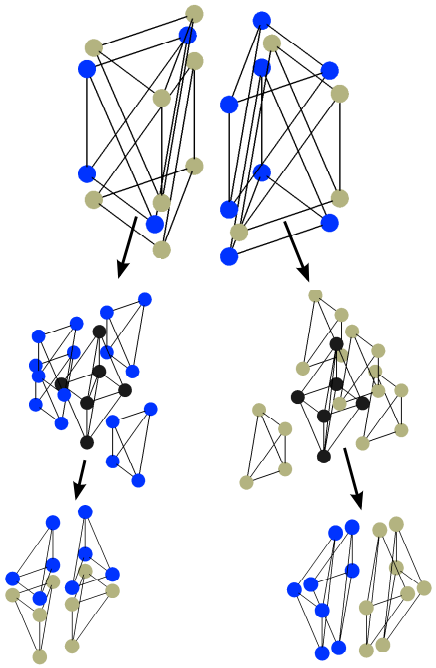
Woptic User's Guide

Optical conductivity with Wannier functions.

Elias Assmann Philipp Wissgott

for version 0.1.0-α



Introduction

To compute the optical conductivity σ in the basis of maximally-localized Wannier orbitals the package WOPTIC is provided. It uses the Green function formalism, which yields

$$\sigma^{\alpha\beta}(\Omega) = \frac{e^2}{(2\pi)^2} \int \mathrm{d}^3k \int \mathrm{d}\omega \; \frac{f(\omega) - f(\omega+\Omega)}{\Omega} \, \mathrm{tr}\left[A(k,\omega)\, V^{\alpha}(k)\, A(k,\omega+\Omega)\, V^{\beta}(k)\right], \qquad (*)$$

where $\sigma^{\alpha\beta}$ is the (α,β) element of the optical conductivity tensor ($\alpha,\beta \in \{x,y,z\}$), V_{uc} the unit cell volume, f the Fermi function, $A = \frac{\mathrm{i}}{2\pi}(G - G^{\dagger})$ the generalized spectral function [1, 2, 3], and V^{α} the group velocity in direction α. The numerical bottleneck in evaluating $(*)$ is the k-summation, since usually many k-points are required to obtain converged results. For a speed-up in k-mesh convergence, WOPTIC therefore employs an adaptively refined tetrahedral tiling of k-space.

WOPTIC consists of two main programs: `woptic_main`, which calculates the optical conductivity, and `refine_tetra`, where the k-mesh is refined; as well as several smaller support programs. The individual programs are normally called by means of the driver script `woptic`. This guide provides technical documentation for WOPTIC. For details on the underlying formalism and algorithm, see Refs. [4, 5, 6].

Acknowledgement Development of this software was supported by Vienna University of Technology, Graz University of Technology, and the European Research Council through grant agreement no. 306447.

Caution Following the many recent changes in WIEN2WANNIER and WOPTIC, some parts of the older version of WOPTIC have not yet been adapted. As such, they must be considered experimental. We keep such untested (or even known to be broken) features in the code and in this guide, where they are marked with a "dangerous bend" sign,  .

Citation In any scientific publications arising from the use of WOPTIC, we ask that you cite Ref. [6],

> E. ASSMANN, P. WISSGOTT, J. KUNEŠ, A. TOSCHI, P. BLAHA, and K. HELD, arXiv:1507.04881,

to acknowledge your use of our code. This is in addition to the appropriate citations to acknowledge other codes used (such as WIEN2K [7], WANNIER90 [8], and WIEN2WANNIER [9]).

Common options and other resources This guide attempts to document the features most relevant to the WOPTIC user; it will not list every option or every file used by every command. Most commands honor the option `--help`, which should provide a definitive list of options for that command. The WOPTIC distribution also includes a terse instruction sheet as `doc/WOPTICHEAT`.

Contact Comments, patches, and the like can be sent to `wien2wannier@ifp.tuwien.ac.at`.

