}(5\cos^2\theta - 1)\sin\theta\cos\varphi$
3	3	fyz2	$\frac{\sqrt{21}}{4\sqrt{2\pi}}(5\cos^2\theta - 1)\sin\theta\sin\varphi$
3	4	fz(x2-y2)	$\frac{\sqrt{105}}{4\sqrt{\pi}}\sin^2\theta\cos\theta\cos 2\varphi$
3	5	fxyz	$\frac{\sqrt{105}}{4\sqrt{\pi}}\sin^2\theta\cos\theta\sin 2\varphi$
3	6	fx(x2-3y2)	$\frac{\sqrt{35}}{4\sqrt{2\pi}}\sin^3\theta(\cos^2\varphi - 3\sin^2\varphi)\cos\varphi$
3	7	fy(3x2-y2)	$\frac{\sqrt{35}}{4\sqrt{2\pi}}\sin^3\theta(3\cos^2\varphi - \sin^2\varphi)\sin\varphi$

Table 3.1: Angular functions $\Theta_{lm_{\rm r}}(\theta, \varphi)$ associated with particular values of l and $m_{\rm r}$ for $l \geq 0$.

l	m_{r}	Name	$\Theta_{lm_{\mathrm{r}}}(\theta, \varphi)$
-1	1	sp-1	$\frac{1}{\sqrt{2}}\mathrm{s} + \frac{1}{\sqrt{2}}\mathrm{px}$
-1	2	sp-2	$\frac{1}{\sqrt{2}}\mathrm{s} - \frac{1}{\sqrt{2}}\mathrm{px}$
-2	1	sp2-1	$\frac{1}{\sqrt{3}}\mathrm{s} - \frac{1}{\sqrt{6}}\mathrm{px} + \frac{1}{\sqrt{2}}\mathrm{py}$
-2	2	sp2-2	$\frac{1}{\sqrt{3}}\mathrm{s} - \frac{1}{\sqrt{6}}\mathrm{px} - \frac{1}{\sqrt{2}}\mathrm{py}$
-2	3	sp2-3	$\frac{1}{\sqrt{3}}\mathrm{s} + \frac{2}{\sqrt{6}}\mathrm{px}$
-3	1	sp3-1	$\frac{1}{2}(\mathrm{s} + \mathrm{px} + \mathrm{py} + \mathrm{pz})$
-3	2	sp3-2	$\frac{1}{2}(\mathrm{s} + \mathrm{px} - \mathrm{py} - \mathrm{pz})$
-3	3	sp3-3	$\frac{1}{2}(\mathrm{s} - \mathrm{px} + \mathrm{py} - \mathrm{pz})$
-3	4	sp3-4	$\frac{1}{2}(\mathrm{s} - \mathrm{px} - \mathrm{py} + \mathrm{pz})$
-4	1	sp3d-1	$\frac{1}{\sqrt{3}}\mathrm{s} - \frac{1}{\sqrt{6}}\mathrm{px} + \frac{1}{\sqrt{2}}\mathrm{py}$
-4	2	sp3d-2	$\frac{1}{\sqrt{3}}\mathrm{s} - \frac{1}{\sqrt{6}}\mathrm{px} - \frac{1}{\sqrt{2}}\mathrm{py}$
-4	3	sp3d-3	$\frac{1}{\sqrt{3}}\mathrm{s} + \frac{2}{\sqrt{6}}\mathrm{px}$
-4	4	sp3d-4	$\frac{1}{\sqrt{2}}\mathrm{pz} + \frac{1}{\sqrt{2}}\mathrm{dz2}$
-4	5	sp3d-5	$-\frac{1}{\sqrt{2}}\mathrm{pz} + \frac{1}{\sqrt{2}}\mathrm{dz2}$
-5	1	sp3d2-1	$\frac{1}{\sqrt{6}}\mathrm{s} - \frac{1}{\sqrt{2}}\mathrm{px} - \frac{1}{\sqrt{12}}\mathrm{dz2} + \frac{1}{2}\mathrm{dx2\text{-}y2}$
-5	2	sp3d2-2	$\frac{1}{\sqrt{6}}\mathrm{s} + \frac{1}{\sqrt{2}}\mathrm{px} - \frac{1}{\sqrt{12}}\mathrm{dz2} + \frac{1}{2}\mathrm{dx2\text{-}y2}$
-5	3	sp3d2-3	$\frac{1}{\sqrt{6}}\mathrm{s} - \frac{1}{\sqrt{2}}\mathrm{py} - \frac{1}{\sqrt{12}}\mathrm{dz2} - \frac{1}{2}\mathrm{dx2\text{-}y2}$
-5	4	sp3d2-4	$\frac{1}{\sqrt{6}}\mathrm{s} + \frac{1}{\sqrt{2}}\mathrm{py} - \frac{1}{\sqrt{12}}\mathrm{dz2} - \frac{1}{2}\mathrm{dx2\text{-}y2}$
-5	5	sp3d2-5	$\frac{1}{\sqrt{6}}\mathrm{s} - \frac{1}{\sqrt{2}}\mathrm{pz} + \frac{1}{\sqrt{3}}\mathrm{dz2}$
-5	6	sp3d2-6	$\frac{1}{\sqrt{6}}\mathrm{s} + \frac{1}{\sqrt{2}}\mathrm{pz} + \frac{1}{\sqrt{3}}\mathrm{dz2}$

Table 3.2: Angular functions $\Theta_{lm_{\mathrm{r}}}(\theta, \varphi)$ associated with particular values of l and m_{r} for $l < 0$, in terms of the orbitals defined in Table 3.1.

r	$R_{\mathrm{r}}(r)$
1	$2\alpha^{3/2}\exp(-\alpha r)$
2	$\frac{1}{2\sqrt{2}}\alpha^{3/2}(2-\alpha r)\exp(-\alpha r/2)$
3	$\sqrt{\frac{4}{27}}\alpha^{3/2}(1-2\alpha r/3+2\alpha^2 r^2/27)\exp(-\alpha r/3)$

Table 3.3: One possible choice for the radial functions $R_{\mathrm{r}}(r)$ associated with different values of r: the set of solutions to the radial part of the hydrogenic Schrödinger equation for $l=0$, i.e., the radial parts of the 1s, 2s, 3s... orbitals, where $\alpha = Z/a = $ `zona`.

Chapter 4

Code Overview

`wannier90` can operate in two modes:

1. *Post-processing mode:* read in the overlaps and projections from file as computed inside a first-principles code. We expect this to be the most common route to using `wannier90`, and is described in Ch. 5;

2. *Library mode:* as a set of library routines to be called from within a first-principles code that passes the overlaps and projections to the `wannier90` library routines and in return gets the unitary transformation corresponding to MLWF. This route should be used if the MLWF are needed within the first-principles code, for example in post-LDA methods such as LDA+U or SIC, and is described in Ch. 6.
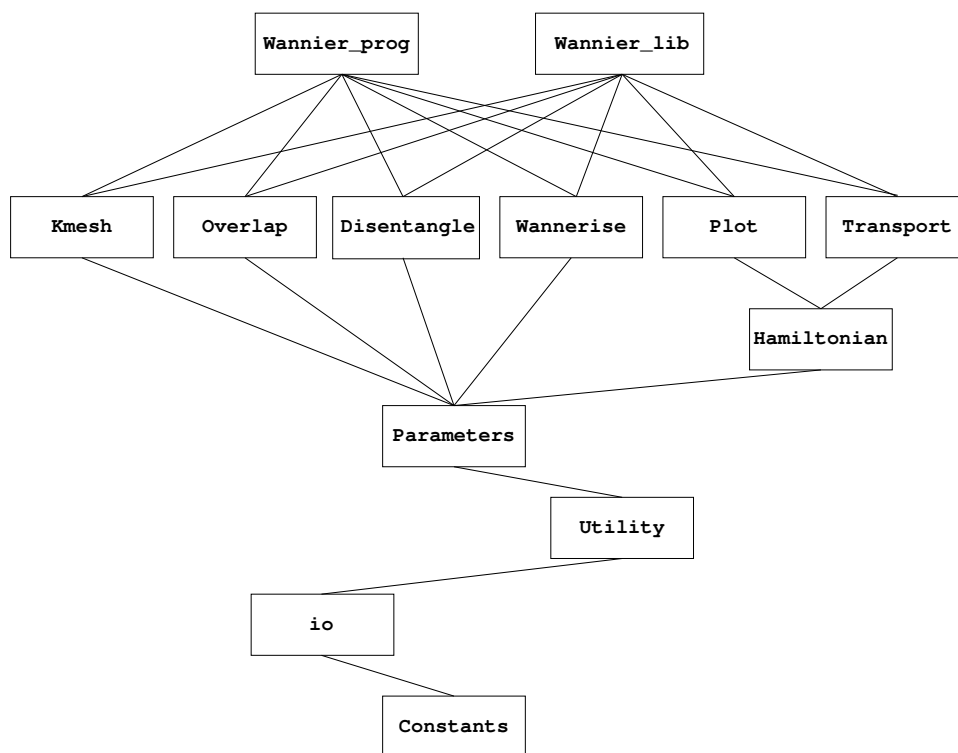
Figure 4.1: Schematic overview of the module structure of `wannier90`. Modules may only use data and subroutines from lower modules.

Chapter 5

`wannier90` as a post-processing tool

This is a description of how to use `wannier90` as a post-processing tool.

The code must be run twice. On the first pass either the logical keyword `postproc_setup` must be set to `.true.` in the input file `seedname.win` or the code must be run with the command line option `-pp`. Running the code then generates the file `seedname.nnkp` which provides the information required to construct the $M_{mn}^{(\mathbf{k},\mathbf{b})}$ overlaps (Ref. [1], Eq. (25)) and $A_{mn}^{(\mathbf{k})}$ (Ref. [1], Eq. (62); Ref. [2], Eq. (22)).

Once the overlaps and projection have been computed and written to files `seedname.mmn` and `seedname.amn`, respectively, set `postproc_setup` to `.false.` and run the code. Output is written to the file `seedname.wout`.

5.1 `seedname.nnkp` file

OUTPUT, if `postproc_setup = .true.`

The file `seedname.nnkp` provides the information needed to determine the required overlap elements $M_{mn}^{(\mathbf{k},\mathbf{b})}$ and projections $A_{mn}^{(\mathbf{k})}$. It is written automatically when the code is invoked with the `-pp` command-line option (or when `postproc_setup=.true.` in `seedname.win`. There should be no need for the user to edit this file.

Much of the information in `seedname.nnkp` is arranged in blocks delimited by the strings `begin block_name` ...`end block_name`, as described below.

5.1.1 Keywords

The first line of the file is a user comment, e.g., the date and time:

`File written on 12Feb2006 at 15:13:12`

The only logical keyword is `calc_only_A`, eg,

`calc_only_A  :  F`

5.1.2 `Real_lattice` block

`begin real_lattice`

```
 2.250000     0.000000     0.000000
 0.000000     2.250000     0.000000
 0.000000     0.000000     2.250000
end real_lattice
```

The real lattice vectors in units of Angstrom.

5.1.3 `Recip_lattice` **block**

```
begin recip_lattice
 2.792527     0.000000     0.000000
 0.000000     2.792527     0.000000
 0.000000     0.000000     2.792527
end recip_lattice
```

The reciprocal lattice vectors in units of inverse Angstrom.

5.1.4 `Kpoints` **block**

```
begin kpoints
  8
  0.00000     0.00000     0.00000
  0.00000     0.50000     0.00000
    .
    .
    .
  0.50000     0.50000     0.50000
end kpoints
```

The first line in the block is the total number of k-points `num_kpts`. The subsequent `num_kpts` lines specify the k-points in crystallographic co-ordinates relative to the reciprocal lattice vectors.

5.1.5 `Projections` **block**

```
begin projections
   n_proj
   centre   l  mr  r
     z-axis   x-axis   zona
   centre   l  mr  r
     z-axis   x-axis   zona
    .
    .
end projections
```

Notes:

`n_proj`: integer; the number of projection centres, equal to the number of MLWF `num_wann`.

centre: three real numbers; projection function centre in crystallographic co-ordinates relative to the direct lattice vectors.

l mr r: three integers; l and m_r specify the angular part $\Theta_{lm_r}(\theta, \varphi)$, and r specifies the radial part $R_r(r)$ of the projection function (see Tables 3.1, 3.2 and 3.3).

z-axis: three real numbers; default is `0.0 0.0 1.0`; defines the axis from which the polar angle θ in spherical polar coordinates is measured.

x-axis: three real numbers; must be orthogonal to `z-axis`; default is `1.0 0.0 0.0` or a vector perpendicular to `z-axis` if `z-axis` is given; defines the axis from with the azimuthal angle φ in spherical polar coordinates is measured.

zona: real number; the value of $\frac{Z}{a}$ associated with the radial part of the atomic orbital. Units are in reciprocal Angstrom.

5.1.6 `spinor_projections` block

```
begin spinor_projections
   n_proj
   centre   l  mr  r
    z-axis   x-axis   zona
     spin spn_quant
   centre   l  mr  r
    z-axis   x-axis   zona
     spin spn_quant
   .
   .
end spinor_projections
```

Notes: Only one of projections and spinor_projections should be defined. Variables are the same as the projections block with the addition of `spin` and `spn_quant`.

spin: integer. '1' or '-1' to denote projection onto up or down states.

spn_quant: three real numbers. Defines the spin quantisation axis in Cartesian coordinates.

5.1.7 `nnkpts` block

```
begin nnkpts
  10
  1   2   0  0  0
  .
  .
end nnkpts
```

First line: **nntot**, the number of nearest neighbours belonging to each k-point of the Monkhorst-Pack mesh

Subsequent lines: **nntot**×**num_kpts** lines, ie, **nntot** lines of data for each k-point of the mesh.

Each line of consists of 5 integers. The first is the k-point number `nkp`. The second to the fifth specify it's nearest neighbours $\mathbf{k} + \mathbf{b}$: the second integer points to the k-point that is the periodic image of the $\mathbf{k} + \mathbf{b}$ that we want; the last three integers give the G-vector, in reciprocal lattice units, that brings the k-point specified by the second integer (which is in the first BZ) to the actual $\mathbf{k} + \mathbf{b}$ that we need.

5.1.8 `exclude_bands` block

```
begin exclude_bands
  8
  1
  2
  .
  .
end exclude_bands
```

To exclude bands (independent of k-point) from the calculation of the overlap and projection matrices, for example to ignore shallow-core states. The first line is the number of states to exclude, the following lines give the states for be excluded.

5.1.9 An example of projections

As a concrete example: one wishes to have a set of four sp^3 projection orbitals on, say, a carbon atom at (0.5,0.5,0.5) in fractional co-ordinates relative to the direct lattice vectors. In this case `seedname.win` will contain the following lines:

```
begin projections
 C:l=-1
end projections
```

and `seedname.nnkp`, generated on the first pass of `wannier90` (with `postproc_setup=T`), will contain:

```
begin projections
   4
   0.50000    0.50000    0.50000    -1  1  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
   0.50000    0.50000    0.50000    -1  2  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
   0.50000    0.50000    0.50000    -1  3  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
   0.50000    0.50000    0.50000    -1  4  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
end projections
```

where the first line tells us that in total four projections are specified, and the subsquent lines provide the projection centre, the angular and radial parts of the orbital (see Section 3.4 for definitions), the z and x axes, and the diffusivity and cut-off radius for the projection orbital.

PWSCF, or any other *ab initio* electronic structure code, then reads `seedname.nnkp` file, calculates the projections and writes them to `seedname.amn`.

5.2 `seedname.mmn` file

INPUT.

The file `seedname.mmn` contains the overlaps $M_{mn}^{(\mathbf{k},\mathbf{b})}$.

First line: a user comment, e.g., the date and time

Second line: 3 integers: `num_bands`, `num_kpts`, `nntot`

Then: `num_kpts` $\times$ `nntot` blocks of data:

First line of each block: 5 integers. The first specifies the $\mathbf{k}$ (i.e., gives the ordinal corresponding to its position in the list of k-points in `seedname.win`). The 2nd to 5th integers specify $\mathbf{k} + \mathbf{b}$. The 2nd integer, in particular, points to the k-point on the list that is a periodic image of $\mathbf{k} + \mathbf{b}$, and in particular is the image that is actually mentioned in the list. The last three integers specify the $\mathbf{G}$ vector, in reciprocal lattice units, that brings the k-point specified by the second integer, and that thus lives inside the first BZ zone, to the actual $\mathbf{k} + \mathbf{b}$ that we need.

Subsequent `num_bands` $\times$ `num_bands` lines of each block: two real numbers per line. These are the real and imaginary parts, respectively, of the actual scalar product $M_{mn}^{(\mathbf{k},\mathbf{b})}$ for $m, n \in [1, \texttt{num\_bands}]$. The order of these elements is such that the first index m is fastest.

5.3 `seedname.amn` file

INPUT.

The file `seedname.amn` contains the projection $A_{mn}^{(\mathbf{k})}$.

First line: a user comment, e.g., the date and time

Second line: 3 integers: `num_bands`, `num_kpts`, `num_wann`

Subsequently `num_bands` $\times$ `num_wann` $\times$ `num_kpts` lines: 3 integers and 2 real numbers on each line. The first two integers are the band indices m and n. The third integer specifies the $\mathbf{k}$ by giving the ordinal corresponding to its position in the list of k-points in `seedname.win`. The real numbers are the real and imaginary parts, respectively, of the actual $A_{mn}^{(\mathbf{k})}$.

5.4 `seedname.eig` file

INPUT.

Required if any of `disentanglement`, `plot_bands`, `plot_fermi_surface` or `hr_plot` are `.true.`

The file `seedname.eig` contains the Kohn-Sham eigenvalues $\varepsilon_{n\mathbf{k}}$ (in eV) at each point in the Monkhorst-Pack mesh.

Each line consist of two integers and a real number. The first integer is the band index, the second integer gives the ordinal corresponding to the k-point in the list of k-points in `seedname.win`, and the real number is the eigenvalue.

