

2024 School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

Calculation of the GW Band Structure and GW-BSE Absorption Spectrum of Silicon Using BerkeleyGW

Hands-on session (Thur.6)

Hands-on based on QE-v7.3.1 and BerkeleyGW-4.0

BerkeleyGW Overview

In this tutorial you will use the BerkeleyGW software package to calculate the GW band structure of silicon and subsequently use the GW's results for the GW to calculate the absorption spectrum via Bethe–Salpeter equation (BSE) approach. An overview of the GW-BSE workflow as implemented in BerkeleyGW is given in Fig. 1.

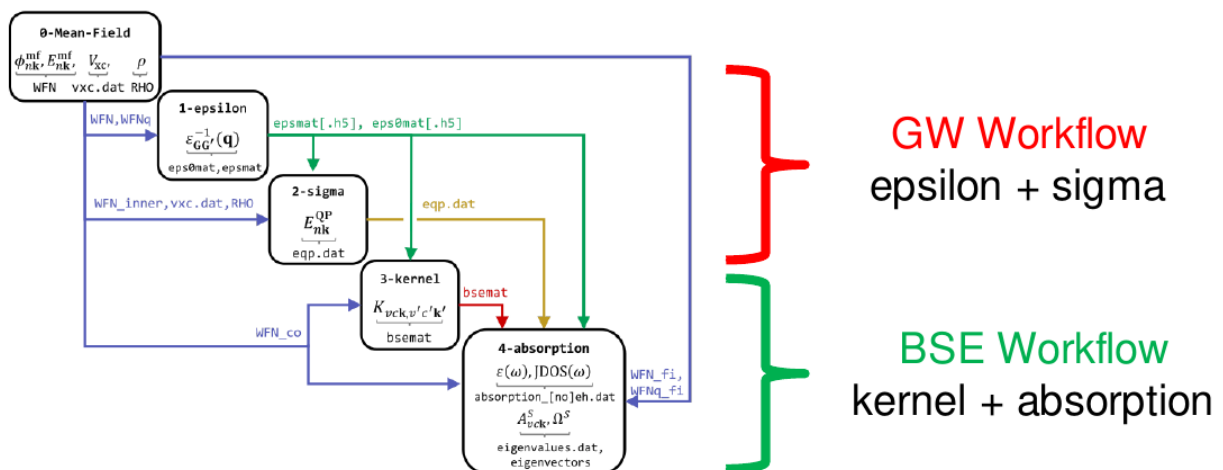


Fig. 1 Shown is the typical workflow, including the required input and output files, for the GW-BSE calculations with BerkeleyGW.

In order to compute GW quasiparticle energies and optical absorption spectra including excitonic effects with BerkeleyGW, one is required to run the following steps:

0. A mean-field program of their choice, such as Quantum ESPRESSO, PARATEC, Abinit, PARSEC, OCTOPUS, JDFT_x and SIESTA, and generate a set of files.
1. **epsilon** module computes the polarizability function, its frequency dependence and generate the dielectric matrix and its inverse ϵ^{-1} .
2. **sigma** module computes the screen coulomb interaction W necessary to compute the self-energy Σ and solves the GW Dyson's equation to compute the quasiparticle energies of the system.
3. **kernel** module computes the direct and exchange BSE kernel matrix elements on a coarse k-point grid.

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4. **absorption** module interpolates the BSE kernel matrix elements onto a fine k-point grid, diagonalize the BSE Hamiltonian, and compute the optical absorption spectrum.

In this tutorial we will use Quantum ESPRESSO to perform the mean-field calculations, generating the various wavefunctions (WFN) and other inputs necessary to run BerkeleyGW. In exercise 1 (1-silicon_gw) we will use the epsilon and sigma modules of BerkeleyGW to evaluate the GW band structure of silicon. In exercise 2 (2-silicon_bse) we will use kernel and absorption modules of BerkeleyGW to evaluate the BSE optical absorption spectrum of silicon.

Setup Instructions

To run this tutorial we will use an interactive session on Stampede3. First copy and extract the tutorial folder:

```
$ cd $SCRATCH
$ mkdir EP-SCHOOL_BGW ; cd EP-SCHOOL_BGW
$ cp /work2/05193/sabyadk/stampede3/EPWSchool2024/tutorials/Thur.6.DelBen.tar .
$ tar -xvf Thur.6.DelBen.tar
```

To start the **interactive session** use the following command:

```
$ /work2/05193/sabyadk/stampede3/EPWSchool2024/BGW/bgw_interactive
```

Note that in order to run the tutorial you need to be on an interactive session. The interactive session will last for 1 hour. After 1 hour the interactive session will expire and you'll need to create a new one by typing the command above. The script will automatically check if you already have an active interactive session and won't allow to have more than one. To check if you already have an active interactive session use the command:

```
$ squeue -u $USER
```

To cancel an existing interactive session use:

```
$ scancel JOBID
```

providing as JOBID argument the job ID number that appears under JOBID column after running `squeue -u $USER` command. Alternatively, if you are on the same command prompt shell where the interactive session was created you can use the keyboard command prompt shortcut `Crt+d`.

To generate some of the plots in the exercise by using the provided python scripts, the `numpy` and `matplotlib` modules are required but might not be installed by default. If these modules are not available use the following two command lines to install them:

```
$ module load python/3.9.18
$ pip install matplotlib
```

Exercise 1 (1-silicon_gw)

In this exercise we will calculate the quasiparticle band structure of silicon using the LDA and GW approximations. We will perform the starting mean-field calculation using Quantum ESPRESSO (QE).