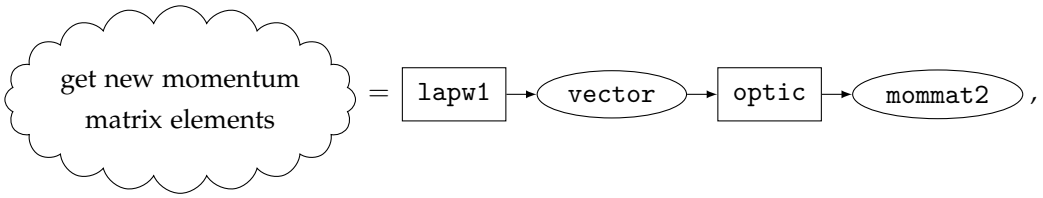
Contents

1 The driver script `woptic`

This is the main user-callable program. It runs the other programs as necessary until a set number of iterations is completed (or an error occurs) — convergence has to be checked manually. If you include an outer window in your `interp` calculation, you should check the localization of $W^{\alpha\beta}(R,\omega)$ and/or the interpolation errors in the optical conductivity.

Since the procedure is a little involved, we provide Fig. 1.1 to give an overview of the files and programs involved in one iteration (but note that not all files that might be involved are shown). The computation of the group velocities $V^{\alpha}(k)$ for the new k-points varies according to the option `matelmode`. WOPTIC implements two modes using the full momentum matrix elements $V^{\alpha}_{ab}(k) = \langle \psi\ ak| \, \widehat{p}_{\alpha} \, |\psi\ bk\rangle$ as group velocities:

`optic` mode takes the matrix elements from WIEN2k's `optic` module,

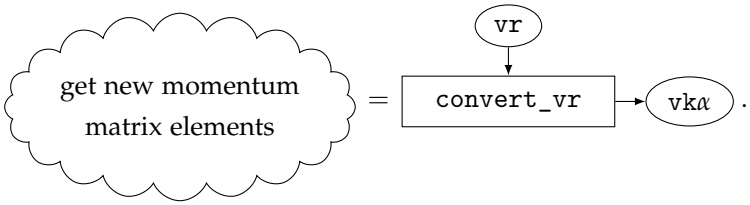


and transforms them to the Wannier basis using the matrices $U(k)$ which diagonalize the Wannier-interpolated Hamiltonian, $U_{nu}(k)H^{\mathrm{w}}_{uv}(k)U^{\dagger}_{vm}(k) = \delta_{nm}\epsilon_n(k)$. But the diagonalization fixes the eigenvectors only up to a phase, which leads to a *random-phase problem* in $(*)$ and associated uncertainties in the optical conductivity. The problem is absent whenever the self-energy is orbital-independent (by symmetry, or in a noninteracting model). In such a case, `optic` mode should be dependable. Otherwise, the results should be checked for the influence of the random-phase problem.

`interp` mode applies Wannier interpolation to the matrix elements directly in order to overcome the random-phase problem. `compute_vr` calculates the Wannier momentum matrix elements in direct space

$$V^{\mathrm{w},\alpha}_{uv}(R) = \frac{1}{N_k}\sum_k \mathrm{e}^{-\mathrm{i}k\cdot R}\, U^{\dagger}_{un}(k)V^{\alpha}_{nm}(k)U_{mv}(k) = \langle w\ u0| \, \widehat{p}_{\alpha} \, |w\ vR\rangle \,,$$

and `convert_vr` interpolates them to the new k-points,[1]



The interpolation works well for the Wannier-Wannier transitions ($V^{\mathrm{W},\alpha}$), but interpolation errors may become large for the mixed transitions governed by $W^{\alpha\beta}(R,\omega)$, where

$$W^{\alpha\beta}_{uv}(k,\omega) = \sum_i V^{\alpha}_{ui}(k) A_{ii}(\omega) V^{\beta}_{iv}(k)$$

with the index i running over the non-Wannier states (i.e. the outer window) and the matrix elements are transformed into the Wannier basis on one side only. Note that the interpolation errors typically only affect the interband optical conductivity; as long as the low-energy degrees of freedom are described by the Wannier functions, the static quantities (dc conductivity and thermopower) should be reliable.