E.g.,

```
        1          1  -6.43858831271328
        2          1   19.3977795287297
        3          1   19.3977795287297
        4          1   19.3977795287298
```

5.5   Interface with PWSCF

Interfaces between `wannier90` and many ab-initio codes as PWSCF, ABINIT (`http://www.abinit.org`), SIESTA (`http://www.icmab.es/siesta/`), FLEUR, VASP and WIEN2K (`http://www.wien2k.at`) are available. Here we describe the seamless interface between `wannier90` and PWSCF, a plane-wave DFT code that comes as part of the QUANTUM ESPRESSO package (see `http://www.quantum-espresso.org`). You will need to download and compile PWSCF (i.e., the `pw.x` code) and the post-processing interface `pw2wannier90.x`. Please refer to the documentation that comes with the QUANTUM ESPRESSO distribution for instructions.

1. Run 'scf'/'nscf' calculation(s) with `pw`

2. Run `wannier90` with `postproc_setup = .true.` to generate `seedname.nnkp`

3. Run `pw2wannier90`. First it reads an input file, e.g., `seedname.pw2wan`, which defines `prefix` and `outdir` for the underlying 'scf' calculation, as well as the name of the file `seedname.nnkp`, and does a consistency check between the direct and reciprocal lattice vectors read from `seedname.nnkp` and those defined in the files specified by `prefix`. `pw2wannier90` generates `seedname.mmn`, `seedname.amn` and `seedname.eig`

4. Run `wannier90` with `postproc_setup = .false.` to disentangle bands (if required), localise MLWF, and use MLWF for plotting, bandstructures, Fermi surfaces etc.

Examples of how the interface with PWSCF works are given in the `wannier90` Tutorial.

5.5.1   `seedname.pw2wan`

A number of keywords may be specified in the `pw2wannier90` input file:

- `outdir` – Location to write output files. Default is './'

- `prefix` – Prefix for the PWSCF calculation. Default is ' '

- `seedname` – Seedname for the `wannier90` calculation. Default is 'wannier'

- `spin_component` – Spin component. Takes values 'up', 'down' or 'none' (default).

- `wan_mode` – Either 'standalone' (default) or 'library'

- `write_unk` – Set to `.true.` to write the periodic part of the Bloch functions for plotting in `wannier90`. Default is `.false.`

- `reduce_unk` – Set to `.true.` to reduce file-size (and resolution) of Bloch functions by a factor of 8. Default is `.false.` (only relevant if `write_unk=.true.`)[1]

---

[1]Note that there is a small bug with this feature in v3.2 (and subsequent patches) of `quantum-espresso`. Please use a later version (if available) or the CVS version of `pw2wannier90.f90`, which has been fixed.

- `wvfn_formatted` – Set to `.true.` to write formatted wavefunctions. Default is `.false.` (only relevant if `write_unk=.true.`)

- `write_amn` – Set to `.false.` if $A_{mn}^{(\mathbf{k})}$ not required. Default is `.true.`

- `write_mmn` – Set to `.false.` if $M_{mn}^{(\mathbf{k,b})}$ not required. Default is `.true.`

- `write_spn` – Set to `.true.` to write out the matrix elements of S between Bloch states (non-collinear spin calculation only). Default is `.false.`

- `spn_formatted` – Set to `.true.` to write spn data as a formatted file. Default is `.false.` (only relevant if `write_spn=.true.`)

- `write_uHu` – Set to `.true.` to write out the matrix elements

$$\langle u_{n\mathbf{k}+\mathbf{b}_1}|H_{\mathbf{k}}|u_{m\mathbf{k}+\mathbf{b}_2}\rangle.$$

  Default is `.false.`

- `uHu_formatted` – Set to `.true.` to write uHu data as a formatted file. Default is `.false.` (only relevant if `write_uHu=.true.`)

- `write_uIu` – Set to `.true.` to write out the matrix elements of

$$\langle u_{n\mathbf{k}+\mathbf{b}_1}|u_{m\mathbf{k}+\mathbf{b}_2}\rangle.$$

  Default is `.false.`

- `uIu_formatted` – Set to `.true.` to write uIu data as a formatted file. Default is `.false.` (only relevant if `write_uIu=.true.`)

- `write_unkg` – Set to `.true.` to write the first few Fourier components of the periodic parts of the Bloch functions.

For examples of use, refer to the `wannier90` Tutorial.

Chapter 6

`wannier90` as a library

This is a description of the interface between any external program and the wannier code. There are two subroutines: `wannier_setup` and `wannier_run`. Calling `wannier_setup` will return information required to construct the $M_{mn}^{(\mathbf{k},\mathbf{b})}$ overlaps (Ref. [1], Eq. (25)) and $A_{mn}^{(\mathbf{k})} = \langle \psi_{m\mathbf{k}} | g_n \rangle$ projections (Ref. [1], Eq. (62); Ref. [2], Eq. (22)). Once the overlaps and projection have been computed, calling `wannier_run` activates the minimisation and plotting routines in `wannier90`.

6.1   Subroutines

6.1.1   `wannier_setup`

```
wannier_setup(seed_name,mp_grid,num_kpts,real_lattice,recip_lattice,
              kpt_latt,num_bands_tot,num_atoms,atom_symbols,atoms_cart,
              gamma_only,spinors,nntot,nnlist,nncell,num_bands,num_wann,proj_site,
              proj_l,proj_m,proj_radial,proj_z,proj_x,proj_zona,
              exclude_bands,proj_s,proj_s_qaxis)
```

- `character(len=*), intent(in) :: seed_name`
  The seedname of the current calculation.

- `integer, dimension(3), intent(in) :: mp_grid`
  The dimensions of the Monkhorst-Pack k-point grid.

- `integer, intent(in) :: num_kpts`
  The number of k-points on the Monkhorst-Pack grid.

- `real(kind=dp), dimension(3,3), intent(in) :: real_lattice`
  The lattice vectors in Cartesian co-ordinates in units of Angstrom.

- `real(kind=dp), dimension(3,3), intent(in) :: recip_lattice`
  The reciprocal lattice vectors in Cartesian co-ordinates in units of reciprocal Angstrom.

- `real(kind=dp), dimension(3,num_kpts), intent(in) :: kpt_latt`
  The positions of the k-points in fractional co-ordinates relative to the reciprocal lattice vectors.

- `integer, intent(in) :: num_bands_tot`
  The total number of bands in the first-principles calculation (note: including semi-core states).

- `integer, intent(in) :: num_atoms`
  The total number of atoms in the system.

- `character(len=20), dimension(num_atoms), intent(in) :: atom_symbols`
  The elemental symbols of the atoms.

- `real(kind=dp), dimension(3,num_atoms), intent(in) :: atoms_cart`
  The positions of the atoms in Cartesian co-ordinates in Angstrom.

- `logical, intent(in) :: gamma_only`
  Set to `.true.` if the underlying electronic structure calculation has been performed with only Γ-point sampling and, hence, if the Bloch eigenstates that are used to construct $A_{mn}^{(\mathbf{k})}$ and $M_{mn}^{(\mathbf{k},\mathbf{b})}$ are real.

- `logical, intent(in) :: spinors`
  Set to `.true.` if underlying electronic structure calculation has been performed with spinor wavefunctions.

- `integer, intent(out) :: nntot`
  The total number of nearest neighbours for each k-point.

- `integer, dimension(num_kpts,num_nnmax), intent(out) :: nnlist`
  The list of nearest neighbours for each k-point.

- `integer,dimension(3,num_kpts,num_nnmax), intent(out) :: nncell`
  The vector, in fractional reciprocal lattice co-ordinates, that brings the `nn`th nearest neighbour of k-point `nkp` to its periodic image that is needed for computing the overlap $M_{mn}^{(\mathbf{k},\mathbf{b})}$.

- `integer, intent(out) :: num_bands`
  The number of bands in the first-principles calculation used to form the overlap matricies (note: excluding eg. semi-core states).

- `integer, intent(out) :: num_wann`
  The number of MLWF to be extracted.

- `real(kind=dp), dimension(3,num_bands_tot), intent(out) :: proj_site`
  Projection function centre in crystallographic co-ordinates relative to the direct lattice vectors.

- `integer, dimension(num_bands_tot), intent(out) :: proj_l`
  l specifies the angular part $\Theta_{lm_\mathrm{r}}(\theta,\varphi)$ of the projection function (see Tables 3.1, 3.2 and 3.3).

- `integer, dimension(num_bands_tot), intent(out) :: proj_m`
  m_r specifies the angular part $\Theta_{lm_\mathrm{r}}(\theta,\varphi)$, of the projection function (see Tables 3.1, 3.2 and 3.3).

- `integer, dimension(num_bands_tot), intent(out) :: proj_radial`
  r specifies the radial part $R_\mathrm{r}(r)$ of the projection function (see Tables 3.1, 3.2 and 3.3).

- `real(kind=dp), dimension(3,num_bands_tot), intent(out) :: proj_z`
  Defines the axis from which the polar angle θ in spherical polar coordinates is measured. Default is `0.0 0.0 1.0`.

- `real(kind=dp), dimension(3,num_bands_tot), intent(out) :: proj_x`
  Must be orthogonal to `z-axis`; default is `1.0 0.0 0.0` or a vector perpendicular to `proj_z` if `proj_z` is given; defines the axis from with the azimuthal angle φ in spherical polar coordinates is measured.

- `real(kind=dp), dimension(num_bands_tot), intent(out) :: proj_zona`
  The value of $\frac{Z}{a}$ associated with the radial part of the atomic orbital. Units are in reciprocal Angstrom.

- `integer, dimension(num_bands_tot), intent(out) :: exclude_bands`
  Kpoints independant list of bands to exclude from the calculation of the MLWF (e.g., semi-core states).

- `integer, dimension(num_bands_tot), optional,intent(out) :: proj_s`
  '1' or '-1' to denote projection onto up or down spin states

- `real(kind=dp), dimension(3,num_bands_tot), intent(out) :: proj_s_qaxisx`
  Defines the spin quantisation axis in Cartesian coordinates.

Conditions:

- ⋆ `num_kpts` = `mp_grid(1)` × `mp_grid(2)` × `mp_grid(3)`.

- ⋆ `num_nnmax` = 12

This subroutine returns the information required to determine the required overlap elements $M_{mn}^{(\mathbf{k},\mathbf{b})}$ and projections $A_{mn}^{(\mathbf{k})}$, i.e., `M_matrix` and `A_matrix`, described in Section 6.1.2.

For the avoidance of doubt, `real_lattice(1,2)` is the $y-$component of the first lattice vector $\mathbf{A}_1$, etc.

The list of nearest neighbours of a particular k-point `nkp` is given by `nnlist(nkp,1:nntot)`.

Additionally, the parameter `shell_list` may be specified in the `wannier90` input file.

6.1.2   `wannier_run`

```
wannier_run(seed_name,mp_grid,num_kpts,real_lattice,recip_lattice,
           kpt_latt,num_bands,num_wann,nntot,num_atoms,atom_symbols,
           atoms_cart,gamma_only,M_matrix_orig,A_matrix,eigenvalues,
           U_matrix,U_matrix_opt,lwindow,wann_centres,wann_spreads,
           spread)
```

- `character(len=*), intent(in) :: seed_name`
  The seedname of the current calculation.

- `integer, dimension(3), intent(in) :: mp_grid`
  The dimensions of the Monkhorst-Pack k-point grid.

- `integer, intent(in) :: num_kpts`
  The number of k-points on the Monkhorst-Pack grid.

- `real(kind=dp), dimension(3,3), intent(in) :: real_lattice`
  The lattice vectors in Cartesian co-ordinates in units of Angstrom.

- `real(kind=dp), dimension(3,3), intent(in) :: recip_lattice`
  The reciprical lattice vectors in Cartesian co-ordinates in units of inverse Angstrom.

- `real(kind=dp), dimension(3,num_kpts), intent(in) :: kpt_latt`
  The positions of the k-points in fractional co-ordinates relative to the reciprocal lattice vectors.

- `integer, intent(in) :: num_bands`
  The total number of bands to be processed.

- `integer, intent(in) :: num_wann`
  The number of MLWF to be extracted.

- `integer, intent(in) :: nntot`
  The number of nearest neighbours for each k-point.

- `integer, intent(in) :: num_atoms`
  The total number of atoms in the system.

- `character(len=20), dimension(num_atoms), intent(in) :: atom_symbols`
  The elemental symbols of the atoms.

- `real(kind=dp), dimension(3,num_atoms), intent(in) :: atoms_cart`
  The positions of the atoms in Cartesian co-ordinates in Angstrom.

- `logical, intent(in) :: gamma_only`
  Set to `.true.` if the underlying electronic structure calculation has been performed with only Γ-point sampling and, hence, if the Bloch eigenstates that are used to construct $A_{mn}^{(\mathbf{k})}$ and $M_{mn}^{(\mathbf{k},\mathbf{b})}$ are real.

- `complex(kind=dp), dimension(num_bands,num_bands,nntot,num_kpts),`
  `                  intent(in) :: M_matrix`
  The matrices of overlaps between neighbouring periodic parts of the Bloch eigenstates at each k-point, $M_{mn}^{((\mathbf{k},\mathbf{b}))}$ (Ref. [1], Eq. (25)).

- `complex(kind=dp), dimension(num_bands,num_wann,num_kpts),`
  `                  intent(in) :: A_matrix`
  The matrices describing the projection of `num_wann` trial orbitals on `num_bands` Bloch states at each k-point, $A_{mn}^{(\mathbf{k})}$ (Ref. [1], Eq. (62); Ref. [2], Eq. (22)).

- `real(kind=dp), dimension(num_bands,num_kpts), intent(in) :: eigenvalues`
  The eigenvalues $\varepsilon_{n\mathbf{k}}$ corresponding to the eigenstates, in eV.

- `complex(kind=dp), dimension(num_wann,num_wann,num_kpts),`
  `                  intent(out) :: U_matrix`
  The unitary matrices at each k-point (Ref. [1], Eq. (59))

- `complex(kind=dp), dimension(num_bands,num_wann,num_kpts),`
  `                optional, intent(out) :: U_matrix_opt`
  The unitary matrices that describe the optimal sub-space at each k-point (see Ref. [2], Section IIIA). The array is packed (see below)

- `logical, dimension(num_bands,num_kpts), optional, intent(out) :: lwindow`
  The element `lwindow(nband,nkpt)` is `.true.` if the band `nband` lies within the outer energy window at kpoint `nkpt`.

- `real(kind=dp), dimension(3,num_wann), optional, intent(out) :: wann_centres`
  The centres of the MLWF in Cartesian co-ordinates in Angstrom.

- `real(kind=dp), dimension(num_wann), optional, intent(out) :: wann_spreads`
  The spread of each MLWF in Å^2.

- `real(kind=dp), dimension(3), optional, intent(out) :: spread`
  The values of Ω, Ω_{I} and $\tilde{\Omega}$ (Ref. [1], Eq. (13)).

Conditions:

- $\star$ `num_wann` $\leq$ `num_bands`

- $\star$ `num_kpts` $=$ `mp_grid(1)` $\times$ `mp_grid(2)` $\times$ `mp_grid(3)`.

If `num_bands` $=$ `num_wann` then `U_matrix_opt` is the identity matrix and `lwindow=.true.`

For the avoidance of doubt, `real_lattice(1,2)` is the $y-$component of the first lattice vector $\mathbf{A}_1$, etc.

$$
\begin{aligned}
\texttt{M\_matrix(m,n,nn,nkp)} &= \langle u_{m\mathbf{k}}|u_{n\mathbf{k+b}}\rangle \\
\texttt{A\_matrix(m,n,nkp)} &= \langle \psi_{m\mathbf{k}}|g_n\rangle \\
\texttt{eigenvalues(n,nkp)} &= \varepsilon_{n\mathbf{k}}
\end{aligned}
$$

where

$$
\begin{aligned}
\mathbf{k} &= \texttt{kpt\_latt(1:3,nkp)} \\
\mathbf{k+b} &= \texttt{kpt\_latt(1:3,nnlist(nkp,nn))} + \texttt{nncell(1:3,nkp,nn)}
\end{aligned}
$$

and $\{|g_n\rangle\}$ are a set of initial trial orbitals. These are typically atom or bond-centred Gaussians that are modulated by appropriate spherical harmonics.

Additional parameters should be specified in the `wannier90` input file.

Chapter 7

Transport Calculations with `wannier90`

By setting `transport = TRUE`, `wannier90` will calculate the quantum conductance and density of states of a one-dimensional system. The results will be written to files `seedname_qc.dat` and `seedname_dos.dat`, respectively.

The system for which transport properties are calculated is determined by the keyword `transport_mode`.

7.1   `transport_mode = bulk`

Quantum conductance and density of states are calculated for a perfectly periodic one-dimensional conductor. If `tran_read_ht = FALSE` the transport properties are calculated using the Hamiltonian in the Wannier function basis of the system found by `wannier90`. Setting `tran_read_ht = TRUE` allows the user to provide an external Hamiltonian matrix file `seedname_htB.dat`, from which the properties are found. See Section 2.9 for more details of the keywords required for such calculations.

7.2   `transport_mode = lcr`

Quantum conductance and density of states are calculated for a system where semi-infinite, left and right leads are connected through a central conductor region. This is known as the *lcr* system. Details of the method is described in Ref. [7].

In `wannier90` two options exist for performing such calculations:

- If `tran_read_ht = TRUE` the external Hamiltonian files `seedname_htL.dat, seedname_htLC.dat, seedname_htC.dat, seedname_htCR.dat, seedname_htR.dat` are read and used to compute the transport properties.

- If `tran_read_ht = FALSE`, then the transport calculation is performed automatically using the Wannier functions as a basis and the 2c2 geometry described in Section 7.3.

7.3 Automated lcr Transport Calculations: The 2c2 Geometry

Calculations using the 2c2 geometry provide a method to calculate the transport properties of an lcr system from a single wannier90 calculation. The Hamiltonian matrices which the five external files provide in the tran_read_ht = TRUE case are instead built from the Wannier function basis directly. As such, strict rules apply to the system geometry, which is shown in Figure 7.1. These rules are as follows:

- Left and right leads must be identical and periodic.

- Supercell must contain two principal layers (PLs) of lead on the left, a central conductor region and two principal layers of lead on the right.

- The conductor region must contain enough lead such that the disorder does not affect the principal layers of lead either side.

