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

Calculations of optical properties with EPW

Hands-on session (Sat.8)

Hands-on based on QE-v7.3.1 and EPW-v5.9

Exercise 1

In this example we are going to calculate the optical absorption of Si for full photon spectra Phys. Rev. B **109**, 195127 (2024). We will learn the basic method to run a QDPT calculation.

```
$ cd $SCRATCH
$ mkdir EP-SCHOOL ; cd EP-SCHOOL
$ cp /work2/05193/sabyadk/stampede3/EPWSchool2024/tutorials/Sat.8.Tiwari.tar.gz .
$ tar -xvzf Sat.8.Tiwari.tar.gz; cd Sat8_Sabya/exercise1
```

▶ 1st step: Run a self-consistent calculation on a homogeneous 6X6X6 $\mathbf{k}$-point grid and a phonon calculation on a homogeneous 3x3x3 $\mathbf{q}$-point grid, and a uniform $\mathbf{k}$-grid calculation on a grid of 6X6X6 using the following jobscript (`submit1.sh`) and input files (`scf.in`, `ph.in`, and `nscf.in`):

Note 1: The homogeneous $\mathbf{k}$ grid for the non self-consistent calculations can be generated using the script `kmesh.pl`

```
$ /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/external/wannier90-3.1.0/utility/kmesh.pl 6 6 6
```

Note 2: EPW calculations require that the fine $\mathbf{k}$ or $\mathbf{q}$ grids are commensurate, i.e., `nkf1, nkf2, nkf3` to be multiple of `nqf1, nqf2, nqf3`.

Note: The `ecutwfc` needs to be much larger for real calculations.

```
$ sbatch submit1.sh
```

submit1.sh

```
#!/bin/bash
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out
#SBATCH -e qe.%j.err
#SBATCH -N 1
#SBATCH -n 48
#SBATCH -t 00:30:00
#SBATCH -A DMR23030
#SBATCH -p skx
#SBATCH --reservation=NSF_Summer_School_Sat


## QE bin directory #############
QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/
################################

### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
MPIRUN="ibrun "
```

```
################################

######## Commands ###############
$MPIRUN $PW .true. -nk 4 -nt 4 -in scf.in > scf.out
$MPIRUN $QE_BIN_DIR/ph.x -nk 4 -nt 4 -pd .true. -input ph.in > ph.out
$MPIRUN $PW .true. -nk 4 -nt 4 -in scf.in > scf.out
$MPIRUN $PW .true. -nk 4 -nt 4 -in nscf.in > nscf.out
################################
```

```
--                                                                                    scf.in
&control
calculation = 'scf'
verbosity = 'high'
restart_mode = 'from_scratch'
outdir = './'
pseudo_dir = '../pseudos/'
prefix = 'si'
&SYSTEM
ibrav = 0
nat = 2
ntyp = 1
ecutwfc = 40
ecutrho = 160
/
&ELECTRONS
conv_thr = 1E-11
diagonalization = 'david'
/
ATOMIC_SPECIES
Si 28.08 Si_r.upf
ATOMIC_POSITIONS crystal
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25

K_POINTS automatic
6 6 6 0 0 0

CELL_PARAMETERS angstrom
0.0  2.7336696142227632  2.7336696142227632
2.7336696142227632  0.0  2.7336696142227632
2.7336696142227632  2.7336696142227632  0.0
```

```
 --                                                                                   ph.in
 &inputph
 prefix   = 'si',
 fildyn   = 'si.dyn',
 fildvscf = 'dvscf',
 tr2_ph   =  1.0d-14
 ldisp    = .true.,
 nq1 = 3,
 nq2 = 3,
 nq3 = 3
 /
```

```
--                                                                                   nscf.in
&CONTROL
calculation = bands
verbosity = 'high'
restart_mode = 'from_scratch'
outdir = './'
pseudo_dir = '../pseudo/'
prefix = 'si'
/
&SYSTEM
ibrav = 0
nat = 2
```

```
ntyp = 1
ecutwfc = 40
ecutrho = 160
nbnd = 36
/
&ELECTRONS
conv_thr = 1E-11
diagonalization = 'david'
/
ATOMIC_SPECIES
Si 28.08 Si_r.upf
ATOMIC_POSITIONS crystal
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25

K_POINTS crystal
 216
0.000 0.000 0.000 0.00463
0.000 0.000 0.167  0.00463
  ...
```