In addition, `Peierls` mode uses the Peierls approximation $V(k) \approx \mathrm{i}\,\nabla_k H(k)$ instead of the momentum matrix elements. It is currently unsupported.

Further reading. See [4] for the original description of WOPTIC in the `optic` and `Peierls` modes. See [5] for a detailed description of `interp` mode and a numerical comparison to `optic` mode including an analysis of the errors commited in each of them. Ref. [1] tests the Peierls approximation against the full momentum matrix elements.

Disentanglement is supported only in `interp` mode in the case where only Wannier-Wannier transitions are included. This may be useful when the Wannier model is expected to describe all the salient features of a system, but disentanglement is necessary, e.g., to remove extraneous states at the band edges.

[1] In the interest of full disclosure, the diagram is accurate in the case where only Wannier-Wannier transitions are taken into account. With mixed transitions, `vr` is supplemented by `vvr` and `vkα` by `vvkαβ`, and `optic` is also called for the mixed [Wannier-Bloch] matrix elements.

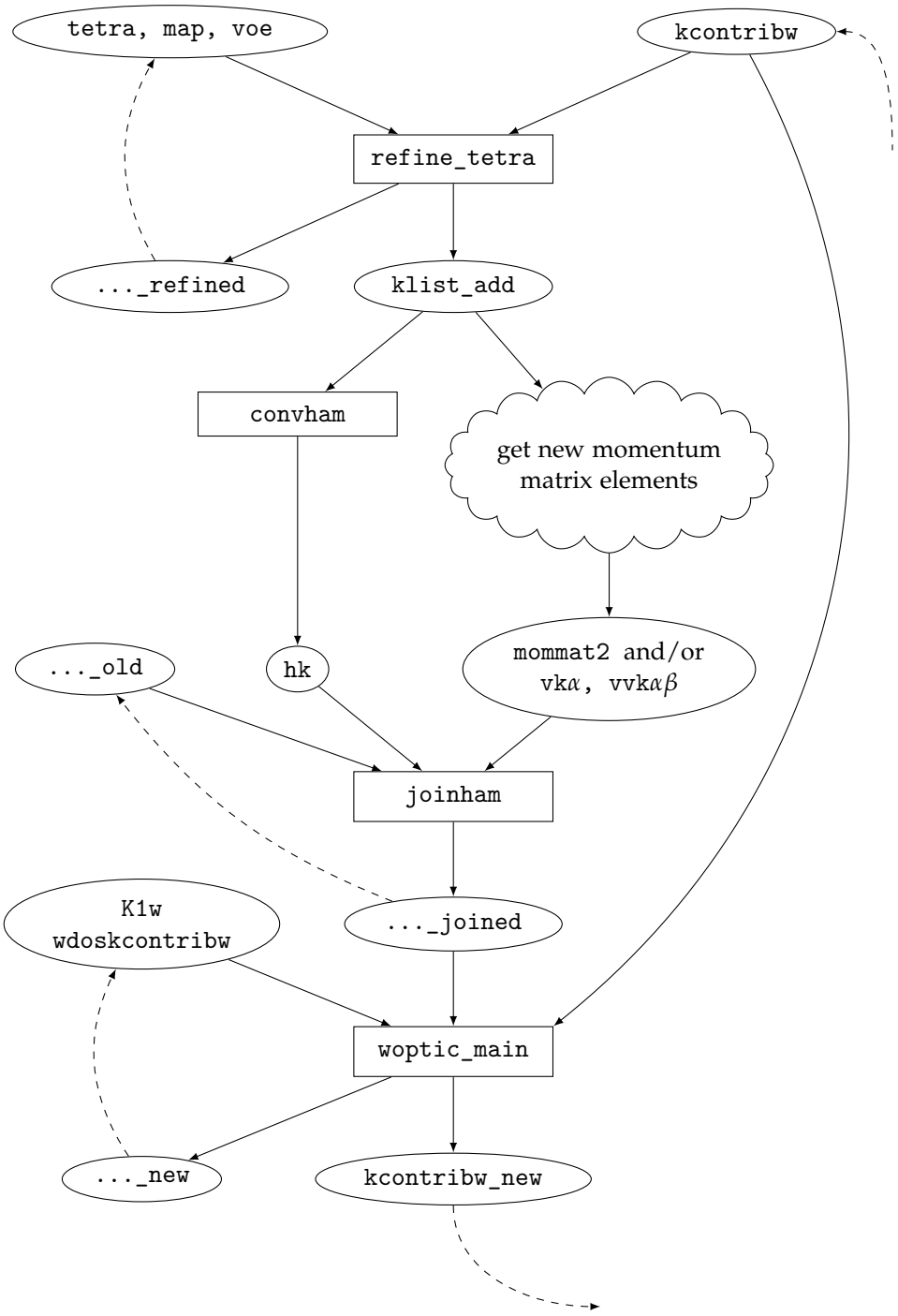


Figure 1.1: Flow of control and information in the main WOPTIC loop: programs (rectangles) and selected files (ellipses). Dashed lines indicate a file is taken from the previous iteration.

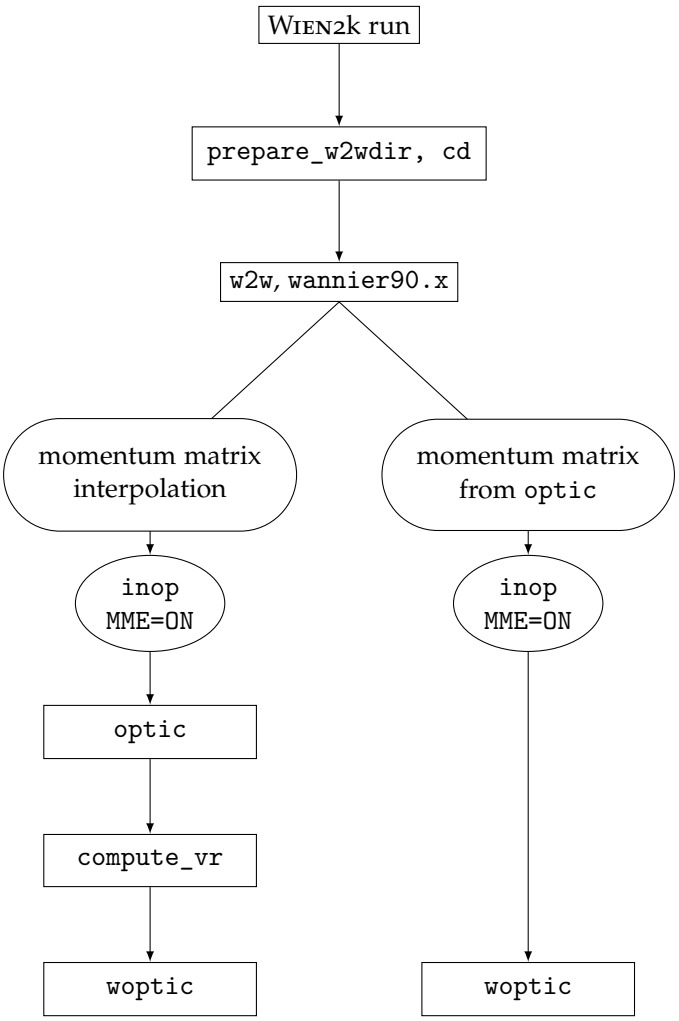


Figure 1.2: Flow of control and information in WOPTIC initialization.