- A single **k**-point (Gamma) must be used.
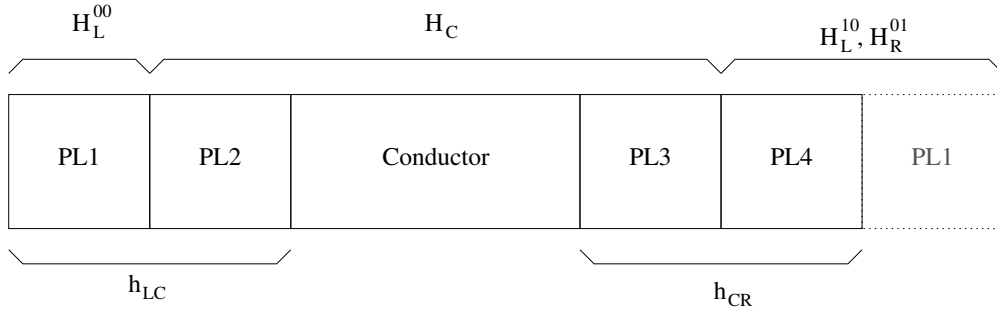
Figure 7.1: Schematic illustration of the supercell required for 2c2 lcr calculations, showing where each of the Hamiltonian matrices are derived from. Four principal layers (PLs) are required plus the conductor region.

In order to build the Hamiltonians, Wannier functions are first sorted according to position and then type if a number of Wannier functions exist with a similar centre (eg. d-orbital type Wannier functions centred on a Cu atom). Next, consistent parities of Wannier function are enforced. To distingiush between different types of Wannier function and assertain relative parities, a signature of each Wannier function is computed. The signature is formed of 20 integrals which have different spatial dependence. They are given by:

$$I = \frac{1}{V} \int_V g(\mathbf{r}) w(\mathbf{r}) d\mathbf{r} \tag{7.1}$$

where V is the volume of the cell, $w(\mathbf{r})$ is the Wannier function and $g(\mathbf{r})$ are the set of functions:

$$g(\mathbf{r}) = \left\{ 1, \sin\left(\frac{2\pi(x-x_c)}{L_x}\right), \sin\left(\frac{2\pi(y-y_c)}{L_y}\right), \sin\left(\frac{2\pi(z-z_c)}{L_z}\right), \sin\left(\frac{2\pi(x-x_c)}{L_x}\right) \sin\left(\frac{2\pi(y-y_c)}{L_y}\right), \right.$$
$$\left. \sin\left(\frac{2\pi(x-x_c)}{L_x}\right) \sin\left(\frac{2\pi(z-z_c)}{L_z}\right), \ldots \right\} \tag{7.2}$$

upto third order in powers of sines. Here, the supercell has dimension (L_x, L_y, L_z) and the Wannier function has centre $\mathbf{r}_c = (x_c, y_c, z_c)$. Each of these integrals may be written as linear combinations of the following sums:

$$S_n(\mathbf{G}) = e^{i\mathbf{G}.\mathbf{r}_c} \sum_m U_{mn} \tilde{u}^*_{m\Gamma}(\mathbf{G}) \tag{7.3}$$

where n and m are the Wannier function and band indexes, $\mathbf{G}$ is a G-vector, U_{mn} is the unitary matrix that transforms from the Bloch reopresentation of the system to the maximally-localised Wannier function basis and $\tilde{u}^*_{m\Gamma}(\mathbf{G})$ are the conjugates of the Fourier transforms of the periodic parts of the Bloch states at the Γ-point. The complete set of $\tilde{u}_{m\mathbf{k}}(\mathbf{G})$ are often outputted by plane-wave DFT codes. However, to calculate the 20 signature integrals, only 32 specific $\tilde{u}_{m\mathbf{k}}(\mathbf{G})$ are required. These are found in an additional file (`seedname.unkg`) that should be provided by the interface between the DFT code and `wannier90` . A detailed description of this file may be found in Section 8.27.

Additionally, the following keywords are also required in the input file:

- `tran_num_ll` : The number of Wannier functions in a principal layer.

- `tran_num_cell_ll` : The number of unit cells in one principal layer of lead

A further parameter related to these calculations is `tran_group_threshold`.

Examples of how 2c2 calculations are preformed can be found in the `wannier90` Tutorial.

Chapter 8

Files

8.1 `seedname.win`

INPUT. The master input file; contains the specification of the system and any parameters for the run. For a description of input parameters, see Chapter 2; for examples, see Section 9.1 and the `wannier90` Tutorial.

8.1.1 Units

The following are the dimensional quantities that are specified in the master input file:

- Direct lattice vectors

- Positions (of atomic or projection) centres in real space

- Energy windows

- Positions of k-points in reciprocal space

- Convergence thresholds for the minimisation of Ω

- `zona` (see Section 3.1)

- `wannier_plot_cube`: cut-off radius for plotting WF in Gaussian cube format

Notes:

- The units (either `ang` (default) or `bohr`) in which the lattice vectors, atomic positions or projection centres are given can be set in the first line of the blocks `unit_cell_cart`, `atoms_cart` and `projections`, respectively, in `seedname.win`.

- Energy is always in eV.

- Convergence thresholds are always in Å^2

- Positions of k-points are always in crystallographic coordinates relative to the reciprocal lattice vectors.

- `zona` is always in reciprocal Angstrom (Å^{-1})

- The keyword `length_unit` may be set to `ang` (default) or `bohr`, in order to set the units in which the quantities in the output file `seedname.wout` are written.

- `wannier_plot_radius` is in Angstrom

The reciprocal lattice vectors $\{\mathbf{B}_1, \mathbf{B}_2, \mathbf{B}_3\}$ are defined in terms of the direct lattice vectors $\{\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3\}$ by the equation

$$\mathbf{B}_1 = \frac{2\pi}{\Omega}\mathbf{A}_2 \times \mathbf{A}_3 \quad \text{etc.,} \tag{8.1}$$

where the cell volume is $V = \mathbf{A}_1 \cdot (\mathbf{A}_2 \times \mathbf{A}_3)$.

8.2   `seedname.mmn`

INPUT. Written by the underlying electronic structure code. See Chapter 5 for details.

8.3   `seedname.amn`

INPUT. Written by the underlying electronic structure code. See Chapter 5 for details.

8.4   `seedname.eig`

INPUT. Written by the underlying electronic structure code. See Chapter 5 for details.

8.5   `seedname.nnkp`

OUTPUT. Written by `wannier90` when `postproc_setup=.TRUE.` (or, alternatively, when `wannier90` is run with the `-pp` command-line option). See Chapter 5 for details.

8.6   `seedname.wout`

OUTPUT. The master output file. Here we give a description of the main features of the output. The verbosity of the output is controlled by the input parameter `iprint`. The higher the value, the more detail is given in the output file. The default value is 1, which prints minimal information.

8.6.1   Header

The header provides some basic information about `wannier90`, the authors, and the execution time of the current run.

```
        +-----------------------------------------------+
        |                                               |
        |                 WANNIER90                     |
        |                                               |
        +-----------------------------------------------+
        |                                               |
        |        Welcome to the Maximally-Localized     |
        |        Generalized Wannier Functions code     |
        |             http://www.wannier.org            |
        |                                               |
        |  Wannier90 v2.0 Authors:                      |
        |     Arash A. Mostofi  (Imperial College London)    |
        |     Giovanni Pizzi    (EPFL)                  |
        |     Ivo Souza         (Universidad del Pais Vasco) |
        |     Jonathan R. Yates (University of Oxford)  |
        |                                               |
        |  Wannier90 Contributors:                      |
        |     Young-Su Lee      (KIST, S. Korea)        |
        |     Matthew Shelley   (Imperial College London)    |
        |     Nicolas Poilvert  (Harvard)              |
        |                                               |
        |  Wannier77 Authors:                           |
        |     Nicola Marzari    (EPFL)                  |
        |     Ivo Souza         (Universidad del Pais Vasco) |
        |     David Vanderbilt  (Rutgers University)    |
        |                                               |
                              .
                              .
        | Copyright (c) 1996-2013                       |
        |        A. A. Mostofi, J. R. Yates, Y.-S. Lee, |
        |        I. Souza, D. Vanderbilt and N. Marzari |
        |                                               |
        |        Release: 2.0    14th October 2013      |
                              .
                              .
        |                                               |
        +-----------------------------------------------+
        |    Execution started on  8Oct2013 at 18:39:42 |
        +-----------------------------------------------+
```

8.6.2 System information

This part of the output file presents information that `wannier90` has read or inferred from the master input file `seedname.win`. This includes real and reciprocal lattice vectors, atomic positions, k-points, parameters for job control, disentanglement, localisation and plotting.

```
                              ------
```

```
                              SYSTEM
                              ------


                        Lattice Vectors (Ang)
                 a_1    3.938486   0.000000   0.000000
                 a_2    0.000000   3.938486   0.000000
                 a_3    0.000000   0.000000   3.938486

             Unit Cell Volume:      61.09251  (Ang^3)


                    Reciprocal-Space Vectors (Ang^-1)
                 b_1    1.595330   0.000000   0.000000
                 b_2    0.000000   1.595330   0.000000
                 b_3    0.000000   0.000000   1.595330


 *-----------------------------------------------------------------------------*
 |   Site       Fractional Coordinate        Cartesian Coordinate (Ang)     |
 +-----------------------------------------------------------------------------+
 | Ba   1  0.00000   0.00000   0.00000  |   0.00000   0.00000   0.00000    |
 | Ti   1  0.50000   0.50000   0.50000  |   1.96924   1.96924   1.96924    |
                                         .
                                         .
 *-----------------------------------------------------------------------------*


                          -----------
                          K-POINT GRID
                          -----------


             Grid size =  4 x  4 x  4     Total points =   64


 *------------------------------- MAIN -------------------------------------*
 |   Number of Wannier Functions              :              9             |
 |   Number of input Bloch states             :              9             |
 |   Output verbosity (1=low, 5=high)         :              1             |
 |   Length Unit                              :             Ang            |
 |   Post-processing setup (write *.nnkp)     :              F             |
                                               .
                                               .
 *-----------------------------------------------------------------------------*
```

8.6.3 Nearest-neighbour k-points

This part of the output files provides information on the b-vectors and weights chosen to satisfy the condition of Eq. 2.1.

```
 *------------------------------- K-MESH -----------------------------------*
 +-----------------------------------------------------------------------------+
 |               Distance to Nearest-Neighbour Shells                        |
 |               ------------------------------------                        |
```

```
|           Shell           Distance (Ang^-1)        Multiplicity       |
|           -----           -----------------        ------------       |
|             1                  0.398833                 6             |
|             2                  0.564034                 12            |
                                    .
                                    .
+----------------------------------------------------------------------+
| The b-vectors are chosen automatically                               |
| The following shells are used:   1                                   |
+----------------------------------------------------------------------+
|                      Shell   # Nearest-Neighbours                     |
|                      -----   -------------------                      |
|                        1               6                             |
+----------------------------------------------------------------------+
| Completeness relation is fully satisfied [Eq. (B1), PRB 56, 12847 (1997)]  |
+----------------------------------------------------------------------+
```

8.6.4 Disentanglement

Then (if required) comes the part where Ω_I is minimised to disentangle the optimally-connected subspace of states for the localisation procedure in the next step.

First, a summary of the energy windows that are being used is given:

```
*----------------------------- DISENTANGLE -----------------------------*
+----------------------------------------------------------------------+
|                           Energy  Windows                            |
|                           --------------                             |
|              Outer:   2.81739  to   38.00000   (eV)                  |
|              Inner:   2.81739  to   13.00000   (eV)                  |
+----------------------------------------------------------------------+
```

Then, each step of the iterative minimisation of Ω_I is reported.

```
            Extraction of optimally-connected subspace
            ------------------------------------------
+-----------------------------------------------------------------+<-- DIS
| Iter     Omega_I(i-1)        Omega_I(i)       Delta (frac.)   Time |<-- DIS
+-----------------------------------------------------------------+<-- DIS
     1      3.82493590          3.66268867       4.430E-02      0.36  <-- DIS
     2      3.66268867          3.66268867       6.911E-15      0.37  <-- DIS
                                    .
                                    .

        <<<        Delta < 1.000E-10  over  3 iterations     >>>
        <<< Disentanglement convergence criteria satisfied >>>

     Final Omega_I     3.66268867 (Ang^2)
```

```
    +--------------------------------------------------------------------+
```

The first column gives the iteration number. For a description of the minimisation procedure and expressions for $\Omega_{\mathrm{I}}^{(i)}$, see the original paper [2]. The procedure is considered to be converged when the fractional difference between $\Omega_{\mathrm{I}}^{(i)}$ and $\Omega_{\mathrm{I}}^{(i-1)}$ is less than `dis_conv_tol` over `dis_conv_window` iterations. The final column gives a running account of the wall time (in seconds) so far. Note that at the end of each line of output, there are the characters "`<- DIS`". This enables fast searching of the output using, for example, the Unix command `grep`:

```
my_shell> grep DIS wannier.wout | less
```

8.6.5 Wannierisation

The next part of the input file provides information on the minimisation of $\widetilde{\Omega}$. At each iteration, the centre and spread of each WF is reported.

```
*---------------------------- WANNIERISE ---------------------------------*
 +-----------------------------------------------------------------+<-- CONV
 | Iter  Delta Spread     RMS Gradient      Spread (Ang^2)      Time |<-- CONV
 +-----------------------------------------------------------------+<-- CONV


 ------------------------------------------------------------------------
 Initial State
  WF centre and spread    1 (  0.000000,  1.969243,  1.969243 )     1.52435832
  WF centre and spread    2 (  0.000000,  1.969243,  1.969243 )     1.16120620
                                          .

                                          .

      0     0.126E+02     0.0000000000        12.6297685260        0.29  <-- CONV
        O_D=        0.0000000 O_OD=       0.1491718 O_TOT=      12.6297685 <-- SPRD
 ------------------------------------------------------------------------
 Cycle:      1
  WF centre and spread    1 (  0.000000,  1.969243,  1.969243 )     1.52414024
  WF centre and spread    2 (  0.000000,  1.969243,  1.969243 )     1.16059775
                                          .

                                          .

  Sum of centres and spreads ( 11.815458, 11.815458, 11.815458 )    12.62663472

      1    -0.313E-02     0.0697660962        12.6266347170        0.34  <-- CONV
        O_D=        0.0000000 O_OD=       0.1460380 O_TOT=      12.6266347 <-- SPRD
 Delta: O_D= -0.4530841E-18 O_OD= -0.3133809E-02 O_TOT= -0.3133809E-02 <-- DLTA
 ------------------------------------------------------------------------
 Cycle:      2
  WF centre and spread    1 (  0.000000,  1.969243,  1.969243 )     1.52414866
  WF centre and spread    2 (  0.000000,  1.969243,  1.969243 )     1.16052405
                                          .

                                          .

  Sum of centres and spreads ( 11.815458, 11.815458, 11.815458 )    12.62646411

      2    -0.171E-03     0.0188848262        12.6264641055        0.38  <-- CONV
```

```
         O_D=       0.0000000 O_OD=       0.1458674 O_TOT=      12.6264641 <-- SPRD
Delta: O_D= -0.2847260E-18 O_OD= -0.1706115E-03 O_TOT= -0.1706115E-03 <-- DLTA
      --------------------------------------------------------------------------
                                       .
                                       .
      --------------------------------------------------------------------------
Final State
 WF centre and spread    1 (  0.000000,  1.969243,  1.969243 )     1.52416618
 WF centre and spread    2 (  0.000000,  1.969243,  1.969243 )     1.16048545
                                       .
                                       .
 Sum of centres and spreads ( 11.815458, 11.815458, 11.815458 )    12.62645344

           Spreads (Ang^2)      Omega I     =    12.480596753
           ================     Omega D     =     0.000000000
                                Omega OD    =     0.145856689
    Final Spread (Ang^2)        Omega Total =    12.626453441
      --------------------------------------------------------------------------
```

It looks quite complicated, but things look more simple if one uses `grep`:

```
my_shell> grep CONV wannier.wout
```

gives

```
+----------------------------------------------------------------------+<-- CONV
| Iter  Delta Spread     RMS Gradient      Spread (Ang^2)      Time  |<-- CONV
+----------------------------------------------------------------------+<-- CONV
    0    0.126E+02      0.0000000000      12.6297685260      0.29  <-- CONV
    1   -0.313E-02      0.0697660962      12.6266347170      0.34  <-- CONV
                                   .
                                   .
   50    0.000E+00      0.0000000694      12.6264534413      2.14  <-- CONV
```

The first column is the iteration number, the second is the change in Ω from the previous iteration, the third is the root-mean-squared gradient of Ω with respect to variations in the unitary matrices $\mathbf{U}^{(\mathbf{k})}$, and the last is the time taken (in seconds). Depending on the input parameters used, the procedure either runs for `num_iter` iterations, or a convergence criterion is applied on Ω. See Section 2.8 for details.

Similarly, the command

```
my_shell> grep SPRD wannier.wout
```

gives

```
         O_D=       0.0000000 O_OD=       0.1491718 O_TOT=      12.6297685 <-- SPRD
         O_D=       0.0000000 O_OD=       0.1460380 O_TOT=      12.6266347 <-- SPRD
                                       .
                                       .
         O_D=       0.0000000 O_OD=       0.1458567 O_TOT=      12.6264534 <-- SPRD
```

which, for each iteration, reports the value of the diagonal and off-diagonal parts of the non-gauge-invariant spread, as well as the total spread, respectively. Recall from Section 1 that $\Omega = \Omega_{\mathrm{I}} + \Omega_{\mathrm{D}} + \Omega_{\mathrm{OD}}$.

8.6.6   Plotting

After WF have been localised, `wannier90` enters its plotting routines (if required). For example, if you have specified an interpolated bandstucture:

```
 *------------------------------------------------------------------------------*
 |                                 PLOTTING                                      |
 *------------------------------------------------------------------------------*

 Calculating interpolated band-structure
```

8.6.7   Summary timings

At the very end of the run, a summary of the time taken for various parts of the calculation is given. The level of detail is controlled by the `timing_level` input parameter (set to 1 by default).

```
 *==============================================================================*
 |                             TIMING INFORMATION                               |
 *==============================================================================*
 |    Tag                                              Ncalls       Time (s)|
 |------------------------------------------------------------------------------|
 |kmesh: get                                     :         1           0.212|
 |overlap: read                                  :         1           0.060|
 |wann: main                                     :         1           1.860|
 |plot: main                                     :         1           0.168|
 *------------------------------------------------------------------------------*

 All done: wannier90 exiting
```

8.7   `seedname.chk`

INPUT/OUTPUT. Information required to restart the calculation or enter the plotting phase. If we have used disentanglement this file also contains the rectangular matrices $\mathbf{U}^{\mathrm{dis}(\mathbf{k})}$.

