User Guide

OpticX
version 0.2

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1 Introduction

OpticX is a code that calculates optical absorbance and nonlinear optical conductivity (shift current). In the current implementation, calculations can only be performed for 2D systems within the independent particle approximation (IPA).

If you use OpticX, we kindly request that you cite the following reference(s):

- J. J. Esteve-Paredes, M. A. García-Blázquez, A. J. Uría-Álvarez, M. Camarasa-Gómez, and J. J. Palacios, *Excitons in nonlinear optical responses: shift current in MoS_2 and GeS monolayers*, npj Comp. Mat. **11**, 13 (2025).

2 Compilation

2.1 Generalities

OpticX is a package written in `Fortran` and requires a Fortran compiler and a BLAS/LAPACK implementation. It supports both OpenBLAS and Intel MKL (Math Kernel Library) implementations for optimized linear algebra operations.

2.2 Instructions for the impatient

Unzip the `opticx.zip` file. Go into the main folder and type:

```
$ make
```

The binary directory `/bin` will contain the binary `opticx.x`.

2.3 Compiler options

The default compiler is `gfortran`. The compiler, as well the compilation flags (optimization, etc.) can be changed using the `FC` and `FFLAGS` in the Makefile.

2.4 Linking options

By default, the code links against OpenBLAS. If you prefer to use the Intel MKL implementation for improved performance (especially, when running the OpticX on Intel CPUs), pass the

```
USE_MKL=1
```

option during compilation. This assumes that Intel MKL is installed system-wide and links to the following libraries `-lmkl_rt -fopenmp -lpthread -lm -ldl`. Otherwise, the code links against `-lopenblas -fopenmp -lgfortran`.

`Optional - Manual path`: If `MKL` is not available system-wide and it is installed in a custom location, uncomment and adjust the lines for `MKLROOT` and `LIBS` accordingly. For example,

```
MKLROOT ?= /opt/intel/oneapi/mkl/latest
LIBS = -L$(MKLROOT)/lib/x86_64-linux-gnu \
       -Wl,--start-group \
       -lmkl_gf_lp64 -lmkl_core -lmkl_gnu_thread \
       -Wl,--end-group -fopenmp -lpthread -lm -ldl
```

3 Examples

For the current version, input files must be placed in the the same folder as the OpticX executable. This version of OpticX contains an example file this directory, labeled `input_false_observable.txt`. In addition to the main input file, a supplementary file `2Dmaterial_tb.dat` is required to run the code. This file must be placed in the `/wannier90_files_input` directory.

Important note: This version of the code requires a manual modification of the `Wannier90` file prior to execution. Specifically, you must delete the first line of the file—which typically includes the creation date and metadata—and replace it with a single line indicating the number of lines preceding the first occurrence of the Bravais lattice vector specification n1 n2 n3. All `Wannier90` files provided in the Atomelix.Databank have already been modified accordingly. You may refer to them for an example of the correct format.

3.1 Evaluation of optical absorbance

3.1.1 Input file example

The example includes a file named `input_false_absorbance.txt`, which contains the following:

```
# 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

Each section of the input file is described below:

`# Periodic dimensions`: currently, only the value `2` is supported.

`# Wannier90_filename`: specifies the `filename` portion of the `filename_tb.dat` file.

`# Xatu_interface`: currently, only `false` is allowed.

`# Bandlist`: lists the band indices to be included in the optical calculation. This follows the same convention as in the XATU code, see the corresponding manual.

`# Ncells`: number of sampling points in the Brillouin zone used in the periodic calculation. This follows the same convention as in the XATU code, see the corresponding manual.

`# Nfermi`: total number of energy bands lying below the Fermi energy in the Wannier-interpolated band structure.

`# OME_sp`: this keyword stands for `OME` "Optical Matrix Elements" and `sp` refers to "single-particle". This flag controls the set of optical matrix elements the code computes prior to evaluating the frequency-dependent optical response. The value `linear` indicates that only the matrix elements relevant for linear-response quantities will be calculated. Since absorbance is derived from the linear optical conductivity, this is the appropriate setting.

`# Response`: specifies the optical response function to be evaluated. In this case, it is set to `absorbance`.

`# Energy_variables`: defines the energy sampling parameters. The four numbers correspond to:

- E_0 (eV): starting energy
- E_f (eV): final energy
- η (eV): broadening parameter
- n_w: number of frequency points

This instructs the code to sample the optical response at n_w evenly spaced points

3.1.3 Running the calculation

To run the calculation, execute the following command:

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

This will generate two output files:

- `sigma_first_sp_real_filename.dat`
- `sigma_first_sp_imag_filename.dat`

These files contain columns of numerical data representing the real and imaginary parts of the optical conductivity tensor, respectively. The columns are organized as follows:

$$E \text{ (eV)},\ \sigma_{xx},\ \sigma_{xy},\ \sigma_{xz},\ \sigma_{yx},\ \sigma_{yy},\ \sigma_{yz},\ \sigma_{zx},\ \sigma_{zy},\ \sigma_{zz}$$

where the conductivity values are given in Hartree atomic units.

3.1.4 Additional notes

Note 1: Although the keyword `absorbance` is used in the input, this version of the code actually computes the optical conductivity. The absorbance is inferred from this quantity.
Note 2: The `# OME_sp` and `# Response` keywords offer flexibility in how the calculation is performed. You can either compute the optical matrix elements and the optical response in a single run or in separate steps. The following examples illustrate this:

1. To compute both the optical matrix elements and the absorbance in a single run:

```
# OME_sp
linear
# Response
absorbance
```

2. To compute only the optical matrix elements:

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

3. To compute only the optical response using previously generated matrix elements:

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

This modular structure can be useful for separating computationally intensive steps or for reusing matrix elements across multiple response calculations.

3.2 Evaluation of shift conductivity

3.2.1 Input file example

The example includes a file named `input_false_shift.txt` with the following content:

```
# 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

Compared to the absorbance input, the only differences lie in the following two fields:
`# OME_sp`: here, the keyword `nonlinear` replaces `linear`, indicating that the code will compute the optical matrix elements required for second-order (nonlinear) optical response calculations.
`# Response`: defines the optical response to be computed. In this case, `shift_shiftvector` is used, where the `_shiftvector` suffix specifies the evaluation method for the shift conductivity. In the current version, only the shift vector approach is implemented.

3.2.3 Running the calculation

To run the calculation, execute the following command:

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

This will produce a file named `shift_shiftvector_filename.dat`, which contains the computed shift conductivity. The columns in the output correspond to:

$$E\ (\text{eV}),\ \sigma^{\text{sh}}_{xxx},\ \sigma^{\text{sh}}_{xyy},\ \sigma^{\text{sh}}_{yyy},\ \sigma^{\text{sh}}_{yxx}$$

Units are given in $(\mu\text{A/V}^2) \cdot \text{nm}$.

3.2.4 Additional notes

Note 1: As in the linear case, the `# OME_sp` and `# Response` keywords can be used flexibly. For example:

1. To compute both the optical matrix elements and the shift conductivity in one run:

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

2. To compute only the nonlinear optical matrix elements:

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

3. To compute the shift conductivity using precomputed matrix elements:

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

This separation can be useful for saving time when exploring multiple nonlinear responses using the same set of matrix elements.