1.1 Synopsis

`woptic [-i` $N_{\mathtt{tot}}$ `] [--restart` I`] [`*more options*`]`

1.2 Options

`-i` $N_{\mathtt{tot}}$ stop after iteration $N_{\mathtt{tot}}$ *(default: 5)*

`--restart` I restart from *`case`*`.wophist.zip` at the beginning of iteration I *(default: 1)*

`--restore` I restore iteration I from *`case`*`.wophist.zip` without continuing

`--theta` Θ refinement harshness *($\Theta = 0$: uniform mesh, $\Theta = 1$: most adaptive; default: 0.5)*

`--inter` focus refinement on larger Ω

`--init` $N_{\mathtt{i}}$ initial uniform refinement steps *(default: 3)*

`--band` compute optical conductivity contributions along *`case`*`.klist_band` to be processed by `kanalysis`

The iterations in `-i`, `--restart`, and `--restore` are "absolute" in the sense that iteration 1 always corresponds to the initial k-mesh. Thus, `woptic --restart 3 -i 5` does three iterations: nos. 3, 4, and 5. Iteration no. 1 starts with a uniform k-mesh whose density is determined by $N_{\mathtt{i}}$. The starting mesh corresponds to $(2^{N_{\mathtt{i}}+1})^3$ k-points in the full BZ.

Let T be a tetrahedron and $\epsilon(T)$ its associated integration error estimate. The precise meaning of the "harshness" $\Theta \in [0,1]$ is: T will be refined if

$$\epsilon(T) \geq \Theta \max_T \epsilon(T) \qquad \texttt{(--theta)}$$

(but may also be refined due to other rules) [4, 6]. The `--inter` option scales the contributions to the error estimates by the frequency,

$$\epsilon(T;\Omega) \leftarrow \Omega \cdot \epsilon(T,\Omega), \qquad \texttt{(--inter)}$$

for the purposes of refinement.

1.3 The input file *case*`.inwop`

The main input file for WOPTIC is

case`.inwop`

```
OPT   interp   F       # mode;      matelmode;    intra-uc hop? (Peierls)
10 0.05 0.05   3 1e-5  # Emax, dE, delta (eV);    omega-div, tol-cutoff
21 23  12 25           # inner window (= WFs);    [outer window]
40.0   0.00            # inv. temp. (eV^-1);      chemical potential (eV)
1.0    F               # Drude-sumrule sep. [eV]; compute orb.resolv.?
T 0                    # read self-energy?        #bands
  21 22 23             # bands with self-energy   (if #b=0: inner window)
F F 1.23 0             # rotate WFs?;       scissors?, shift (eV), #bands
  24 25                # bands to shift
```

end of *case*`.inwop`

This file is read using Fortran list-oriented reads, i.e., items are separated by white space.

line 1 `mode, matelmode, intrahop` — modes of operation

`mode`	`OPT`	compute the optical conductivity
	`JOINT`	compute the joint density of states (noninteracting only)
`matelmode`	`1 | Peierls`	use $\mathrm{d}H^{\mathrm{w}}/\mathrm{d}k$ as momentum matrix elements
	`2 | interp`	Wannier-interpolated momentum matrix elements
	`3 | optic`	matrix elements computed by WIEN2k's `optic`
	`4 | Bloch`	for testing (noninteracting only)
	`5 | LDA`	for testing (noninteracting only; should be similar to `optic-joint-kram`)
`intrahop`	*`logical`*	whether to use intra-UC hopping in `Peierls` mode [2, 3] (needs *`case`*`.intrahop`)

Only modes `interp` and `optic` are thoroughly tested; `Peierls`, `Bloch`, and `LDA` must be considered experimental.

line 2 $\Omega_{\mathtt{max}}$, $\Delta\Omega$, δ, $N_{\omega/\Omega}$, ϵ — frequency grids and broadening