8.8   `seedname.r2mn`

OUTPUT. Written if `write_r2mn = true`. The matrix elements $\langle m|r^2|n\rangle$ (where m and n refer to MLWF)

8.9 `seedname_band.dat`

OUTPUT. Written if `bands_plot=.TRUE.`; The raw data for the interpolated band structure.

8.10 `seedname_band.gnu`

OUTPUT. Written if `bands_plot=.TRUE.` and `bands_plot_format=gnuplot`; A `gnuplot` script to plot the interpolated band structure.

8.11 `seedname_band.agr`

OUTPUT. Written if `bands_plot=.TRUE.` and `bands_plot_format=xmgrace`; A `grace` file to plot the interpolated band structure.

8.12 `seedname_band.kpt`

OUTPUT. Written if `bands_plot=.TRUE.`; The k-points used for the interpolated band structure, in units of the reciprocal lattice vectors. This file can be used to generate a comparison band structure from a first-principles code.

8.13 `seedname.bxsf`

OUTPUT. Written if `fermi_surface_plot=.TRUE.`; A Fermi surface plot file suitable for plotting with XCrySDen.

8.14 `seedname_w.xsf`

OUTPUT. Written if `wannier_plot=.TRUE.` and `wannier_plot_format=xcrysden`. Contains the wth WF in real space in a format suitable for plotting with XCrySDen or VMD, for example.

8.15 `seedname_w.cube`

OUTPUT. Written if `wannier_plot=.TRUE.` and `wannier_plot_format=cube`. Contains the wth WF in real space in Gaussian cube format, suitable for plotting in XCrySDen, VMD, gopenmol etc.

8.16 `UNKp.s`

INPUT. Read if `wannier_plot=.TRUE.` and used to plot the MLWF. Read if `transport_mode=lcr` and `tran_read_ht=.FALSE.` for use in automated lcr transport calculations.

The periodic part of the Bloch states represented on a regular real space grid, indexed by k-point `p` (from 1 to `num_kpts`) and spin `s` ('1' for 'up', '2' for 'down').

The name of the wavefunction file is assumed to have the form:

```
    write(wfnname,200) p,spin
200 format ('UNK',i5.5,'.',i1)
```

The first line of each file should contain 5 integers: the number of grid points in each direction (`ngx`, `ngy` and `ngz`), the k-point number `ik` and the total number of bands `num_band` in the file. The full file will be read by `wannier90` as:

```
read(file_unit) ngx,ngy,ngz,ik,nbnd
do loop_b=1,num_bands
  read(file_unit) (r_wvfn(nx,loop_b),nx=1,ngx*ngy*ngz)
end do
```

The file can be in formatted or unformatted style, this is controlled by the logical keyword `wvfn_formatted`.

8.17   `seedname_centres.xyz`

OUTPUT. Written if `write_xyz=.TRUE.`; xyz format atomic structure file suitable for viewing with your favourite visualiser (`jmol`, `gopenmol`, `vmd`, etc.).

8.18   `seedname_hr.dat`

OUTPUT. Written if `hr_plot=.TRUE.`. The first line gives the date and time at which the file was created. The second line states the number of Wannier functions `num_wann`. The third line gives the number of Wigner-Seitz grid-points `nrpts`. The next block of `nrpts` integers gives the degeneracy of each Wigner-Seitz grid point, with 15 entries per line. Finally, the remaining $\text{num\_wann}^2 \times \text{nrpts}$ lines each contain, respectively, the components of the vector $\mathbf{R}$ in terms of the lattice vectors $\{\mathbf{A}_i\}$, the indices m and n, and the real and imaginary parts of the Hamiltonian matrix element $H_{mn}^{(\mathbf{R})}$ in the WF basis, e.g.,

```
 Created on 24May2007 at 23:32:09
       20
       17
    4   1   2   1   4   1   1   2   1   4   6   1   1   1   2
    1   2
    0   0  -2   1   1   -0.001013    0.000000
    0   0  -2   2   1    0.000270    0.000000
    0   0  -2   3   1   -0.000055    0.000000
    0   0  -2   4   1    0.000093    0.000000
    0   0  -2   5   1   -0.000055    0.000000
    .
    .
    .
```

8.19   `seedname_qc.dat`

OUTPUT. Written if `transport = .TRUE.`. The first line gives the date and time at which the file was created. In the subsequent lines, the energy value in units of eV is written in the left column, and the quantum conductance in units of $\frac{2e^2}{h}$ ($\frac{e^2}{h}$ for a spin-polarized system) is written in the right column.

```
## written on 14Dec2007 at 11:30:17
   -3.000000        8.999999
   -2.990000        8.999999
   -2.980000        8.999999
   -2.970000        8.999999
      .
      .
      .
```

8.20   `seedname_dos.dat`

OUTPUT. Written if `transport = .TRUE.`. The first line gives the date and time at which the file was created. In the subsequent lines, the energy value in units of eV is written in the left column, and the density of states in an arbitrary unit is written in the right column.

```
## written on 14Dec2007 at 11:30:17
   -3.000000        6.801199
   -2.990000        6.717692
   -2.980000        6.640828
   -2.970000        6.569910
      .
      .
      .
```

8.21   `seedname_htB.dat`

INPUT/OUTPUT. Read if `transport_mode = bulk` and `tran_read_ht = .TRUE.`. Written if `tran_write_ht = .TRUE.`. The first line gives the date and time at which the file was created. The second line gives `tran_num_bb`. The subsequent lines contain `tran_num_bb`×`tran_num_bb` H_{mn} matrix, where the indices m and n span all `tran_num_bb` WFs located at 0th principal layer. Then `tran_num_bb` is recorded again in the new line followed by H_{mn}, where m^{th} WF is at 0th principal layer and n^{th} at 1st principal layer. The H_{mn} matrix is written in such a way that m is the fastest varying index.

```
written on 14Dec2007 at 11:30:17
  150
  -1.737841   -2.941054    0.052673   -0.032926    0.010738   -0.009515
   0.011737   -0.016325    0.051863   -0.170897   -2.170467    0.202254
      .
      .
```

```
      .
 -0.057064    -0.571967    -0.691431     0.015155    -0.007859     0.000474
 -0.000107    -0.001141    -0.002126     0.019188    -0.686423   -10.379876
 150
  0.000000     0.000000     0.000000     0.000000     0.000000     0.000000
  0.000000     0.000000     0.000000     0.000000     0.000000     0.000000
      .
      .
      .
  0.000000     0.000000     0.000000     0.000000     0.000000    -0.001576
  0.000255    -0.000143    -0.001264     0.002278     0.000000     0.000000
```

8.22 seedname_htL.dat

INPUT. Read if `transport_mode = lcr` and `tran_read_ht = .TRUE.`. The file must be written in the same way as in `seedname_htB.dat`. The first line can be any comment you want. The second line gives `tran_num_ll`. `tran_num_ll` in `seedname_htL.dat` must be equal to that in `seedname.win`. The code will stop otherwise.

```
Created by a WANNIER user
  105
   0.316879     0.000000    -2.762434     0.048956     0.000000    -0.016639
   0.000000     0.000000     0.000000     0.000000     0.000000    -2.809405
      .
      .
      .
   0.000000     0.078188     0.000000     0.000000    -2.086453    -0.001535
   0.007878    -0.545485   -10.525435
  105
   0.000000     0.000000     0.000315    -0.000294     0.000000     0.000085
   0.000000     0.000000     0.000000     0.000000     0.000000     0.000021
      .
      .
      .
   0.000000     0.000000     0.000000     0.000000     0.000000     0.000000
   0.000000     0.000000     0.000000
```

8.23 seedname_htR.dat

INPUT. Read if `transport_mode = lcr` and `tran_read_ht = .TRUE.` and `tran_use_same_lead = .FALSE.`. The file must be written in the same way as in `seedname_htL.dat`. `tran_num_rr` in `seedname_htR.dat` must be equal to that in `seedname.win`.

8.24 `seedname_htC.dat`

INPUT. Read if `transport_mode = lcr` and `tran_read_ht = .TRUE.`. The first line can be any comment you want. The second line gives `tran_num_cc`. The subsequent lines contain `tran_num_cc`×`tran_num_cc` H_{mn} matrix, where the indices m and n span all `tran_num_cc` WFs inside the central conductor region. `tran_num_cc` in `seedname_htC.dat` must be equal to that in `seedname.win`.

```
Created by a WANNIER user
   99
 -10.499455   -0.541232    0.007684   -0.001624   -2.067078   -0.412188
   0.003217    0.076965    0.000522   -0.000414    0.000419   -2.122184
   .
   .
   .
  -0.003438    0.078545    0.024426    0.757343   -2.004899   -0.001632
   0.007807   -0.542983  -10.516896
```

8.25 `seedname_htLC.dat`

INPUT. Read if `transport_mode = lcr` and `tran_read_ht = .TRUE.`. The first line can be any comment you want. The second line gives `tran_num_ll` and `tran_num_lc` in the given order. The subsequent lines contain `tran_num_ll`×`tran_num_lc` H_{mn} matrix. The index m spans `tran_num_ll` WFs in the surface principal layer of semi-infinite left lead which is in contact with the conductor region. The index n spans `tran_num_lc` WFs in the conductor region which have a non-negligible interaction with the WFs in the semi-infinite left lead. Note that `tran_num_lc` can be different from `tran_num_cc`.

```
Created by a WANNIER user
  105     99
    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
   .
   .
   .
  -0.000003    0.000009    0.000290    0.000001   -0.000007   -0.000008
   0.000053   -0.000077   -0.000069
```

8.26 `seedname_htCR.dat`

INPUT. Read if `transport_mode = lcr` and `tran_read_ht = .TRUE.`. The first line can be any comment you want. The second line gives `tran_num_cr` and `tran_num_rr` in the given order. The subsequent lines contain `tran_num_cr`×`tran_num_rr` H_{mn} matrix. The index m spans `tran_num_cr` WFs in the conductor region which have a non-negligible interaction with the WFs in the semi-infinite right lead. The index n spans `tran_num_rr` WFs in the surface principal layer of semi-infinite right lead which is in contact with the conductor region. Note that `tran_num_cr` can be different from `tran_num_cc`.

```
Created by a WANNIER user
  99    105
  -0.000180    0.000023    0.000133   -0.000001    0.000194    0.000008
  -0.000879   -0.000028    0.000672   -0.000257   -0.000102   -0.000029
   .
   .
   .
   0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
   0.000000    0.000000    0.000000
```

8.27 `seedname.unkg`

INPUT. Read if `transport_mode = lcr` and `tran_read_ht = .FALSE.`. The first line is the number
of G-vectors at which the $\tilde{u}_{m\mathbf{k}}(\mathbf{G})$ are subsequently printed. This number should always be 32 since
32 specific $\tilde{u}_{m\mathbf{k}}$ are required. The following lines contain the following in this order: The band index
m, a counter on the number of G-vectors, the integer co-efficient of the G-vector components a, b, c
(where $\mathbf{G} = a\mathbf{b}_1 + b\mathbf{b}_2 + c\mathbf{b}_3$), then the real and imaginary parts of the corresponding $\tilde{u}_{m\mathbf{k}}(\mathbf{G})$ at the
Γ-point. We note that the ordering in which the G-vectors and $\tilde{u}_{m\mathbf{k}}(\mathbf{G})$ are printed is not important,
but the specific G-vectors are critical. The following example displays for a single band, the complete
set of $\tilde{u}_{m\mathbf{k}}(\mathbf{G})$ that are required. Note the G-vectors (a, b, c) needed.

```
    32
 1    1    0    0    0    0.4023306    0.0000000
 1    2    0    0    1   -0.0000325    0.0000000
 1    3    0    1    0   -0.3043665    0.0000000
 1    4    1    0    0   -0.3043665    0.0000000
 1    5    2    0    0    0.1447143    0.0000000
 1    6    1   -1    0    0.2345179    0.0000000
 1    7    1    1    0    0.2345179    0.0000000
 1    8    1    0   -1    0.0000246    0.0000000
 1    9    1    0    1    0.0000246    0.0000000
 1   10    0    2    0    0.1447143    0.0000000
 1   11    0    1   -1    0.0000246    0.0000000
 1   12    0    1    1    0.0000246    0.0000000
 1   13    0    0    2    0.0000338    0.0000000
 1   14    3    0    0   -0.0482918    0.0000000
 1   15    2   -1    0   -0.1152414    0.0000000
 1   16    2    1    0   -0.1152414    0.0000000
 1   17    2    0   -1   -0.0000117    0.0000000
 1   18    2    0    1   -0.0000117    0.0000000
 1   19    1   -2    0   -0.1152414    0.0000000
 1   20    1    2    0   -0.1152414    0.0000000
 1   21    1   -1   -1   -0.0000190    0.0000000
 1   22    1   -1    1   -0.0000190    0.0000000
 1   23    1    1   -1   -0.0000190    0.0000000
 1   24    1    1    1   -0.0000190    0.0000000
 1   25    1    0   -2   -0.0000257    0.0000000
 1   26    1    0    2   -0.0000257    0.0000000
```

```
1   27    0    3    0  -0.0482918   0.0000000
1   28    0    2   -1  -0.0000117   0.0000000
1   29    0    2    1  -0.0000117   0.0000000
1   30    0    1   -2  -0.0000257   0.0000000
1   31    0    1    2  -0.0000257   0.0000000
1   32    0    0    3   0.0000187   0.0000000
2    1    0    0    0  -0.0000461   0.0000000
.
.
.
```

Chapter 9

Sample Input Files

9.1   Master input file: `seedname.win`

```
num_wann        : 4
mp_grid         : 4 4 4
num_iter        : 100
postproc_setup  : true

begin unit_cell_cart
ang
-1.61 0.00 1.61
 0.00 1.61 1.61
-1.61 1.61 0.00
end unit_cell_cart

begin atoms_frac
C   -0.125  -0.125  -0.125
C    0.125   0.125   0.125
end atoms_frac

bands_plot        : true
bands_num_points  : 100
bands_plot_format : gnuplot

begin kpoint_path
L 0.50000 0.50000 0.50000 G 0.00000 0.00000 0.00000
G 0.00000 0.00000 0.00000 X 0.50000 0.00000 0.50000
X 0.50000 0.00000 0.50000 K 0.62500 0.25000 0.62500
end kpoint_path

begin projections
C:l=0,l=1
end projections

begin kpoints
```

```
0.00 0.00 0.00
0.00 0.00 0.25
0.00 0.50 0.50
 .
 .
 .
0.75 0.75 0.50
0.75 0.75 0.75
end kpoints
```

9.2   seedname.nnkp

Running wannier90 on the above input file would generate the following nnkp file:

```
File written on  9Feb2006 at 15:13: 9

calc_only_A   :  F

begin real_lattice
  -1.612340    0.000000    1.612340
   0.000000    1.612340    1.612340
  -1.612340    1.612340    0.000000
end real_lattice

begin recip_lattice
  -1.951300   -1.951300    1.951300
   1.951300    1.951300    1.951300
  -1.951300    1.951300   -1.951300
end recip_lattice

begin kpoints
     64
  0.00000    0.00000    0.00000
  0.00000    0.25000    0.00000
  0.00000    0.50000    0.00000
  0.00000    0.75000    0.00000
  0.25000    0.00000    0.00000
   .
   .
   .
  0.50000    0.75000    0.75000
  0.75000    0.00000    0.75000
  0.75000    0.25000    0.75000
  0.75000    0.50000    0.75000
  0.75000    0.75000    0.75000
end kpoints
```

```
begin projections
   8
  -0.12500    -0.12500    -0.12500      0  1  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
  -0.12500    -0.12500    -0.12500      1  1  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
  -0.12500    -0.12500    -0.12500      1  2  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
  -0.12500    -0.12500    -0.12500      1  3  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
   0.12500     0.12500     0.12500      0  1  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
   0.12500     0.12500     0.12500      1  1  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
   0.12500     0.12500     0.12500      1  2  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
   0.12500     0.12500     0.12500      1  3  1
     0.000  0.000  1.000   1.000  0.000  0.000   2.00
end projections

begin nnkpts
    8
   1     2       0   0   0
   1     4       0  -1   0
   1     5       0   0   0
   1    13      -1   0   0
   1    17       0   0   0
   1    22       0   0   0
   1    49       0   0  -1
   1    64      -1  -1  -1
   2     1       0   0   0
   2     3       0   0   0
   2     6       0   0   0
   2    14      -1   0   0
   2    18       0   0   0
   2    23       0   0   0
   2    50       0   0  -1
   2    61      -1   0  -1
   .
   .
   .
  64     1       1   1   1
  64    16       0   0   1
  64    43       0   0   0
  64    48       0   0   0
  64    52       1   0   0
  64    60       0   0   0
  64    61       0   1   0
  64    63       0   0   0
```

```
end nnkpts

begin exclude_bands
    4
    1
    2
    3
    4
end exclude_bands
```

Part III

postw90.x

Chapter 10

Parameters

10.1 Introduction

The `wannier90.x` code described in Part II calculates the maximally-localized Wannier functions. The `wannier90.x` code is a serial executable (i.e., it cannot be executed in parallel on different CPUs).

For users of the previous `wannier90` 1.2 release, the `wannier90.x` executable has only a few minor changes with respect to the 1.2 release.

The `postw90.x` executable contains instead a series of modules that take the Wannier functions calculated by `wannier90.x` and use them to calculate different properties. This executable is parallel (by means of MPI libraries), so it can be run on multiple CPUs. The information on the calculated Wannier functions is read from the checkpoint `seedname.chk` file. Note that this is written in an unformatted machine-dependent format. If you need to use this file on a different machine, or you want to use a version of `postw90.x` compiled with a different compiler, refer to Sec. A.2 in the Appendices for a description of how to export/import this file.

10.2 Usage

`postw90.x` can be run in parallel using MPI libraries to reduce the computation time.

For serial execution use: `postw90.x [seedname]`

- `seedname`: If a seedname string is given the code will read its input from a file `seedname.win`. The default value is `wannier`. One can also equivalently provide the string `seedname.win` instead of `seedname`.

For parallel execution use: `mpirun -np NUMPROCS postw90.x [seedname]`

- `NUMPROCS`: substitute with the number of processors that you want to use.