The basic goals are the following:

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1. Understand the basic workflow of BerkeleyGW, and the relation between the k-grids, wavefunctions, and the `epsilon`, `sigma`, and `inteqp` codes.
 2. Run a basic GW calculation on silicon with the generalized plasmon pole (GPP) model.
 3. Construct an interpolated band structure via scissors parameters and `Inteqp`.

To run the exercise, after you created an interactive session (see **Setup Instruction** section), enter the directory:

```
$ cd $SCRATCH/EP-SCHOOL_BGW/bgw_tutorial/1-silicon_gw/
```

and follow the instructions given in the `README.md` files.

At the end of the exercise you'll be able to plot the LDA and GW band structures. Figure 2 shows the results for your reference.

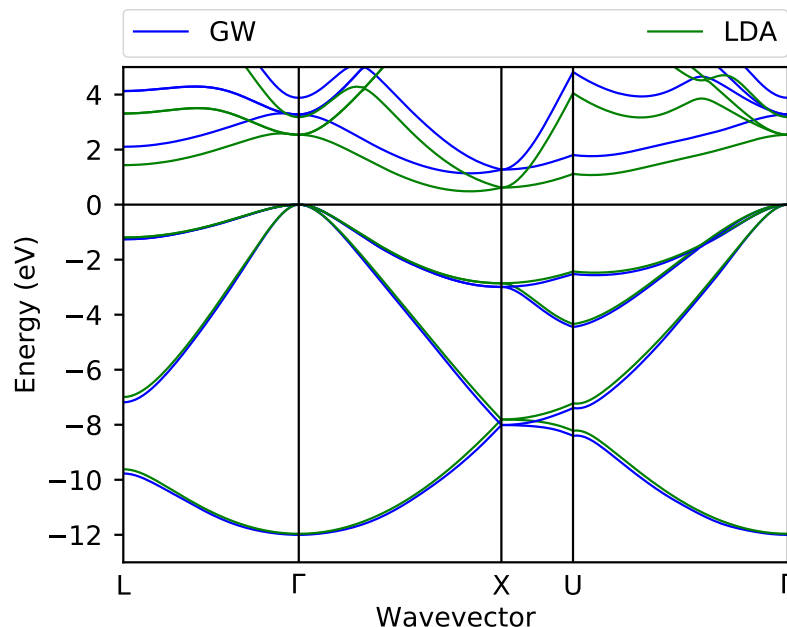


Fig. 2 Shown are the band structures of silicon at the LDA and GW computed by BerkeleyGW in this exercise.

Exercise 2 (2-silicon_bse)

In this exercise we will calculate the optical absorption spectrum of silicon within the GW-BSE formalism. We'll continue from where we left off in the previous exercise where you calculated the quasiparticle band structure of silicon within the GW approximation.

The basic goals are the following:

1. Learn how to use the `kernel` and `absorption` codes.
2. Plot the optical absorption spectrum of silicon with and without electron-hole (e-h) interactions.

The stretch goals are:

1. Check the convergence of the BSE spectrum with respect to the number of bands and k-point sampling included in the calculation.

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2. Use scissors corrections with the absorption code.
 3. Compare results with RPA spectrum with local fields.

Note that for running this exercise you would need the results from exercise 1. To facilitate the execution we will reuse the pre-ran solutions from the `1-silicon_gw` example that we ran prior to the workshop. However, you can also change the script to reuse the files from your own previous calculations.

To run the exercise, after you created an interactive session (see **Setup Instruction** section), enter the directory:

```
$ cd $SCRATCH/EP-SCHOOL_BGW/bgw_tutorial/2-silicon_bse/
```

and follow the instructions given in the `README.md` files.

At the end of the exercise you'll be able to plot the optical absorption spectra of silicon, BerkeleyGW will provide the spectrum both including and excluding the electron-hole. Figure 3 shows the results for your reference.

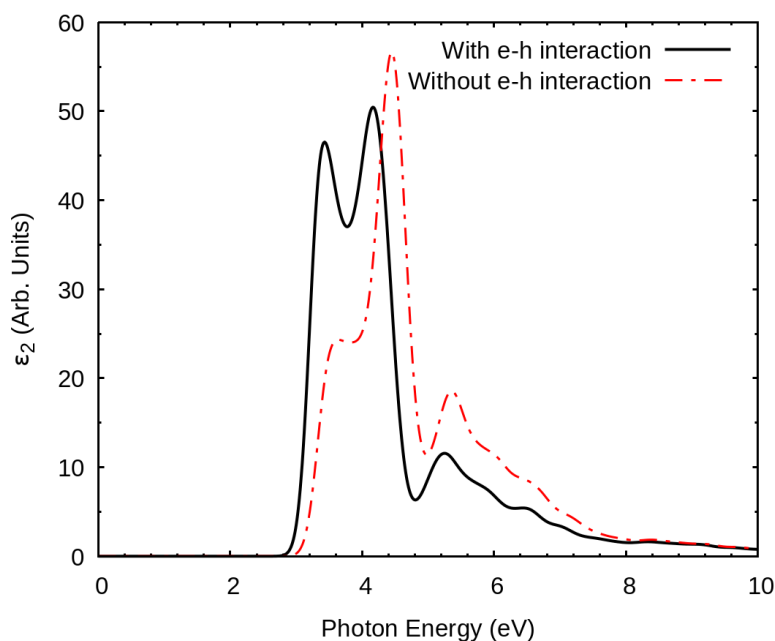


Fig. 3 Shown are the absorption spectra computed by BerkeleyGW including and excluding electron-hole interactions.