$\Omega_{\mathtt{max}}$	eV	maximum external frequency for which $\sigma(\Omega = \Omega_{\mathrm{max}})$ is computed
$\Delta\Omega$	eV	Ω grid spacing
δ	eV	broadening parameter for noninteracting bands (where $\Sigma \leftarrow \mathrm{i}\delta$)
$N_{\omega/\Omega}$	*`int`*	internal frequency density ($N_{\omega/\Omega}$ internal ω per external Ω)
ϵ	*`real`*	tolerance for ω-integration limits ($-\Omega_{\mathrm{max}} \lesssim \omega \lesssim 0$)

line 3 `Wlo, Whi, [Blo, Bhi]` — band windows

`Wlo, Whi`	*`int`*	band indices corresponding to WFs
`Blo, Bhi`	*`int`*	the outer ("Bloch") window *(optional, default:* *`Wlo, Whi`*`)`

line 4 β, μ — grand-canonical ensemble parameters

β	eV^{-1}	the inverse temperature *(To convert to temperature in Kelvin: $T \mathrel{\widehat{=}} 11604/\beta$.)*
μ	eV	the chemical potential *(applied only to the interacting bands [see* *`iself`*`], use the DMFT value; for noninteracting calculations, set` $\mu = 0$`)*

line 5 `Drudesep, orbresolv`

`Drudesep`	eV	cutoff for Drude sumrule integration
`orbresolv`	*`logical`*	whether to compute observables per-orbital

line 6 `selfE, Nself` — self-energy specification

`selfE`	*`logical`*	whether to read self-energy $\Sigma_i(\omega)$ from *`case`*`.selfE`
`Nself`	*`int`*	number of bands with self-energy, or 0 *(in this case,* *`Whi`*$-$*`Wlo`*$+1$*)*

line 7 `iself` — interacting bands *(ignored if* *`selfE=.false.`* *or* *`Nself=0`*`)`

`iself`	*`int(Nself)`*	indices of interacting bands *(if* *`Nself=0`*`: inner window)`

line 8 `wfrot, shift, Eshift, Nshift` — WF rotation and scissors operator

`wfrot`	*`logical`*	whether to apply unitary matrix from *`case`*`.wfrot` to WF basis

`shift`	*`logical`*	whether to apply rigid "scissors" shift
`Eshift`	eV	shift value
`Nshift`	*`int`*	number of bands to shift

line 9 `ishift` — scissor bands

`ishift`	*`int(Nshift)`*	indices of bands to shift

1.4 Output files

Over the course of the iterations, `woptic` writes diagnostic information to standard output and lists the executed commands in `:log`. In particular, the current values of the quantities `thermopower`, `dc conductivity`, and `sumrules` are extracted from `woptic_main`'s output file *`case`*`.outputwop`, as well as the integration error `estimator` from `refine_tetra`'s `case.outputref`. The latter is given in arbitrary units and should decrease over the iterations.

The optical conductivity is written to *`case`*`.optcondw`. For comparison with WIEN2k's standard `optic` module, note that there is a factor ≈ 1112.65 between `optic`'s output (given in Gaussian CGS units of $10^{15}\,\mathrm{s}^{-1}$ in *`case`*`.sigmak`) and WOPTIC's (in SI units of $\mathrm{S\,cm}^{-1}$). Expressed in the SI, the conversion is $\texttt{optic} = \text{WOPTIC} \cdot 4\pi\,\epsilon_0\,10^{15}\,\mathrm{Hz\,\Omega\,cm}$.

The density of states is written to *`case`*`.wdos`. The files *`case`*`.optcondw` and *`case`*`.wdos` always correspond to the latest iteration. Together with certain other files, they are archived in *`case`*`.wophist.zip` with a suffix `.`I for iteration I.

2 Support Programs

In this section, the sub-programs called by `woptic` are documented, roughly in order of decreasing user-callability.

2.1 `wopticlean` — remove left-over files from woptic runs

`wopticlean` preserves files which serve as input to `woptic` and its sub-programs, as well as the archive file *`case`*`.wophist.zip`. The number of files considered for deletion is substantial; to check which ones are, use the `--recon` option or the source.