Note that the `mpirun` command and command-line flags may be different in your MPI implementation: read your MPI manual or ask your computer administrator.

Note also that this requires that the `postw90.x` executable has been compiled in its parallel version (follow the instructions in the file `README.install` in the main directory of the wannier90 distribution) and that the MPI libraries and binaries are installed and correctly configured on your machine.

10.3   `seedname.win` File

The `postw90.x` uses the same `seedname.win` input file of `wannier90.x`. The input keywords of `postw90.x` must thus be added to this file, using the same syntax described in Sec. 2.2.

Note that `wannier90.x` checks if the syntax of the input file is correct, but then ignores the value of the flags that refer only to modules of `postw90.x`, so one can safely run `wannier90.x` on a file that contains also `postw90.x` flags.

Similarly, `postw90.x` ignores flags that refer only to `wannier90.x` (as number of iterations, restart flags, . . .). However, some parts of the input file must be there, as for instance the number of Wannier functions, etc.

The easiest thing to do is therefore to simply *add* the `postw90` input keywords to the `seedname.win` file that was used to obtain the Wannier functions.

10.4   List of available modules

The currently available modules in `postw90.x` are:

- `dos`: Calculation of the density of states (DOS), projected density of states (PDOS), net spin etc.

- `kpath`: Calculation of k-space quantities such as energy bands and Berry curvature along a piecewise linear path in the BZ (see examples 17 and 18 of the tutorial).

- `kslice`: Calculation of k-space quantities on a planar slice of the BZ (see examples 17 and 18 of the tutorial).

- `berry`: Calculation of properties related to the BZ integral of the Berry curvature and Berry connection, including anomalous Hall conductivity, orbital magnetisation, and optical conductivity (see Chap. 11 and examples 18 and 19 of the tutorial).

- `BoltzWann`: Calculation of electronic transport properties for bulk materials using the semiclassical Boltzmann transport equation (see Chap. 12 and example 16 of the tutorial).

- `geninterp` (Generic Band Interpolation): Calculation band energies (and band derivatives) on a generic list of k points (see Chap. 13).

10.5   Keyword List

On the next pages the list of available `postw90` input keywords is reported. In particular, Table 10.1 reports keywords that affect the generic behavior of all modules of `postw90`. Often, these are "global" variables that can be overridden by module-specific keywords (as for instance the `kmesh` flag). The subsequent tables describe the input parameters for each specific module.

A description of the behaviour of the global flags is described Sec. 10.6; the description of the flags specific to the modules can be found in the following sections.

Keyword	Type	Description
Global Parameters of `postw90`		
KMESH	I	Dimensions of the uniform interpolation k-mesh (one or three integers)
KMESH_SPACING	R	Minimum spacing between k points in Å^{-1}
ADPT_SMR	L	Use adaptive smearing
ADPT_SMR_FAC	R	Adaptive smearing prefactor
ADPT_SMR_MAX	P	Maximum allowed value for the adaptive energy smearing (eV)
SMR_TYPE	S	Analytical form used for the broadened delta function
SMR_FIXED_EN_WIDTH	P	Energy smearing (if non-adaptive)
NUM_ELEC_PER_STATE	I	Number of electrons per state
SCISSORS_SHIFT	P	Scissors shift applied to the conduction bands (eV)
NUM_VALENCE_BANDS	I	Number of valence bands
SPIN_DECOMP	L	Decompose various properties into up-spin, down-spin, and possibly spin-flip parts
SPIN_AXIS_POLAR	P	Polar angle of the spin quantization axis (deg)
SPIN_AXIS_AZIMUTH	P	Azimuthal angle of the spin quantization axis (deg)
SPIN_MOMENT*	L	Determines whether to evaluate the spin magnetic moment per cell
uHu_FORMATTED	L	Read a formatted `seedname.uHu` file
SPN_FORMATTED	L	Read a formatted `seedname.spn` file
BERRY_CURV_UNIT	S	Unit of Berry curvature

Table 10.1: `seedname.win` file keywords controlling the general behaviour of the modules in `postw90`. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

The keyword `spin_moment` does not affect the behavior of the modules in `postw90`, and does not really belong to any of them. It is listed here for lack of a better place.

Keyword	Type	Description
dos Parameters		
DOS	L	Calculate the density of states and related properties
DOS_TASK	S	List of properties to compute
DOS_ENERGY_MIN	P	Lower limit of the energy range for computing the DOS (eV)
DOS_ENERGY_MAX	P	Upper limit of the energy range for computing the DOS (eV)
DOS_ENERGY_STEP	R	Step for increasing the energy in the specified range (eV)
DOS_PROJECT	I	List of WFs onto which the DOS is projected
[DOS_]KMESH	I	Dimensions of the uniform interpolation k-mesh (one or three integers)
[DOS_]KMESH_SPACING	R	Minimum spacing between k points in Å^{-1}
[DOS_]ADPT_SMR	L	Use adaptive smearing for the DOS
[DOS_]ADPT_SMR_FAC	R	Adaptive smearing prefactor
[DOS_]ADPT_SMR_MAX	P	Maximum allowed value for the adaptive energy smearing (eV)
[DOS_]SMR_FIXED_EN_WIDTH	P	Energy smearing (if non-adaptive) for the DOS (eV)
[DOS_]SMR_TYPE	S	Analytical form used for the broadened delta function when computing the DOS.

Table 10.2: `seedname.win` file keywords controlling the `dos` module. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

Keyword	Type	Description
kpath Parameters		
KPATH	L	Calculate properties along a piecewise linear path in the BZ
KPATH_TASK	L	List of properties to evaluate
KPATH_NUM_POINTS	I	Number of points in the first kpath segment
KPATH_BANDS_COLOUR	S	Property used to colour the energy bands along the path

Table 10.3: `seedname.win` file keywords controlling the `kpath` module. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

Keyword	Type	Description
kslice Parameters		
KSLICE	L	Calculate properties on a slice in the BZ
KSLICE_TASK	S	List of properties to evaluate
KSLICE_CORNER	R	Position of the corner of the slice
KSLICE_B1	R	First vector defining the slice
KSLICE_B2	R	Second vector defining the slice
KSLICE_2DKMESH	I	Dimensions of the uniform interpolation k-mesh on the slice (one or two integers)
KSLICE_FERMI_LEVEL	P	Energy level for plotting constant-energy contour lines (eV)
KSLICE_FERMI_LINES_COLOUR	S	Property used to colour the Fermi lines

Table 10.4: `seedname.win` file keywords controlling the `kslice` module. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

Keyword	Type	Description
berry Parameters		
BERRY	L	Calculate Berry-type quantities
BERRY_TASK	L	List of properties to compute
[BERRY_]KMESH	I	Dimensions of the uniform interpolation k-mesh (one or three integers)
[BERRY_]KMESH_SPACING	R	Minimum spacing between k points in Å^{-1}
BERRY_CURV_ADPT_KMESH	I	Linear dimension of the adaptively refined k-mesh used to compute the anomalous Hall conductivity
BERRY_CURV_ADPT_KMESH_THRESH	P	Threshold magnitude of the Berry curvature for adaptive refinement
KUBO_FREQ_MIN	P	Lower limit of the frequency range for optical spectra and JDOS (eV)
KUBO_FREQ_MAX	P	Upper limit of the frequency range for optical spectra and JDOS (eV)
KUBO_FREQ_STEP	R	Step for increasing the optical frequency in the specified range
KUBO_EIGVAL_MAX	P	Maximum energy eigenvalue included when evaluating the Kubo-Greenwood conductivity and JDOS
[KUBO_]ADPT_SMR	L	Use adaptive energy smearing for the optical conductivity and JDOS
[KUBO_]ADPT_SMR_FAC	R	Adaptive smearing prefactor
[KUBO_]ADPT_SMR_MAX	P	Maximum allowed value for the adaptive energy smearing (eV)
[KUBO_]SMR_TYPE	S	Analytical form used for the broadened delta function when computing the optical conductivity and JDOS
[KUBO_]SMR_FIXED_EN_WIDTH	P	Energy smearing (if non-adaptive) for the optical conductivity and JDOS (eV)

Table 10.5: `seedname.win` file keywords controlling the `berry` module. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

Keyword	Type	Description
BoltzWann Parameters		
BOLTZWANN	L	Calculate Boltzmann transport co-efficients
[BOLTZ_]KMESH	I	Dimensions of the uniform interpolation k-mesh (one or three integers)
[BOLTZ_]KMESH_SPACING	R	Minimum spacing between k points in Å^{-1}
BOLTZ_2D_DIR	S	Non-periodic direction (for 2D systems only)
BOLTZ_RELAX_TIME	P	Relaxation time in fs
BOLTZ_MU_MIN	P	Minimum value of the chemical potential μ in eV
BOLTZ_MU_MAX	P	Maximum value of the chemical potential μ in eV
BOLTZ_MU_STEP	R	Step for μ in eV
BOLTZ_TEMP_MIN	P	Minimum value of the temperature T in Kelvin
BOLTZ_TEMP_MAX	P	Maximum value of the temperature T in Kelvin
BOLTZ_TEMP_STEP	R	Step for T in Kelvin
BOLTZ_TDF_ENERGY_STEP	R	Energy step for the TDF (eV)
BOLTZ_TDF_SMR_FIXED_EN_WIDTH	P	Energy smearing for the TDF (eV)
BOLTZ_TDF_SMR_TYPE	S	Smearing type for the TDF
BOLTZ_CALC_ALSO_DOS	L	Calculate also DOS while calculating the TDF
BOLTZ_DOS_ENERGY_MIN	P	Minimum value of the energy for the DOS in eV
BOLTZ_DOS_ENERGY_MAX	P	Maximum value of the energy for the DOS in eV
BOLTZ_DOS_ENERGY_STEP	R	Step for the DOS in eV
[BOLTZ_DOS_]SMR_TYPE	S	Smearing type for the DOS
[BOLTZ_DOS_]ADPT_SMR	L	Use adaptive smearing for the DOS
[BOLTZ_DOS_]ADPT_SMR_FAC	R	Adaptive smearing prefactor
[BOLTZ_DOS_]ADPT_SMR_MAX	P	Maximum allowed value for the adaptive energy smearing (eV)
[BOLTZ_DOS_SMR_]FIXED_EN_WIDTH	P	Energy smearing (if non-adaptive) for the DOS (eV)

Table 10.6: `seedname.win` file keywords controlling the `BoltzWann` module (calculation of the Boltzmann transport coefficients in the Wannier basis). Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

Keyword	Type	Description
geninterp Parameters		
GENINTERP	L	Calculate bands for given set of k points
GENINTERP_ALSOFIRSTDER	L	Calculate also first derivatives
GENINTERP_SINGLE_FILE	L	Write a single file or one for each process

Table 10.7: `seedname.win` file keywords controlling the Generic Band Interpolation (`geninterp`) module. Argument types are represented by, I for a integer, R for a real number, P for a physical value, L for a logical value and S for a text string.

10.6   Global variables

10.6.1   `integer :: kmesh(:)`

Dimensions of the interpolation grid used in `postw90.x`.

Not to be confused with the `mp_grid` *input flag, which instead specifies the Monkhorst–Pack grid used in the ab-initio calculation!*

If three integers $l\ m\ n$ are given, the reciprocal-space cell subtended by the three primitive translations is sampled on a uniform $l \times m \times n$ grid (including Γ). If only one integer m is given, an $m \times m \times m$ grid is used.

If you use a module which needs a k-mesh, either `kmesh_spacing` or `kmesh` must be defined.

10.6.2   `real(kind=dp) :: kmesh_spacing`

An alternative way of specifying the interpolation grid. This flag defines the minimum distance for neighboring k points along each of the three directions in k space.

The units are Å^{-1}.

If you use a module which needs a k-mesh, either `kmesh_spacing` or `kmesh` must be defined.

10.6.3   `logical :: adpt_smr`

Determines whether to use an adaptive scheme for broadening the DOS and similar quantities defined on the energy axis. If `true`, the values for the smearing widths are controlled by the flag `adpt_smr_fac`.

The default value is `true`.

10.6.4   `real(kind=dp) :: adpt_smr_fac`

The width $\eta_{n\mathbf{k}}$ of the broadened delta function used to determine the contribution to the spectral property (DOS, ...) from band n at point $\mathbf{k}$ is calculated as

$$\eta_{n\mathbf{k}} = \alpha |\nabla_{\mathbf{k}} \varepsilon_{n\mathbf{k}}| \Delta k,$$

where $\varepsilon_{n\mathbf{k}}$ is the energy eigenvalue and the dimensionless factor α is given by `adpt_smr_fac`. Δk is taken to be the largest of the mesh spacings along the three reciprocal lattice vectors $\mathbf{b_1}$, $\mathbf{b_2}$, and $\mathbf{b_3}$. If the calculated value of $\eta_{n\mathbf{k}}$ exceeds `adpt_smr_max`, the latter value is used.

The default value is $\sqrt{2}$.

10.6.5   `real(kind=dp) :: adpt_smr_max`

See description given immediately above.

The units are eV. The default value is 1.0.

10.6.6   `character(len=120) :: smr_type`

Defines the analytical form used for the broadened delta function in the computation of the DOS and similar quantities defined on the energy axis.

- `gauss`: Gaussian smearing

- `m-pN`: derivative of the N-th order Methfessel-Paxton function ($N \geq 0$). Example: `m-p2` for the second-order Methfessel-Paxton function. If only `m-p` is provided, the first-order function is used, i.e., it is equivalent to `m-p1`.

- `m-v` or `cold`: derivative of the Marzari–Vanderbilt cold-smearing function

- `f-d`: derivative of the Fermi-Dirac distribution function

The default value is `gauss`.

10.6.7   `logical :: smr_fixed_en_width`

Energy width for the smearing function for the DOS. Used only if `adpt_smr` is `false`.

The units are eV. The default value is 0 eV. Note that if the width is smaller than twice the energy step (e.g. `dos_energy_step` for the `dos` module), the DOS will be unsmeared (thus the default is to have an unsmeared properties when `adpt_smr` is set to `false`.).

10.6.8   `integer :: num_elec_per_state`

Number of electrons per state. It can only take the values one or two.

The default value is 1 if `spinors=true`, 2 otherwise.

10.6.9   `real(kind=dp) :: scissors_shift`

Scissors shift applied to the conduction bands.

The units are eV. The default value is 0 eV (i.e., no scissors shift applied).

10.6.10   `integer :: num_valence_bands`

Number of valence bands of the system. Used in different modules and for the scissors shift.

No default value.

10.6.11   `logical :: spin_decomp`

If `true`, extra columns are added to some output files (such as `seedname-dos.dat` for the `dos` module, and analogously for the `berry` and `BoltzWann` modules).

For the `dos` and `BoltzWann` modules, two further columns are generated, which contain the decomposition of the required property (e.g., total or orbital-projected DOS) of a spinor calculation into up-spin and down-spin parts (relative to the quantization axis defined by the input variables `spin_axis_polar` and `spin_axis_azimuth`). For the `berry` module with `berry_task = kubo`, three extra columns are added to `seedname-jdos.dat`, containing the decomposition of the JDOS into up → up, down → down, and spin-flip transitions. In the same way, six extra columns are added to the data files `seedname-kubo*.dat` where the complex optical conductivity is stored.

The file `seedname.spn` must be present at input. Furthermore, if this variable is set to `true` it requires `num_elec_per_state = 1`.

The default value is `false`.

10.6.12   real(kind=dp) ::   spin_axis_polar

Polar angle of the spin quantization axis.

The units are degrees. The default value is 0.

10.6.13   real(kind=dp) ::   spin_axis_azimuth

Azimuthal angle of the spin quantization axis.

The units are degrees. The default value is 0.

10.6.14   logical ::   spin_moment

Determines whether to evaluate the spin moment.

The default value is `false`.

10.6.15   logical ::   uHu_formatted

If `uHu_formatted=true`, then the uHu matrix elements will be read from disk as formatted (ie ASCII) files; otherwise they will be read as unformatted files.

The default value of this parameter is `false`.

10.6.16   logical ::   spn_formatted

If `spn_formatted=true`, then the spin matrix elements will be read from disk as formatted (ie ASCII) files; otherwise they will be read as unformatted files. Unformatted is generally preferable as the files will take less disk space and I/O is significantly faster. However such files will not be transferable between all machine architectures and formatted files should be used if transferability is required (i.e., for test cases).

The default value is `false`.

10.6.17 `character(len=20) :: berry_curv_unit`

Unit in which the Berry curvature is specified at input (in `berry_curv_adpt_kmesh_thresh`) or written to file (when `kpath_task=curv` or `kslice_task=curv`).

- `ang2`: Angstrom^2

- `bohr2`: Bohr^2 (atomic units)

The default value is `ang2`.

10.7   DOS

Note that the behavior of the `dos` module is also influenced by the value of some global flags (listed in Table 10.1), as `spin_decomp`, `spin_axis_polar`, `spin_axis_azimuth`, `scissors_shift`, etc. Some of the global flags can be possibly overridden by local flags of the DOS module, listed below, which have the same name of the global flag but are prefixed by `dos_`.

10.7.1   logical ::   dos

Determines whether to enter the DOS routines.

The default value is `false`.

10.7.2   character(len=20) ::   dos_task

The quantity to compute when `dos=true`

The valid options for this parameter are:

- `dos_plot` Density of states. An output data file `seedname-dos.dat` is created, containing the energy values in eV in the first column, and the total DOS per unit cell and unit energy range (in eV^{-1}) in the second. Two additional columns are present if `spin_decomp=true`

The default value is `dos_plot`.

10.7.3   real(kind=dp) ::   dos_energy_min

Lower limit of the energy range for computing the DOS. Units are eV.

The default value is the minimum value of the energy eigenvalues stored in `seedname.eig`, minus 0.6667.

10.7.4   real(kind=dp) ::   dos_energy_max

Upper limit of the energy range for computing the DOS. Units are eV.

If an inner energy window was specified, the default value is the upper bound of the innter energy window, plus 0.6667. Otherwise it is the maximum value of the energy eigenvalues stored in `seedname.eig`, plus 0.6667.

10.7.5   real(kind=dp) ::   dos_energy_step

Energy step for the grid of energies used to plot the dos. Units are eV.

The default value is 0.01 eV.