During the run, notice the irreducible (IBZ) q-point grid:

```
Dynamical matrices for ( 3, 3, 3)  uniform grid of q-points
(   4 q-points):
  N         xq(1)         xq(2)         xq(3)
  1   0.000000000   0.000000000   0.000000000
  2   0.235702260   0.235702260  -0.235702260
  3   0.471404521   0.000000000   0.000000000
  4  -0.000000000  -0.471404521   0.471404521
```

You will notice three .out files (scf.out, nscf.out, and ph.out).

▶ 2nd step: Gather the `.dyn`, `.dvscf`, and `patterns` files into a new `save` directory using the pp.py python script.

```
$ python /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/EPW/bin/pp.py
```

The script will ask you to provide the `prefix` of your calculation (here "si").

▶ 3rd step: Run the epw calculation to obtain the electron-phonon matrix in Wannier representation using epw1.in.

```
$ sbatch submit2.sh
```

submit2.sh

```
#!/bin/bash
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out
#SBATCH -e qe.%j.err
#SBATCH -N 1
#SBATCH -n 48
#SBATCH -t 00:30:00
#SBATCH -A DMR23030
#SBATCH -p skx
#SBATCH --reservation=NSF_Summer_School_Sat

## QE bin directory #############
QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/
###################################

### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
```

```
MPIRUN="ibrun "
#################################

######## Commands ###############
$MPIRUN $EPW -nk 48 -input epw1.in > epw1.out
#$MPIRUN $EPW -nk 48 -input epw2.in > epw2.out
#################################
```

```
--                                                                                    epw1.in
&inputepw
prefix = 'si'
amass(1) = 28.08
outdir = './'
elph = .true.
epbwrite = .false.
epbread = .false.
epwwrite = .true.
epwread = .false.
etf_mem = 1
nbndsub = 8
asr_typ = 'crystal'
use_ws = .true.
wannierize = .true.
num_iter = 500
iprint = 2
dis_win_max = 30
dis_froz_max = 11.654
dis_froz_min = 0
fsthick = 1.2
temps = 1
degaussw = 0.005
dvscf_dir = './save'
band_plot = .true.
nk1 = 6
nk2 = 6
nk3 = 6
nq1 = 3
nq2 = 3
nq3 = 3
wdata(1) = 'guiding_centres = .true.'
wdata(2) = 'dis_num_iter = 500'
wdata(3) = 'num_print_cycles  = 10'
wdata(4) = 'dis_mix_ratio = 1'
wdata(5) = 'use_ws_distance = t'
wdata(5) = 'exclude_bands = 20-36'
dis_froz_min = -6.672
dis_win_min = -10
proj(1) = 'Si : sp3'
filkf = 'LGX.txt'
filqf = 'LGX.txt'
/
```

With the above input, we are instructing EPW to:

- Representing electron-phonon coupling in Wannier representation. Notice the starting Wannier orbitals.

```
Initial Wannier projections
(   0.00000   0.00000   0.00000) :  l =  -3 mr =   1
(   0.00000   0.00000   0.00000) :  l =  -3 mr =   2
(   0.00000   0.00000   0.00000) :  l =  -3 mr =   3
(   0.00000   0.00000   0.00000) :  l =  -3 mr =   4
(   0.25000   0.25000   0.25000) :  l =  -3 mr =   1
(   0.25000   0.25000   0.25000) :  l =  -3 mr =   2
(   0.25000   0.25000   0.25000) :  l =  -3 mr =   3
(   0.25000   0.25000   0.25000) :  l =  -3 mr =   4
```