Synopsis

`wopticlean [--recursive] [--mrproper] [--recon] [`*`directory ...`*`]`

Options and arguments

`-r|--recursive` Operate recursively on *all* directories below

`-A|--mrproper` delete also files whose basename does not match the containing directory

`-n|--recon` dry-run; print file names that would be deleted

The arguments specify *`directories`* to operate on *(default: `.`)*. Before a big cleanup (especially when using `-A` or `-r`), you are advised to do a dry-run.

2.2 `compute_vr` — compute $V^{\mathrm{w}}(R)$

`compute_vr` computes the dipole matrix elements $V^{\mathrm{W},\alpha}(R)$ and $W^{\alpha\beta}(R,\omega)$ in direct space by applying the matrices $U(k)$ and a Fourier transform for use with the `interp` mode. You should check these matrix elements (especially $W^{\alpha\beta}$) for decay in R when using this mode.

Synopsis

`compute_vr [--text]` *`case`*

Option

`--text` output *case*`.vvr` in plain text

Files read

case`.inwop` input file
case`.chk` WANNIER90 checkpoint file
case`_hr.dat` Hamiltonian in direct space
case`.mommat2` momentum matrix elements
case`.struct` WIEN2k master input file *(mixed transitions)*
case`.energy` energies from `lapw1` *(mixed transitions)*
case`.fermi` Fermi energy *(mixed transitions)*
case`.inwf` `w2w` input file *(disentanglement)*

Files written

case`.outputvr` log file
case`.vr` $V^{\mathrm{W},\alpha}(R)$
case`.vvr` $W^{\alpha\beta}(R,\omega)$ *(mixed transitions)*

2.3 `kanalysis` — $\sigma(k,\omega)$ on a BZ path

This program generates files that can be used for analysis of the contributions to the optical conductivity in WOPTIC. Required is a run of `woptic` with the `--band` option, such that it computes the contributions to the optical conductivity along *case*`.klist_band` and stores them in *case*`.kcontribw_band`. `kanalysis` reads this file and generates 2D data in ω- and k-space readable e.g. by gnuplot.

Synopsis

`kanalysis` $n_\Omega^{\mathtt{min}}$ *case* [*mode*]

Arguments

$n_\Omega^{\mathtt{min}}$ minimum frequency index for output
mode *(optional)* by default, the output includes extra newlines for convenient plotting with gnuplot (`splot "`*case*`.optanalysis_band" with pm3d`); if `mode` $=1$, these newlines are omitted

2.4 `obtain_dist` — intra-UC hopping for `Peierls`

In WOPTIC, for the generalized `Peierls` approximation [2], the distances between the Wannier centers are required. This program reads *case*`_centres.xyz` which is produced by WANNIER90 and generates *case*`.intrahop` which can then be used by WOPTIC.

Synopsis

```
obtain_dist case
```

2.5 inwopcheck — parse inwop file

A helper program for woptic. Reads an inwop file and outputs information suitable for reading in a shell script or for inspection.

Synopsis

```
inwopcheck case.inwop
```

2.6 woptic_main — k-integration

woptic_main computes the optical conductivity contributions $\sigma(k,\omega)$ on the k-mesh constructed by refine_tetra and performs the k- and ω-integration. It is normally called by woptic, but it may be useful to call it manually after a woptic run.

Synopsis

```
woptic_main [--band] case
```

Option

--band compute optical conductivity contributions along *case*.klist_band to be processed by kanalysis

Files used by woptic_main are listed below. *Updated* files are written with a suffix _new. Which files precisely are used depends on the options in effect, this dependence is partially indicated below.