10.7.6 integer :: dos_project(:)

If present postw90 computes, instead of the total DOS, the partial DOS projected onto the WFs listed. The WFs are numbered according to the file seedname.wout.

For example, to project onto WFs 2, 6, 7, 8, and 12:

dos_project : 2, 6-8, 12

The DOS projected onto a set $\mathcal{S}$ of orbitals is calculated as

$$\rho_{\mathcal{S}}(E) = \frac{1}{N_k} \sum_{\mathbf{k}} \sum_{n} \langle \psi_{n\mathbf{k}}^{(\mathrm{H})} | \hat{P}_{\mathbf{k}}(\mathcal{S}) | \psi_{n\mathbf{k}}^{(\mathrm{H})} \rangle \delta(\varepsilon_{n\mathbf{k}} - E) \tag{10.1}$$

$$\hat{P}_{\mathbf{k}}(\mathcal{S}) = \sum_{m \in \mathcal{S}} | \psi_{n\mathbf{k}}^{(\mathrm{W})} \rangle \langle \psi_{n\mathbf{k}}^{(\mathrm{W})} |, \tag{10.2}$$

where N_k is the number of mesh points used to sample the BZ, and the superscript (H) and (W) refer to *Hamiltonian gauge* and *Wannier gauge* [8].

10.7.7 integer :: dos_kmesh(:)

Overrides the kmesh global variable (see Sec. 10.6).

10.7.8 real(kind=dp) :: dos_kmesh_spacing

Overrides the kmesh_spacing global variable (see Sec. 10.6).

10.7.9 logical :: dos_adpt_smr

Overrides the adpt_smr global variable (see Sec. 10.6).

10.7.10 real(kind=dp) :: dos_adpt_smr_fac

Overrides the adpt_smr_fac global variable (see Sec. 10.6).

10.7.11 real(kind=dp) :: dos_adpt_smr_max

Overrides the adpt_smr_max global variable (see Sec. 10.6).

10.7.12 logical :: dos_smr_fixed_en_width

Overrides the smr_fixed_en_width global variable (see Sec. 10.6).

Note that if the width is smaller than twice the energy step dos_energy_step, the DOS will be unsmeared (thus the default is to have an unsmeared DOS).

10.7.13   `character(len=20) :: dos_smr_type`

Overrides the `smr_type` global variable (see Sec. 10.6).

10.8 kpath

10.8.1 `logical :: kpath`

Determines whether to enter the kpath routines.

The default value is `false`.

10.8.2 `character(len=20) :: kpath_task`

The quantities to plot when `kpath=true`

The valid options for this parameter are:

- `bands` Energy bands, in eV. The following files are created:

  · `seedname-bands.dat` (data file)
  · `seedname-bands.gnu` (`gnuplot` script)
  · `seedname-bands.py` (`python` script)
  · `seedname-path.kpt` (list of k-points along the path, written in the `pwscf` format)

- `curv` Minus the Berry curvature given by Eq. (11.18) of Ch. 11, in units of `berry_curv_unit`. The following files are created:

  · `seedname-curv.dat` (data file)
  · `seedname-curv_{x,y,z}.gnu` (`gnuplot` scripts)
  · `seedname-curv_{x,y,z}.py` (`python` scripts)

- `morb` The integrand of the k-space orbital magnetization formula [Eq. (11.20) of Ch. 11] in eV·Å^2. Four output files are created:

  · `seedname-morb.dat` (data file)
  · `seedname-morb_{x,y,z}.gnu` (`gnuplot` scripts)
  · `seedname-morb_{x,y,z}.py` (`python` scripts)

- Any combination of the above. The following combinations are of special interest

  `kpath_task = bands+curv`

  `kpath_task = bands+morb`

  They generate the following files:

  · `seedname-bands.dat` (data file)
  · `seedname-{curv,morb}.dat` (data file)
  · `seedname-bands+{curv,morb}_{x,y,z}.py` (`python` scripts)

  Two-panel figures are produced, with the energy bands within ±0.65 eV of the Fermi level in the top panel, and the Berry curvature (or k-space orbital magnetization) in the bottom panel.

The default value is `bands`.

10.8.3   `integer :: kpath_num_points`

If `kpath = true`, then the number of points along the first section of the bandstructure plot given by `kpoint_path`. Other sections will have the same density of k-points.

The default value is 100.

10.8.4   `character(len=20) :: kpath_bands_colour`

When `kpath_task=bands`, colour code the energy bands according to the specified quantity.

The valid options for this parameter are:

- `spin` Spin projection (in units of $\hbar/2$) along the quantization axis defined by the variables `spin_axis_polar` and `spin_axis_azimuth`, for a spinor calculation

- `none` no colour coding

The default value is `none`.

10.9 kslice

10.9.1 logical :: kslice

Determines whether to enter the kslice routines.

The default value is `false`.

10.9.2 character(len=20) :: kslice_task

The quantity to plot when `kslice=true`

The valid options for this parameter are:

- `fermi_lines` Lines of intersection between constant-energy surfaces and the slice. The energy level is specified by the keyword `kslice_fermi_level`. Output files:

  - `seedname-kslice-fermi-spn.dat` (data file when `kslice_fermi_lines_colour = spin`)
  - `seedname-bnd_n.dat` (gnuplot data files when `kslice_fermi_lines_colour = none`)
  - `seedname-kslice-coord.dat` (python data files when `kslice_fermi_lines_colour = none`)
  - `seedname-kslice-bands.dat` (python data file when `kslice_fermi_lines_colour = none`)
  - `seedname-kslice-fermi_lines.gnu` (gnuplot script)
  - `seedname-kslice-fermi_lines.py` (python script)

- `curv[+fermi_lines]` Heatmap of the Berry curvature of the occupied states [together with the constant-energy contours]. The unit of Berry curvature is `berry_curv_unit`.

  Output files:

  - `seedname-kslice-coord.dat` (data files)
  - `seedname-kslice-curv.dat` (data file)
  - [`seedname-kslice-bands.dat`] (data file)
  - `seedname-kslice-curv_{x,y,z}[+fermi_lines].py` (python scripts)

- `morb[+fermi_lines]` Heatmap of the k-space orbital magnetization in eV·Å^2 [together with the constant-energy contours]. Output files:

  - `seedname-kslice-coord.dat` (data files)
  - `seedname-kslice-morb.dat` (data file)
  - [`seedname-kslice-bands.dat`] (data file)
  - `seedname-kslice-morb_{x,y,z}[+fermi_lines].py` (python scripts)

The default value is `fermi_lines`.

Note: When `kslice_fermi_lines_colour = none` the `gnuplot` scripts draw the k-slices with a square shape, even when `kslice_b1` and `kslice_b2` below are not at right angles, or do not have equal lengths. (The `python` scripts draw the slices with the correct parallelogram shape.)

10.9.3 `real(kind=dp) :: kslice_corner(3)`

Reduced coordinates of the lower-left corner of the slice in k-space.

The default value is $(0.0, 0.0, 0.0)$

10.9.4 `real(kind=dp) :: kslice_b1(3)`

Reduced coordinates of the first reciprocal-space vector defining the slice.

The default value is $(1.0, 0.0, 0.0)$.

10.9.5 `real(kind=dp) :: kslice_b2(3)`

Reduced coordinates of the second reciprocal-space vector defining the slice.

The default value is $(0.0, 1.0, 0.0)$.

10.9.6 `integer :: kslice_2dkmesh(2)`

Dimensions of the k-point grid covering the slice. If two integers m n are given, the slice is sampled on a uniform $m \times n$ grid. If only one integer m is given, an $m \times m$ grid is used.

The default value for `kslice_kmesh` is 50.

10.9.7 `real(kind=dp) :: kslice_fermi_level`

Energy level in eV of the constant-energy contours when `kslice_task = fermi_lines`.

The default value is `fermi_energy`, if defined. Otherwise, no default value is given.

10.9.8 `character(len=20) :: kslice_fermi_lines_colour`

When `kslice_task=fermi_lines` (but not when combined with `curv` or `morb`), colour code the Fermi lines according to the specified quantity.

The valid options for this parameter are:

- `spin` Spin projection (in units of $\hbar/2$) along the quantization axis defined by the variables `spin_axis_polar` and `spin_axis_azimuth`, for a spinor calculation

- `none` no colour coding

The default value is `none`.

10.10 berry

10.10.1 logical :: berry

Determines whether to enter the berry routines.

The default value is `false`.

10.10.2 character(len=120) :: berry_task

The quantity to compute when `berry=true`

The valid options for this parameter are:

- **kubo** Complex optical conductivity and joint density of states. Output files:

  · `seedname-kubo-S_{xx,yy,zz,xy,xz,yz}.dat` (data files). First column: optical frequency $\hbar\omega$ in eV. Second and third columns: real and imaginary parts of the symmetric conductivity $\sigma^{\mathrm{S}}_{\alpha\beta}(\hbar\omega) = \sigma^{\mathrm{S}}_{\beta\alpha}(\hbar\omega)$ in S/cm. Six additional columns are present if `spin_decomp = true`.

  · `seedname-kubo-A_{yz,zx,xy}.dat` (data files). First column: optical frequency $\hbar\omega$ in eV. Second and third columns: real and imaginary parts of the antisymmetric conductivity $\sigma^{\mathrm{A}}_{\alpha\beta}(\hbar\omega) = -\sigma^{\mathrm{A}}_{\beta\alpha}(\hbar\omega)$ in S/cm. Six additional columns are present if `spin_decomp = true`.

  · `seedname-jdos.dat` (data file). First column: energy difference $\hbar\omega$ in eV between conduction (c) and valence (v) states with the same crystal momentum **k**. Second column: joint density of states $\rho_{cv}(\hbar\omega)$ (number of states per unit cell per unit energy range, in eV^{-1}). Three additional columns are present if `spin_decomp = true`.

- **ahc** Anomalous Hall conductivity, in S/cm. The three independent components $\sigma_x = \sigma_{yz}$, $\sigma_y = \sigma_{zx}$, and $\sigma_z = \sigma_{xy}$ are computed. Output files:

  · `seedname-ahc-fermiscan.dat` (data file) . The first column contains the Fermi level ε_F in eV, and the following three column the values of $\sigma_{x,y,z}(\varepsilon_F)$. This file is written if a range of Fermi energies is specified via `fermi_energy_min` and `fermi_energy_max`. If a single Fermi energy is given, the AHC is printed in `seedname.wpout` only.

- **morb** Orbital magnetisation, in bohr magnetons per cell.

  Output files:

  · `seedname-morb-fermiscan.dat` (data file). The first column contains the Fermi level ε_F in eV, and the following three column the values of $M^{\mathrm{orb}}_{x,y,z}(\varepsilon_F)$. This file is written if a range of Fermi energies is specified via `fermi_energy_min` and `fermi_energy_max`. If a single Fermi energy is given, $\mathbf{M}^{\mathrm{orb}}$ is printed in `seedname.wpout` only.

There is no default value.

10.10.3 integer :: berry_kmesh(:)

Overrides the `kmesh` global variable (see Sec. 10.6).

10.10.4 `real(kind=dp) ::  berry_kmesh_spacing`

Overrides the `kmesh_spacing` global variable (see Sec. 10.6).

10.10.5 `integer ::  berry_curv_adpt_kmesh`

If a positive integer n is given and `berry_task=ahc`, an $n \times n \times n$ mesh is placed around points on the uniform mesh (defined by either `berry_kmesh` or `berry_kmesh_spacing`) where the magnitude of the k-space Berry curvature exceeds the threshold value specified in `berry_curv_adpt_kmesh_thresh`. This can be used to densify the BZ integration mesh around spikes in the Berry curvature.

The default value is 1.

10.10.6 `real(kind=dp) ::  berry_curv_adpt_kmesh_thresh`

Magnitude of the Berry curvature (in units of `berry_curv_unit`) that triggers adaptive mesh refinement when `berry_task=ahc`.

The default value is 100.0.

10.10.7 `real(kind=dp) ::  kubo_freq_min`

Lower limit of the frequency range for computing the optical conductivity and JDOS. Units are eV.

The default value 0.0.

10.10.8 `real(kind=dp) ::  kubo_freq_max`

Upper limit of the frequency range for computing the optical conductivity and JDOS. Units are eV.

If an inner energy window was specified, the default value is `dis_froz_max-fermi_energy`+0.6667. Otherwise it is the difference between the maximum and the minimum energy eigenvalue stored in `seedname.eig`, plus 0.6667.

10.10.9 `real(kind=dp) ::  kubo_freq_step`

Difference between consecutive values of the optical frequency between `kubo_freq_min` and `kubo_freq_max`. Units are eV.

The default value is 0.01.

10.10.10 `real(kind=dp) ::  kubo_eigval_max`

Maximum energy eigenvalue of the eigenstates to be included in the evaluation of the optical conductivity and JDOS. Units are eV.

If an inner energy window was specified, the default value is the upper bound of the inner energy window plus 0.6667. Otherwise it is the maximum energy eigenvalue stored in `seedname.eig` plus 0.6667.

10.10.11   `logical :: kubo_adpt_smr`

Overrides the `adpt_smr` global variable (see Sec. 10.6).

10.10.12   `real(kind=dp) :: kubo_adpt_smr_fac`

Overrides the `adpt_smr_fac` global variable (see Sec. 10.6).

10.10.13   `real(kind=dp) :: kubo_adpt_smr_max`

Overrides the `adpt_smr_max` global variable (see Sec. 10.6).

10.10.14   `logical :: kubo_smr_fixed_en_width`

Overrides the `smr_fixed_en_width` global variable (see Sec. 10.6).

10.10.15   `character(len=120) :: kubo_smr_type`

Overrides the `smr_type` global variable (see Sec. 10.6).

10.11   BoltzWann

10.11.1   `logical :: boltzwann`

Determines whether to enter the `BoltzWann` routines.

The default value is `false`.

10.11.2   `integer :: boltz_kmesh(:)`

It determines the interpolation k mesh used to calculate the TDF (from which the transport coefficient are calculated). If `boltz_calc_also_dos` is `true`, the same k mesh is used also for the DOS. Overrides the `kmesh` global variable (see Sec. 10.6).

10.11.3   `real(kind=dp) :: boltz_kmesh_spacing`

Overrides the `kmesh_spacing` global variable (see Sec. 10.6).

10.11.4   `character(len=4) :: boltz_2d_dir`

For two-dimensional systems, the direction along which the system is non-periodic. It can assume the following values: `x` for a 2D system on the yz plane, `y` for a 2D system on the xz plane, `z` for a 2D system on the xy plane, or `no` for a 3D system with periodicity along all threee directions.

This value is used when calculating the Seebeck coefficient, where the electrical conductivity tensor needs to be inverted. If the value is different from zero, only the relevant 2×2 sub-block of the electrical conductivity is inverted.

The default value is `no`.

10.11.5   `real(kind=dp) :: boltz_relax_time`

The relaxation time to be used for the calculation of the TDF and the transport coefficients.

The units are fs. The default value is 10 fs.

10.11.6   `real(kind=dp) :: boltz_mu_min`

Minimum value for the chemical potential μ for which we want to calculate the transport coefficients.

The units are eV. No default value.

10.11.7   `real(kind=dp) :: boltz_mu_max`

Maximum value for the chemical potential μ for which we want to calculate the transport coefficients.

The units are eV. No default value.

10.11.8 `real(kind=dp) ::  boltz_mu_step`

Energy step for the grid of chemical potentials μ for which we want to calculate the transport coefficients.

The units are eV. No default value.

10.11.9 `real(kind=dp) ::  boltz_temp_min`

Minimum value for the temperature T for which we want to calculate the transport coefficients.

The units are K. No default value.

10.11.10 `real(kind=dp) ::  boltz_temp_max`

Maximum value for the temperature T for which we want to calculate the transport coefficients.

The units are K. No default value.

10.11.11 `real(kind=dp) ::  boltz_temp_step`

Energy step for the grid of temperatures T for which we want to calculate the transport coefficients.

The units are K. No default value.

10.11.12 `real(kind=dp) ::  boltz_tdf_energy_step`

Energy step for the grid of energies for the TDF.

The units are eV. The default value is 0.001 eV.

10.11.13 `character(len=120) ::  boltz_tdf_smr_type`

The type of smearing function to be used for the TDF. The available strings are the same of the global `smr_type` input flag.

The default value is the one given via the `smr_type` input flag (if defined).

10.11.14 `real(kind=dp) ::  boltz_tdf_smr_fixed_en_width`

Energy width for the smearing function. Note that for the TDF, a standard (non-adaptive) smearing scheme is used.

The units are eV. The default value is 0 eV. Note that if the width is smaller than twice the energy step `boltz_tdf_energy_step`, the TDF will be unsmeared (thus the default is to have an unsmeared TDF).

10.11.15   logical :: boltz_calc_also_dos

Whether to calculate also the DOS while calculating the TDF.

If one needs also the DOS, it is faster to calculate the DOS using this flag instead of using independently the routines of the `dos` module, since in this way the interpolation on the k points will be performed only once.

The default value is `false`.

10.11.16   real(kind=dp) :: boltz_dos_energy_min

The minimum value for the energy grid for the calculation of the DOS.

The units are eV. The default value is `minval(eigval)-0.6667`, where `minval(eigval)` i s the minimum eigenvalue returned by the ab-initio code on the ab-initio q me sh.

10.11.17   real(kind=dp) :: boltz_dos_energy_max

The maximum value for the energy grid for the calculation of the DOS.

The units are eV. The default value is `maxval(eigval)+0.6667`, where `maxval(eigval)` i s the maximum eigenvalue returned by the ab-initio code on the ab-initio q me sh.

10.11.18   real(kind=dp) :: boltz_dos_energy_step

Energy step for the grid of energies for the DOS.

The units are eV. The default value is 0.001 eV.

10.11.19   character(len=120) :: boltz_dos_smr_type

Overrides the `smr_type` global variable (see Sec. 10.6).

10.11.20   logical :: boltz_dos_adpt_smr

Overrides the `adpt_smr` global variable (see Sec. 10.6).

10.11.21   real(kind=dp) :: boltz_dos_adpt_smr_fac

Overrides the `adpt_smr_fac` global variable (see Sec. 10.6).

10.11.22   real(kind=dp) :: boltz_dos_adpt_smr_max

Overrides the `adpt_smr_max` global variable (see Sec. 10.6).

