User Guide

Opticx (pre-alpha version)

Juan José Esteve-Paredes[1]

[1] *Centro de Física de Materiales, Universidad del País Vasco (UPV/EHU), 20018 Donostia-San Sebastián, Spain*

May 19, 2025

Contents

Last iteration of this user guide: 19-05-2025.

1 Theoretical framework

In a future version, we will briefly explain here the quantities that can be calculated with the code.

2 Compilation

Unzip the `opticx_test_19052025.zip` file. Go into the generated folder, then do:

```
$ make
```

The binary directory `/bin` should contain the opticx binary `opticx.x`. Jobs will be run from this directory.

3 Examples of usage

As a general rule, an input file telling the program the relevant parameter for the calculation will be placed in the `/bin` directory. The alpha version package contains an example file in such directory, called `input_false.txt`. The `_false` denotes that only calculations in the independent particle approximation (IPA) can be performed in this test version. Even more, we will limit test to 2D systems.

Apart from the input file, we only need a `2Dmaterial_tb.dat` file to start running the code. These files will be placed in the `/wannier90_files_input` folder. Important note: in this test version, a modification is required to be done in the wannier90 file before running the code. Please erase the first line of the file, which contains the date of creation of the file and other information, and write instead the number of lines before the first line containing the Bravais coefficients n1 n2 n3 appears. The wannier90 files in the Atomelix.Databank already include in this modification, see them to visualize an example.

Below I provide a step-by-step guide to compute the frequency dependent optical absorbance and shift conductivity for a given wannierization. These are the only two quantities that can be evaluated in this version.

3.1 Evaluation of optical absorbance

3.1.1 Input file example

The test version includes a file called `input_false_absorbance.txt` with the following text inside:

```
# Periodic dimensions
2
# Wannier90_filename
GeS_wannier_04062024
# Xatu_interface
false
# Bandlist
-1 0 1 2
# Ncells
102
```

```
# Nfermi
20
# OME_sp
linear
# Response
absorbance
# Energy_variables
1 9 0.025 400
```

3.1.2 Description of the input file

I will briefly describe every section:

`# Periodic dimensions`: only `2` is allowed by now.

`# Wannier90_filename`: the `filename` part of the `filename_tb.dat` file.

`# Xatu_interface`: only `false` is allowd by now.

`# Bandlist`: bands taken into account for the optical calculation. Same meaning than in the XATU code.

`# Ncells`: number of reciprocal space points per periodic calculation for the Brillouin Zone sampling. Same meaning than in the XATU code.

`# Nfermi`: number of total energy bands below the bandgap in the wannierized band structure.

`# OME_sp`: the acronym `OME` stands for "Optical matrix elements", while `sp` means "single-particle". This part controls the set of optical matrix elements that the code evaluates before computing the frequency-dependent optical response. The word `linear` means that only optical matrix elements relevant for linear-response quantities will be calculated, as we are interested in optical absorbance in this case (which is related to the linear conductivity).

`# Response`: the optical response that will be evaluated in this case.

`# Energy_variables`: this part controls the energy variables for the calculation. In order, the 4 numbers are: E_0 (eV), E_f (eV), η (eV), and n_w number of frequency points. This is, we will sample the optical response in n_w points in the interval $E \in (E_0, E_f)$.

3.1.3 Running the calculation

To run the calculation, do:

```
$ ./bin/opticx input_false_absorbance.txt
```

Two files called `sigma_first_sp_real_filename.dat` and `sigma_first_sp_imag_filename.dat` will be generated with columns of numbers, containing the real and imaginary parts of the optical conducitivity. Every column correspond to: E (eV), σ_{xx}, σ_{xy}, σ_{xz}, σ_{yx}, σ_{yy}, σ_{yz}, σ_{zx}, σ_{zy}, σ_{zz} (conductivity is in Hartree units).

3.1.4 Additional notes

Finally, some additional notes:

Note 1: note that even though we use the `absorbance` keyword, this version of the code actually evaluates the optical conductivity.

Note 2: the parts `# OME_sp` and `# Response` keywords can be used in several ways. First,

```
# OME_sp
linear
```

```
# Response
absorbance
```

evaluates the optical matrix elements (a file will be generated containing them) and the optical absorbance in the same run. These two tasks can be performed in separated runs. This is, one can also do

```
# OME_sp
linear
# Response
none
```

to only evaluate the optical matrix elements. In a subsequent run, one will set

```
# OME_sp
none
# Response
absorbance
```

to evaluate the optical response.

3.2 Evaluation of shift conductivity

3.2.1 Input file example

The test version includes a file called `input_false_shift.txt` with the following text inside:

```
# Periodic dimensions
2
# Wannier90_filename
GeS_wannier_04062024
# Xatu_interface
false
# Bandlist
-1 0 1 2
# Ncells
102
# Nfermi
20
# OME_sp
nonlinear
# Response
shift_shiftvector
# Energy_variables
1 9 0.025 400
```

3.2.2 Description of the input file

The only two sections that are different than in the absorbance example are:

`# OME_sp`: In this case the word `linear` in the previous example is replaced `nonlinear`. Now more optical matrix elements are evaluated, which are needed for calculations related the second-order optical conductivity.

`# Response`: the optical response that will be evaluated in this case. We will use `shift_shiftvector`, where the `_shiftvector` part of the string denotes the method that will be used to evaluate the shift conductivity. In this test version, only the shift vector method is available.

3.2.3 Running the calculation

To run the calculation, do:

```
$ ./bin/opticx input_false_shift.txt
```

A file called `shift_shiftvector_filename.dat` will be generated with columns of numbers, containing the shift conductivity response. Every column corresponds to: E (eV), $\sigma^{\rm sh}_{xxx}$, $\sigma^{\rm sh}_{xyy}$, $\sigma^{\rm sh}_{yyy}$, $\sigma^{\rm sh}_{yxx}$.Units are $(\mu{\rm A/V}^2)\cdot{\rm nm}$.

3.2.4 Additional notes

Finally, some additional notes:

Note 1: note that the evaluation of nonlinear optical matrix elements will be much heavier than in the linear case.

Note 2: as in the linear response case, the parts `# OME_sp` and `# Response` keywords can be used in several ways. First,

```
# OME_sp
nonlinear
# Response
shift_shiftvector
```

evaluates the set optical matrix elements relevant for nonlinear calculations (a file will be generated containing them) and the shift conductivitty in the same run. These two tasks can be performed in separated runs. This is, one can also do

```
# OME_sp
nonlinear
# Response
none
```

to only evaluate the optical matrix elements. In a subsequent run, one will set

```
# OME_sp
none
# Response
shift_shiftvector
```

to evaluate the optical response.