Files read

***case*.inwop** woptic main input file *(always)*

***case*.struct** Wien2k master input file *(always)*

***case*.symop** symmetry operations from optic *(always)*

***case*.klist** symmetrized k-points *(always)*

***case*.tetra** symmetrized tetrahedra *(always)*

***case*.energy** energies from lapw1

***case*.fermi** Fermi energy

***case*.mommat2** matrix elements from optic

***case*.chk** WANNIER90 checkpoint file *(testing mode)*

***case*.vkα** Wannier-interpolated matrix elements *(interp)*

case.vvk$\alpha\beta$ Wannier-interpolated mixed matrix elements *(interp)*

case.hk Wannier Hamiltonian $H^{\mathrm{W}}(R)$

case.selfE self-energy $\Sigma(\omega)$ *(selfE)*

case.wfrot Wannier function rotation matrix *(wfrot)*

case.klist_full unsymmetrized k-points *(Peierls)*

case.tetra_full unsymmetrized tetrahedra *(Peierls)*

case.map mapping of `klist_full` to `klist` *(Peierls)*

case.intrahop WF center distance matrix *(Peierls & intrahop)*

Files written

case.outputwop diagnostic output *(always)*

case.optcondw optical conductivity *(always)*

case.wdos (joint) density of states *(always)*

case.optcondw_orb$\alpha\beta$ orbitally resolved optical conductivity *(orbresolv)*

Files updated

case.kcontribw optical conductivity contributions

case.K1w thermopower contributions

case.wdoskcontribw DOS contributions

2.7 `refine_tetra` — k-mesh refinement

`refine_tetra` uses the optical conductivity contributions $\sigma(k,\omega)$ to compute integration error estimates and refine the k-mesh. It is normally called by `woptic`.

Synopsis

```
refine_tetra [options] case
```

Options

--theta Θ $0 \leq \Theta \leq 1$ defines the "harshness" of refinement *(see corresponding option of woptic)*

--init N_{i} initial refinement with N_{i} steps *(see corresponding option of woptic)*

-inter give larger weight to higher-energy contributions *(see corresponding option of woptic)*

Files used by `refine_tetra` are listed below. *Updated* files are written with a suffix `_refined`.

Files read

case.inwop woptic main input file

case.struct Wien2k master input file

Files written

case.kcontribw function values for estimator on case.klist

case.outputref log file

Files updated

case.klist symmetrized k-points

case.klist_full unsymmetrized k-points

case.tetra symmetrized tetrahedra

case.tetra_full unsymmetrized tetrahedra

case.voe list of k-points on tetrahedral edges

case.map internal mapping of case.klist_full to case.klist

2.8 joinham — combine hk / mommat2 / vkα / vvkαβ files

joinham combines _old files from the previous iteration with new files corresponding to added k-points. It is normally called by woptic.

Synopsis

```
joinham case |
joinham hk mommat |
joinham hk1 hk2 hkout |
joinham hk1 hk2 hkout mom1 mom2 momout
```

Arguments

hk* a file of type case.hk, case.vkα, or case.vvkαβ

mom* a file of type case.mommat2

In the first form, case.hk_old is joined with case.hk, and, if they exist, case.mommat2_old with case.mommat. In the second form, hk_old is joined with hk and mom_old with mom. In both cases, output file names are suffixed with _joined. Unformatted mom files are handled automatically and result in unformatted output.

2.9 convert_vr — Fourier-interpolate $V^{w}(k)$

convert_vr computes case.vkα and case.vvkαβ from case.vr and case.vvr by Fourier transform. The procedure is analogous to convham, case.hk, and case_hr.dat.

Synopsis

`convert_vr [--text] case`

Option

`-t, --text` write *case*`.vvk`$\alpha\beta$ in plain text instead of `unformatted` (*case*`.vk`α is always plain text)

Files read

***case*`.struct`** WIEN2k master input file

***case*`.klist`** target k-points

***case*`.inwop`** `woptic` input file

***case*`.vr`** direct-space matrix elements $V^{W,\alpha}(R)$

***case*`.vvr`** direct-space mixed matrix elements $W^{\alpha\beta}(R,\omega)$ *(mixed transitions)*

Files written

***case*`.outputvk`** log file

***case*`.vk{x,y,z}`** k-space matrix elements $V^{W,\alpha}(k)$

***case*`.vvk{xx,xy,xz,yy,yz,zz}`** k-space mixed matrix elements $W^{\alpha\beta}(R,\omega)$ *(mixed transitions)*

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