10.11.23 `logical :: boltz_dos_smr_fixed_en_width`

Overrides the `smr_fixed_en_width` global variable (see Sec. 10.6).

10.12   Generic Band Interpolation

10.12.1 `logical :: geninterp`

Determines whether to enter the Generic Band Interpolation routines.

The default value is `false`.

10.12.2 `logical :: geninterp_alsofirstder`

Whether to calculate also the first derivatives of the bands at the given k points.

The default value is `false`.

10.12.3 `logical :: geninterp_single_file`

Whether to write a single `seedname_geninterp.dat` file (all I/O is done by the root node); or instead multiple files (one for each node) with names `seedname_geninterp_NNNNN.dat`, where `NNNNN` is the node number. See also the discussion in Sec. 13.1.2 on how to use this flag.

The default value is `true`.

Chapter 11

Overview of the `berry` module

The `berry` module of `postw90` is called by setting `berry = true` and choosing one or more of the available options for `berry_task`. The routines in the `berry` module which compute the k-space Berry curvature and orbital magnetization are also called when `kpath = true` and `kpath_task = {curv,morb}`, or when `kslice = true` and `kslice_task = {curv,morb}`.

11.1   Background: Berry connection and curvature

The Berry connection is defined in terms of the cell-periodic Bloch states $|u_{n\mathbf{k}}\rangle = e^{-i\mathbf{k}\cdot\mathbf{r}}|\psi_{n\mathbf{k}}\rangle$ as

$$\mathbf{A}_n(\mathbf{k}) = \langle u_{n\mathbf{k}}|i\boldsymbol{\nabla}_\mathbf{k}|u_{n\mathbf{k}}\rangle, \tag{11.1}$$

and the Berry curvature is the curl of the connection,

$$\boldsymbol{\Omega}_n(\mathbf{k}) = \boldsymbol{\nabla}_\mathbf{k} \times \mathbf{A}_n(\mathbf{k}) = -\mathrm{Im}\langle\boldsymbol{\nabla}_\mathbf{k} u_{n\mathbf{k}}| \times |\boldsymbol{\nabla}_\mathbf{k} u_{n\mathbf{k}}\rangle. \tag{11.2}$$

These two quantities play a central role in the description of several electronic properties of crystals [9]. In the following we will work with a matrix generalization of the Berry connection,

$$\mathbf{A}_{nm}(\mathbf{k}) = \langle u_{n\mathbf{k}}|i\boldsymbol{\nabla}_\mathbf{k}|u_{m\mathbf{k}}\rangle = \mathbf{A}^*_{mn}(\mathbf{k}), \tag{11.3}$$

and write the curvature as an antisymmetric tensor,

$$\Omega_{n,\alpha\beta}(\mathbf{k}) = \epsilon_{\alpha\beta\gamma}\Omega_{n,\gamma}(\mathbf{k}) = -2\mathrm{Im}\langle\nabla_{k_\alpha} u_{n\mathbf{k}}|\nabla_{k_\beta} u_{n\mathbf{k}}\rangle. \tag{11.4}$$

11.2   `berry_task=kubo`: optical conductivity and joint density of states

The Kubo-Greenwood formula for the optical conductivity of a crystal in the independent-particle approximation reads

$$\sigma_{\alpha\beta}(\hbar\omega) = \frac{ie^2\hbar}{N_k\Omega_c}\sum_\mathbf{k}\sum_{n,m}\frac{f_{m\mathbf{k}} - f_{n\mathbf{k}}}{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}}}\frac{\langle\psi_{n\mathbf{k}}|v_\alpha|\psi_{m\mathbf{k}}\rangle\langle\psi_{m\mathbf{k}}|v_\beta|\psi_{n\mathbf{k}}\rangle}{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}} - (\hbar\omega + i\eta)}. \tag{11.5}$$

Indices α, β denote Cartesian directions, Ω_c is the cell volume, N_k is the number of k-points used for sampling the Brillouin zone, and $f_{n\mathbf{k}} = f(\varepsilon_{n\mathbf{k}})$ is the Fermi-Dirac distribution function. $\hbar\omega$ is the optical frequency, and $\eta > 0$ is an adjustable smearing parameter with units of energy.

The off-diagonal velocity matrix elements can be expressed in terms of the connection matrix [10],

$$\langle \psi_{n\mathbf{k}} | \mathbf{v} | \psi_{m\mathbf{k}} \rangle = -\frac{i}{\hbar}(\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}}) \mathbf{A}_{nm}(\mathbf{k}) \quad (m \neq n). \tag{11.6}$$

The conductivity becomes

$$\sigma_{\alpha\beta}(\hbar\omega) = \frac{1}{N_k} \sum_{\mathbf{k}} \sigma_{\mathbf{k},\alpha\beta}(\hbar\omega) \tag{11.7}$$

$$\sigma_{\mathbf{k},\alpha\beta}(\hbar\omega) = \frac{ie^2}{\hbar\Omega_c} \sum_{n,m}(f_{m\mathbf{k}} - f_{n\mathbf{k}}) \frac{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}}}{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}} - (\hbar\omega + i\eta)} A_{nm,\alpha}(\mathbf{k}) A_{mn,\beta}(\mathbf{k}). \tag{11.8}$$

Let us decompose it into Hermitian (dissipative) and anti-Hermitean (reactive) parts. Note that

$$\overline{\delta}(\varepsilon) = \frac{1}{\pi} \text{Im} \left[\frac{1}{\varepsilon - i\eta} \right], \tag{11.9}$$

where $\overline{\delta}$ denotes a "broadended" delta-function. Using this identity we find for the Hermitean part

$$\sigma^{\text{H}}_{\mathbf{k},\alpha\beta}(\hbar\omega) = -\frac{\pi e^2}{\hbar\Omega_c} \sum_{n,m}(f_{m\mathbf{k}} - f_{n\mathbf{k}})(\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}}) A_{nm,\alpha}(\mathbf{k}) A_{mn,\beta}(\mathbf{k}) \overline{\delta}(\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}} - \hbar\omega). \tag{11.10}$$

Improved numerical accuracy can be achieved by replacing the Lorentzian (11.9) with a Gaussian, or other shapes. The analytical form of $\overline{\delta}(\varepsilon)$ is controlled by the keyword `[kubo_]smr_type`.

The anti-Hermitean part of Eq. (11.8) is given by

$$\sigma^{\text{AH}}_{\mathbf{k},\alpha\beta}(\hbar\omega) = \frac{ie^2}{\hbar\Omega_c} \sum_{n,m}(f_{m\mathbf{k}} - f_{n\mathbf{k}}) \text{Re} \left[\frac{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}}}{\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}} - (\hbar\omega + i\eta)} \right] A_{nm,\alpha}(\mathbf{k}) A_{mn,\beta}(\mathbf{k}). \tag{11.11}$$

Finally the joint density of states is

$$\rho_{cv}(\hbar\omega) = \frac{1}{N_k} \sum_{\mathbf{k}} \sum_{n,m} f_{n\mathbf{k}}(1 - f_{m\mathbf{k}}) \overline{\delta}(\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}} - \hbar\omega). \tag{11.12}$$

Equations (11.9–11.12) contain the parameter η, whose value can be chosen using the keyword `[kubo_]smr_fixed_en_width`. Better results can often be achieved by adjusting the value of η for each pair of states, i.e., $\eta \rightarrow \eta_{nm\mathbf{k}}$. This is done as follows (see description of the keyword `adpt_smr_fac`)

$$\eta_{nm\mathbf{k}} = \alpha |\boldsymbol{\nabla}_{\mathbf{k}}(\varepsilon_{m\mathbf{k}} - \varepsilon_{n\mathbf{k}})| \Delta k. \tag{11.13}$$

The energy eigenvalues $\varepsilon_{n\mathbf{k}}$, band velocities $\boldsymbol{\nabla}_{\mathbf{k}}\varepsilon_{n\mathbf{k}}$, and off-diagonal Berry connection $\mathbf{A}_{nm}(\mathbf{k})$ entering the previous four equations are evaluated over a k-point grid by Wannier interpolation, as described in Refs. [8, 11]. After averaging over the Brillouin zone, the Hermitean and anti-Hermitean parts of the conductivity are assembled into the symmetric and antisymmetric tensors

$$\sigma^{\text{S}}_{\alpha\beta} = \text{Re}\sigma^{\text{H}}_{\alpha\beta} + i\text{Im}\sigma^{\text{AH}}_{\alpha\beta} \tag{11.14}$$

$$\sigma^{\text{A}}_{\alpha\beta} = \text{Re}\sigma^{\text{AH}}_{\alpha\beta} + i\text{Im}\sigma^{\text{H}}_{\alpha\beta}, \tag{11.15}$$

whose independent components are written as a function of frequency onto nine separate files.

11.3   `berry_task=ahc`: anomalous Hall conductivity

The antisymmetric tensor $\sigma^{\mathrm{A}}_{\alpha\beta}$ is odd under time reversal, and therefore vanishes in non-magnetic systems, while in ferromagnets with spin-orbit coupling it is generally nonzero. The imaginary part $\mathrm{Im}\sigma^{\mathrm{H}}_{\alpha\beta}$ describes magnetic circular dichroism, and vanishes as $\omega \to 0$. The real part $\mathrm{Re}\sigma^{\mathrm{AH}}_{\alpha\beta}$ describes the anomalous Hall conductivity (AHC), and remains finite in the static limit.

The intrinsic dc AHC is obtained by setting $\eta = 0$ and $\omega = 0$ in Eq. (11.11). The contribution from point $\mathbf{k}$ in the Brillouin zone is

$$\sigma^{\mathrm{AH}}_{\mathbf{k},\alpha\beta}(0) = \frac{2e^2}{\hbar\Omega_c} \sum_{n,m} f_{n\mathbf{k}}(1 - f_{m\mathbf{k}})\mathrm{Im}\langle\nabla_{k_\alpha} u_{n\mathbf{k}}|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\nabla_{k_\beta} u_{n\mathbf{k}}\rangle, \tag{11.16}$$

where we replaced $f_{n\mathbf{k}} - f_{m\mathbf{k}}$ with $f_{n\mathbf{k}}(1 - f_{m\mathbf{k}}) - f_{m\mathbf{k}}(1 - f_{n\mathbf{k}})$.

This expression is not the most convenient for *ab initio* calculations, as the sums run over the complete set of occupied and empty states. In practice the sum over empty states can be truncated, but a relatively large number should be retained to obtain accurate results. Using the resolution of the identity $1 = \sum_m |u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|$ and noting that the term $\sum_{n,m} f_{n\mathbf{k}}f_{m\mathbf{k}}(\ldots)$ vanishes identically, we arrive at the celebrated formula for the intrinsic AHC in terms of the Berry curvature,

$$\sigma^{\mathrm{AH}}_{\alpha\beta}(0) = \frac{e^2}{\hbar} \frac{1}{N_k\Omega_c} \sum_{\mathbf{k}} (-1)\Omega_{\alpha\beta}(\mathbf{k}), \tag{11.17}$$

$$\Omega_{\alpha\beta}(\mathbf{k}) = \sum_n f_{n\mathbf{k}}\Omega_{n,\alpha\beta}(\mathbf{k}). \tag{11.18}$$

Note that only *occupied* states enter this expression. Once we have a set of Wannier functions spanning the valence bands (together with a few low-lying conduction bands, typically) Eq. (11.17) can be evaluated by Wannier interpolation as described in Refs. [8, 12], with no truncation involved.

11.4   `berry_task=morb`: orbital magnetization

The ground-state orbital magnetization of a crystal is given by [9, 13]

$$\mathbf{M}^{\mathrm{orb}} = \frac{e}{\hbar} \frac{1}{N_k\Omega_c} \sum_{\mathbf{k}} \mathbf{M}^{\mathrm{orb}}(\mathbf{k}), \tag{11.19}$$

$$\mathbf{M}^{\mathrm{orb}}(\mathbf{k}) = \sum_n \frac{1}{2} f_{n\mathbf{k}} \, \mathrm{Im} \, \langle\boldsymbol{\nabla}_{\mathbf{k}} u_{n\mathbf{k}}| \times (H_{\mathbf{k}} + \varepsilon_{n\mathbf{k}} - 2\varepsilon_F) |\boldsymbol{\nabla}_{\mathbf{k}} u_{n\mathbf{k}}\rangle, \tag{11.20}$$

where ε_F is the Fermi energy. The Wannier-interpolation calculation is described in Ref. [12]. Note that the definition of $\mathbf{M}^{\mathrm{orb}}(\mathbf{k})$ used here differs by a factor of $-1/2$ from the one in Eq. (97) and Fig. 2 of that work.

11.5   Needed matrix elements

All the quantities entering the formulas for the optical conductivity and AHC can be calculated by Wannier interpolation once the Hamiltonian and position matrix elements $\langle\mathbf{0}n|H|\mathbf{R}m\rangle$ and $\langle\mathbf{0}n|\mathbf{r}|\mathbf{R}m\rangle$ are known [8, 11]. Those matrix elements are readily available at the end of a standard MLWF

calculation with `wannier90`. In particular, $\langle \mathbf{0}n|\mathbf{r}|\mathbf{R}m \rangle$ can be calculated by Fourier transforming the overlap matrices in Eq. (1.7),

$$\langle u_{n\mathbf{k}}|u_{m\mathbf{k}+\mathbf{b}} \rangle.$$

Further Wannier matrix elements are needed for the orbital magnetization [12]. In order to calculate them using Fourier transforms, one more piece of information must be taken from the k-space *ab-initio* calculation, namely, the matrices

$$\langle u_{n\mathbf{k}+\mathbf{b}_1}|H_{\mathbf{k}}|u_{m\mathbf{k}+\mathbf{b}_2} \rangle$$

over the *ab-initio* k-point mesh [12]. These are evaluated by `pw2wannier90`, the interface routine between `pwscf` and `wannier90`, by adding to the input file `seedname.pw2wan` the line

$$\text{write\_uHu} = \text{.true.}$$

Chapter 12

Electronic transport calculations with the `BoltzWann` module

By setting `boltzwann = TRUE`, `postw90` will call the `BoltzWann` routines to calculate some transport coefficients using the Boltzmann transport equation in the relaxation time approximation.

In particular, the transport coefficients that are calculated are: the electrical conductivity $\boldsymbol{\sigma}$, the Seebeck coefficient $\mathbf{S}$ and the coefficient $\mathbf{K}$ (defined below; it is the main ingredient of the thermal conductivity).

The list of parameters of the `BoltzWann` module are summarized in Table 10.6. An example of a Boltzmann transport calculation can be found in the `wannier90` Tutorial.

Note: By default, the code assumes to be working with a 3D bulk material, with periodicity along all three spatial directions. If you are interested in studying 2D systems, set the correct value for the `boltz_2d_dir` variable (see Sec. 10.11.4 for the documentation). This is important for the evaluation of the Seebeck coefficient.

Please cite the following paper [14] when publishing results obtained using the `BoltzWann` module:

> G. Pizzi, D. Volja, B. Kozinsky, M. Fornari, and N. Marzari,
> *BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties*
> *with a maximally-localized Wannier functions basis,*
> Comp. Phys. Comm. 185, 422 (2014), DOI:10.1016/j.cpc.2013.09.015.

12.1 Theory

The theory of the electronic transport using the Boltzmann transport equations can be found for instance in Refs. [15–17]. Here we briefly summarize only the main results.

The current density $\mathbf{J}$ and the heat current (or energy flux density) $\mathbf{J}_Q$ can be written, respectively, as

$$\mathbf{J} = \boldsymbol{\sigma}(\mathbf{E} - \mathbf{S}\boldsymbol{\nabla}T) \tag{12.1}$$

$$\mathbf{J}_Q = T\boldsymbol{\sigma}\mathbf{S}\mathbf{E} - \mathbf{K}\boldsymbol{\nabla}T, \tag{12.2}$$

where the electrical conductivity $\boldsymbol{\sigma}$, the Seebeck coefficient $\mathbf{S}$ and $\mathbf{K}$ are 3×3 tensors, in general.

Note: the thermal conductivity $\boldsymbol{\kappa}$ (actually, the electronic part of the thermal conductivity), which is defined as the heat current per unit of temperature gradient in open-circuit experiments (i.e., with $\mathbf{J} = 0$) is not precisely $\mathbf{K}$, but $\boldsymbol{\kappa} = \mathbf{K} - \mathbf{S}\boldsymbol{\sigma}\mathbf{S}T$ (see for instance Eq. (7.89) of Ref. [15] or Eq. (XI-57b) of Ref. [16]). The thermal conductivity $\boldsymbol{\kappa}$ can be then calculated from the $\boldsymbol{\sigma}$, $\mathbf{S}$ and $\mathbf{K}$ tensors output by the code.

These quantities depend on the value of the chemical potential μ and on the temperature T, and can be calculated as follows:

$$[\boldsymbol{\sigma}]_{ij}(\mu, T) = e^2 \int_{-\infty}^{+\infty} d\varepsilon \left(-\frac{\partial f(\varepsilon, \mu, T)}{\partial \varepsilon} \right) \Sigma_{ij}(\varepsilon), \tag{12.3}$$

$$[\boldsymbol{\sigma}\mathbf{S}]_{ij}(\mu, T) = \frac{e}{T} \int_{-\infty}^{+\infty} d\varepsilon \left(-\frac{\partial f(\varepsilon, \mu, T)}{\partial \varepsilon} \right) (\varepsilon - \mu)\Sigma_{ij}(\varepsilon), \tag{12.4}$$

$$[\mathbf{K}]_{ij}(\mu, T) = \frac{1}{T} \int_{-\infty}^{+\infty} d\varepsilon \left(-\frac{\partial f(\varepsilon, \mu, T)}{\partial \varepsilon} \right) (\varepsilon - \mu)^2 \Sigma_{ij}(\varepsilon), \tag{12.5}$$

where $[\boldsymbol{\sigma}\mathbf{S}]$ denotes the product of the two tensors $\boldsymbol{\sigma}$ and $\mathbf{S}$, $f(\varepsilon, \mu, T)$ is the usual Fermi–Dirac distribution function

$$f(\varepsilon, \mu, T) = \frac{1}{e^{(\varepsilon - \mu)/K_B T} + 1}$$

and $\Sigma_{ij}(\varepsilon)$ is the Transport Distribution Function (TDF) tensor, defined as

$$\Sigma_{ij}(\varepsilon) = \frac{1}{V} \sum_{n, \mathbf{k}} v_i(n, \mathbf{k}) v_j(n, \mathbf{k}) \tau(n, \mathbf{k}) \delta(\varepsilon - E_{n,k}).$$

In the above formula, the sum is over all bands n and all states $\mathbf{k}$ (including spin, even if the spin index is not explicitly written here). $E_{n,\mathbf{k}}$ is the energy of the $n-$th band at $\mathbf{k}$, $v_i(n, \mathbf{k})$ is the $i-$th component of the band velocity at $(n, \mathbf{k})$, δ is the Dirac's delta function, V is the cell volume, and finally τ is the relaxation time. In the *relaxation-time approximation* adopted here, τ is assumed as a constant, i.e., it is independent of n and $\mathbf{k}$ and its value (in fs) is read from the input variable `boltz_relax_time`.

12.2 Files

12.2.1 `seedname_boltzdos.dat`

OUTPUT. Written by `postw90` if `boltz_calc_also_dos` is `true`. Note that even if there are other general routines in `postw90` which specifically calculate the DOS, it may be convenient to use the routines in `BoltzWann` setting `boltz_calc_also_dos = true` if one must also calculate the transport coefficients. In this way, the (time-demanding) band interpolation on the k mesh is performed only once, resulting in a much shorter execution time.

The first lines are comments (starting with # characters) which describe the content of the file. Then, there is a line for each energy ε on the grid, containing a number of columns. The first column is the energy ε. The following is the DOS at the given energy ε. The DOS can either be calculated using the adaptive smearing scheme[1] if `boltz_dos_adpt_smr` is `true`, or using a "standard" fixed smearing, whose type and value are defined by `boltz_dos_smr_type` and `boltz_dos_smr_fixed_en_width`, respectively.

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[1]Note that in `BoltzWann` the adaptive (energy) smearing scheme also implements a simple adaptive $k-$mesh scheme: if at any given k point one of the band gradients is zero, then that k point is replaced by 8 neighboring k points. Thus, the final results for the DOS may be slightly different with respect to that given by the `dos` module.

If spin decomposition is required (input flag `spin_decomp`), further columns are printed, with the spin-up projection of the DOS, followed by spin-down projection.

12.2.2 `seedname_tdf.dat`

OUTPUT. This file contains the Transport Distribution Function (TDF) tensor $\boldsymbol{\Sigma}$ on a grid of energies.

The first lines are comments (starting with # characters) which describe the content of the file. Then, there is a line for each energy ε on the grid, containing a number of columns. The first is the energy ε, the followings are the components if $\boldsymbol{\Sigma}(\varepsilon)$ in the following order: Σ_{xx}, Σ_{xy}, Σ_{yy}, Σ_{xz}, Σ_{yz}, Σ_{zz}. If spin decomposition is required (input flag `spin_decomp`), 12 further columns are provided, with the 6 components of $\boldsymbol{\Sigma}$ for the spin up, followed by those for the spin down.

The energy ε is in eV, while $\boldsymbol{\Sigma}$ is in $\dfrac{1}{\hbar^2} \cdot \dfrac{\text{eV} \cdot \text{fs}}{\text{Å}}$.

12.2.3 `seedname_elcond.dat`

OUTPUT. This file contains the electrical conductivity tensor $\boldsymbol{\sigma}$ on the grid of T and μ points.

The first lines are comments (starting with # characters) which describe the content of the file. Then, there is a line for each (μ, T) pair, containing 8 columns, which are respectively: μ, T, σ_{xx}, σ_{xy}, σ_{yy}, σ_{xz}, σ_{yz}, σ_{zz}. (The tensor is symmetric).

The chemical potential is in eV, the temperature is in K, and the components of the electrical conductivity tensor ar in SI units, i.e. in $1/\Omega/\text{m}$.

12.2.4 `seedname_sigmas.dat`

OUTPUT. This file contains the tensor $\boldsymbol{\sigma}\mathbf{S}$, i.e. the product of the electrical conductivity tensor and of the Seebeck coefficient as defined by Eq. (12.4), on the grid of T and μ points.

The first lines are comments (starting with # characters) which describe the content of the file. Then, there is a line for each (μ, T) pair, containing 8 columns, which are respectively: μ, T, $(\sigma S)_{xx}$, $(\sigma S)_{xy}$, $(\sigma S)_{yy}$, $(\sigma S)_{xz}$, $(\sigma S)_{yz}$, $(\sigma S)_{zz}$. (The tensor is symmetric).

The chemical potential is in eV, the temperature is in K, and the components of the tensor ar in SI units, i.e. in A/m/K.

12.2.5 `seedname_seebeck.dat`

OUTPUT. This file contains the Seebeck tensor $\mathbf{S}$ on the grid of T and μ points.

Note that in the code the Seebeck coefficient is defined as zero when the determinant of the electrical conductivity $\boldsymbol{\sigma}$ is zero. If there is at least one (μ, T) pair for which $\det \boldsymbol{\sigma} = 0$, a warning is issued on the output file.

The first lines are comments (starting with # characters) which describe the content of the file. Then, there is a line for each (μ, T) pair, containing 11 columns, which are respectively: μ, T, S_{xx}, S_{xy}, S_{xz}, S_{yx}, S_{yy}, S_{yz}, S_{zx}, S_{zy}, S_{zz}.

NOTE: therefore, the format of the columns of this file is different from the other three files (elcond, sigmas and kappa)!

The chemical potential is in eV, the temperature is in K, and the components of the Seebeck tensor ar in SI units, i.e. in V/K.

12.2.6   `seedname_kappa.dat`

OUTPUT. This file contains the tensor $\mathbf{K}$ defined in Sec. 12.1 on the grid of T and μ points.

The first lines are comments (starting with $\#$ characters) which describe the content of the file. Then, there is a line for each (μ, T) pair, containing 8 columns, which are respectively: μ, T, K_{xx}, K_{xy}, K_{yy}, K_{xz}, K_{yz}, K_{zz}. (The tensor is symmetric).

The chemical potential is in eV, the temperature is in K, and the components of the $\mathbf{K}$ tensor are the SI units for the thermal conductivity, i.e. in W/m/K.

Chapter 13

Generic Band interpolation

By setting `geninterp = TRUE`, `postw90` will calculate the band energies (and possibly the band derivatives, if also `geninterp_alsofirstder` is set to `TRUE`) on a generic list of k points provided by the user.

The list of parameters of the Generic Band Interpolation module are summarized in Table 10.7. The list of input k points for which the band have to be calculated is read from the file named `seedname_geninterp.kpt`. The format of this file is described below.

13.1 Files

13.1.1 seedname_geninterp.kpt

INPUT. Read by `postw90` if `geninterp` is `true`.

The first line is a comment (its maximum allowed length is 500 characters).

The second line must contain `crystal` (or `rel`) if the k-point coordinates are given in relative (crystallographic) units, i.e., in fractional units with respect to the primitive reciprocal lattice vectors. Otherwise, it must contain `frac` (or `abs`) if instead the $k-$point coordinates are given in absolute coordinates (in units of $2\pi/\text{Å}$) along the k_x, k_y and k_z axes.

The third line must contain the number n of following k points.

The following n lines must contain the list of k points in the format

```
kpointidx k1 k2 k3
```

where `kpointidx` is an integer identifying the given k point, and `k1`, `k2` and `k3` are the three coordinates of the k points in the chosen units.

13.1.2 seedname_geninterp.dat or seedname_geninterp_NNNNN.dat

OUTPUT. This file/these files contain the interpolated band energies (and also the band velocities if the input flag `geninterp_alsofirstder` is `true`).

If the flag `geninterp_single_file` is `true`, then a single file `seedname_geninterp.dat` is written by the code at the end of the calculation. If instead one sets `geninterp_single_file` to `false`, each process writes its own output file, named `seedname_geninterp_00000.dat`, `seedname_geninterp_00001.dat`, . . .

This flag is useful when one wants to parallelize the calculation on many nodes, and it should be used especially for systems with a small number of Wannier functions, when one wants to compute the bands on a large number of k points (if the flag `geninterp_single_file` is `true`, instead, all the I/O is made by the root node, which is a significant bottleneck).

Important! The files are not deleted before the start of a calculation, but only the relevant files are overwritten. Therefore, if one first performs a calculation and then a second one with a smaller number of processors, care is needed to avoid to mix the results of the older calculations with those of the new one. In case of doubt, either check the date stamp in the first line of the `seedname_geninterp_*.dat` files, or simply delete the `seedname_geninterp_*.dat` files before starting the new calculation.

To join the files, on can simply use the following command:

```
cat seedname_geninterp_*.dat > seedname_geninterp.dat
```

or, if one wants to remove the comment lines:

```
rm seedname_geninterp.dat
for i in seedname_geninterp_*.dat ; do grep -v \# "$i" >> \
seedname_geninterp.dat ; done
```

The first few lines of each files are comments (starting with $\#$), containing a datestamp, the comment line as it is read from the input file, and a header. The following lines contain the band energies (and derivatives) for each band and k point (the energy index runs faster than the k-point index). For each of these lines, the first four columns contain the k-point index as provided in the input, and the k coordinates (always in absolute coordinates, in units of $2\pi/\text{Å}$). The fifth column contains the band energy.

If `geninterp_alsofirstder` is `true`, three further columns are printed, containing the three first derivatives of the bands along the k_x, k_y and k_z directions.

The k point coordinates are in units of $2\pi/\text{Å}$, the band energy is in eV.

Part IV

Appendices

Appendix A

Utilities

The `wannier90` code is shipped with a few utility programs that may be useful in some occasions. In this chapter, we describe their use.

A.1 `kmesh.pl`

The `wannier90` code requires the definition of a full Monkhorst–Pack grid of k points. In the input file the size of this mesh is given by means of the `mp_grid` variable. E.g., setting

```
mp_grid = 4 4 4
```

tells `wannier90` that we want to use a $4 \times 4 \times 4$ k grid.

One has then to specify (inside the `kpoints` block in the the `seedname.win` file) the list of k points of the grid. Here, the `kmesh.pl` Perl script becomes useful, being able to generate the required list.

The script can be be found in the `utility` directory of the `wannier90` distribution. To use it, simply type:

```
./kmesh.pl nx ny nz
```

where `nx`, `ny` and `nz` define the size of the Monkhorst–Pack grid that we want to use (for instance, in the above example of the $4 \times 4 \times 4$ k grid, `nx=ny=nz=4`).

This produces on output the list of k points in Quantum Espresso format, where (apart from a header) the first three columns of each line are the k coordinates, and the fourth column is the weight of each k point. This list can be used to create the input file for the ab-initio `nscf` calculation.

If one wants instead to generate the list of the k coordinates without the weight (in order to copy and paste the output inside the `seedname.win` file), one simply has to provide a fourth argument on the command line. For instance, for a $4 \times 4 \times 4$ k grid, use

```
./kmesh.pl 4 4 4 wannier
```

and then copy the output inside the in the `kpoints` block in the `seedname.win` file.

We suggest to always use this utility to generate the k grids. This allows to provide the k point coordinates with the accuracy required by wannier90, and moreover it makes sure that the k grid used in the ab-initio code and in wannier90 are the same.

A.2 w90chk2chk.x

During the calculation of the Wannier functions, wannier90 produces a .chk file that contains some information to restart the calculation.

This file is also required by the postw90 code. In particular, the postw90 code requires at least the .chk file, the .win input file, and (almost always) the .eig file. Specific modules may require further files: see the documentation of each module.

However, the .chk file is written in a machine-dependent format. If one wants to run wannier90 on a machine, and then continue the calculation with postw90 on a different machine (or with postw90 compiled with a different compiler), the file has to be converted first in a machine-independent "formatted" format on the first machine, and then converted back on the second machine.

To this aim, use the w90chk2chk.x executable. Note that this executable is not compiled by default: you can obtain it by executing

```
make w90chk2chk
```

in the main wannier90 directory.

A typical use is the following:

1. Calculate the Wannier functions with wannier90

2. At the end of the calculation you will find a seedname.chk file. Run (in the folder with this file) the command

   ```
   w90chk2chk.x -export seedname
   ```

   or equivalently

   ```
   w90chk2chk.x -u2f seedname
   ```

   (replacing seedname with the seedname of your calculation).

   This command reads the seedname.chk file and creates a formatted file seedname.chk.fmt that is safe to be transferred between different machines.

3. Copy the seedname.chk.fmt file (together with the seedname.win and seedname.eig files) on the machine on which you want to run postw90.

4. On this second machine (after having compiled w90chk2chk.x) run

   ```
   w90chk2chk.x -import seedname
   ```

   or equivalently

```
w90chk2chk.x -f2u seedname
```

This command reads the `seedname.chk.fmt` file and creates an unformatted file `seedname.chk` ready to be used by `postw90`.

5. Run the `postw90` code.

A.3 PL_assessment

The function of this utility is to assess the length of a principal layer (in the context of a Landauer-Buttiker quantum conductance calculation) of a periodic system using a calculation on a single unit cell with a dense k-point mesh.

The utility requires the real-space Hamiltonian in the MLWF basis, `seedname_hr.dat`.

The `seedname_hr.dat` file should be copied to a directory containing executable for the utility. Within that directory, run:

```
\$> ./PL_assess.x  nk1 nk2 nk3 num_wann
```

where:

`nk1` is the number of k-points in x-direction `nk2` is the number of k-points in y-direction `nk3` is the number of k-points in z-direction `num_wann` is the number of wannier functions of your system

e.g.,

```
\$> ./PL_assess.x  1 1 20 16
```

Note that the current implementation only allows for a single k-point in the direction transverse to the transport direction.

When prompted, enter the seedname.

The programme will return an output file `seedname_pl.dat`, containing four columns

1. Unit cell number, R

2. Average 'on-site' matrix element between MLWFs in the home unit cell, and the unit cell R lattice vectors away

3. Standard devaition of the quantity in (2)

4. Maximum absolute value in (2)

A.4 w90vdw

This utility provides an implementation of a method for calculating van der Waals energies based on the idea of density decomposition via MLWFs.

For theoretical details, please see the following publication and references therein:

Lampros Andrinopoulos, Nicholas D. M. Hine and Arash A. Mostofi, "Calculating dispersion interactions using maximally localized Wannier functions", *J. Chem. Phys.* **135**, 154105 (2011).

For further details of this program, please see the documentation in `utility/w90vdw/doc/` and the related examples in `utility/w90vdw/examples/`.

A.5   `w90pov`

An utility to create Pov files (to render the Wannier functions using the PovRay utility) is provided inside `utility/w90pov`.

Please refer to the documentation inside `utility/w90pov/doc` for more information.

Appendix B

Frequently Asked Questions

B.1   General Questions

B.1.1   What is `wannier90`?

`wannier90` is a computer package, written in Fortran90, for obtaining maximally-localised Wannier functions, using them to calculate bandstructures, Fermi surfaces, dielectric properties, sparse Hamiltonians and many things besides.

B.1.2   Where can I get `wannier90`?

The most recent release of `wannier90` is always available on our website `http://www.wannier.org`.

B.1.3   Where can I get the most recent information about `wannier90`?

The latest news about `wannier90` can be followed on our website `http://www.wannier.org`.

B.1.4   Is `wannier90` free?

Yes! `wannier90` is available for use free-of-charge under the GNU General Public Licence. See the file `LICENCE` that comes with the `wannier90` distribution or the GNU hopepage at `http://www.gnu.org`.

B.2   Getting Help

B.2.1   Is there a Tutorial available for `wannier90`?

Yes! The `examples` directory of the `wannier90` distribution contains input files for a number of tutorial calculations. The `doc` directory contains the accompanying tutorial handout.

B.2.2   Where do I get support for `wannier90`?

There are a number of options:

1. The `wannier90` User Guide, available in the `doc` directory of the distribution, and from the webpage (`http://www.wannier.org/user_guide.html`)

2. The `wannier90` webpage for the most recent announcements (`http://www.wannier.org`)

3. The `wannier90` mailing list (see `http://www.wannier.org/forum.html`)

B.2.3   Is there a mailing list for `wannier90`?

Yes! You need to register: go to `http://www.wannier.org/forum.html` and follow the instructions.

B.3   Providing Help: Finding and Reporting Bugs

B.3.1   I think I found a bug. How do I report it?

- Check and double-check. Make sure it's a bug.

- Check that it is a bug in `wannier90` and not a bug in the software interfaced to `wannier90`.

- Check that you're using the latest version of `wannier90`.

- Send us an email. Make sure to describe the problem and to attach all input and output files relating to the problem that you have found.

B.3.2   I have got an idea! How do I report a wish?

We're always happy to listen to suggestions. Email your idea to the `wannier90` developers.

B.3.3   I want to help! How can I contribute to `wannier90`?

Great! There's always plenty of functionality to add. Email us to let us know about the functionality you'd like to contribute.

B.3.4   I like `wannier90`! Should I donate anything to its authors?

Our Swiss bank account number is... just kidding! There is no need to donate anything, please just cite our paper in any publications that arise from your use of `wannier90`:

[ref]A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt and N. Marzari, `wannier90`: A Tool for Obtaining Maximally-Localized Wannier Functions, *Comput. Phys. Commun.*, 178, 685 (2008) and `http://arxiv.org/abs/0708.0650`.

B.4 Installation

B.4.1 How do I install `wannier90`?

Follow the instructions in the file `README.install` in the main directory of the `wannier90` distribution.

B.4.2 Are there `wannier90` binaries available?

Not at present.

B.4.3 Is there anything else I need?

Yes. `wannier90` works on top of an electronic structure calculation.

At the time of writing there are public, fully functioning, interfaces between `wannier90` and PWSCF, ABINIT (`http://www.abinit.org`), SIESTA (`http://www.icmab.es/siesta/`), VASP (`https://www.vasp.at`), WIEN2K (`http://www.wien2k.at`), FLEUR (`http://www.fleur.de`).

To use `wannier90` in combination with PWSCF code (a plane-wave, pseudopotential, density-functional theory code, which is part of the `quantum-espresso` package) you will need to download PWSCF from the webpage `http://www.quantum-espresso.org`. Then compile PWSCF and the `wannier90` interface program `pw2wannier90`. For instructions, please refer to the documentation that comes with the `quantum-espresso` distribution.

For examples of how to use PWSCF and `wannier90` in conjunction with each other, see the `wannier90` Tutorial.

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