These correspond to the sp3 projection that we have chosen in the epw1.in **proj(1) = 'Si : sp3'**. Projections in epw are a choice and require manual intervention. One can choose SCDM for automatic projections in order to avoid choosing wannier orbitals. Notice in si.wout file,

```
 Final State
  WF centre and spread    1  (  0.449910, -0.449904,  0.449982 )     2.58934555
  WF centre and spread    2  ( -0.449836, -0.449899, -0.449886 )     2.58939169
  WF centre and spread    3  ( -0.449919,  0.449900,  0.449900 )     2.58937680
  WF centre and spread    4  (  0.449903,  0.449888, -0.449892 )     2.58939402
  WF centre and spread    5  (  1.816701,  1.816754,  1.816707 )     2.58936159
  WF centre and spread    6  (  1.816779,  0.916909,  0.916956 )     2.58935527
  WF centre and spread    7  (  0.916890,  1.816758,  0.916871 )     2.58931994
  WF centre and spread    8  (  0.916897,  0.916935,  1.816721 )     2.58936108
```

The spreads should be small (ideally). After the epw1.out calculation is finished.

Next, plot using the python codes provided in py_codes

```
$ python ../py_codes/plot_band.py
```

You will notice the bandstructure file pop out which would look something like,

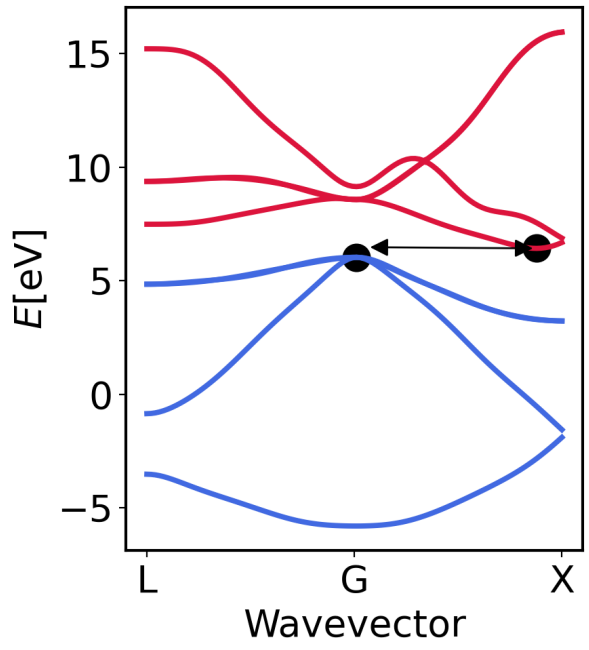

Fig. 1 Silicon bandstructure. The arrow shows the minima of conduction band and maxima of valence band. We see that the gap is about 0.6 eV which is lower than experimental gap.

We see that the gap is about 0.6 eV which is lower than experimental gap. The reason is that PBE (GGA) underestimates the gap. It can be corrected by using GW eigenvalues as you must have learnt in indabs tutorial. We will correct the gap at the end using a rigid scissor shift.

- We have written on disk the `si.epmatwp` file, hence, we restart the QDPT calculation with the ep matrix files. Comment the first line and uncomment the second line in submit2.sh (commands).

▶ 4th step: Run the EPW restart calculation using submit2.sh. Uncomment second line in commands of submit2.sh and comment the first line.

```
$ sbatch submit2.sh
```

submit2.sh

```
#!/bin/bash
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out
#SBATCH -e qe.%j.err
#SBATCH -N 1
#SBATCH -n 48
#SBATCH -t 00:30:00
#SBATCH -A DMR23030
#SBATCH -p skx
#SBATCH --reservation=NSF_Summer_School_Sat

## QE bin directory #############
QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/
#################################

### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
MPIRUN="ibrun "
#################################

######## Commands ###############
#$MPIRUN $EPW -nk 48 -input epw1.in > epw1.out
$MPIRUN $EPW -nk 48 -input epw2.in > epw2.out
#################################
```

epw2.in

```
--
&inputepw
prefix = 'si'            !Prefix used
amass(1) = 28.08         !Atomic mass
outdir = './'            !Ourput directory
elph = .true.            !Perform electron-phonon calculations
epwwrite = .false.       !Write epmatwp for restart
epwread = .true.         !Read epmatwp file and few others for restart
etf_mem = 1              !Optimization
nbndsub = 8              !Number of bands
asr_typ = 'crystal'      !Acoustic sum-rule
use_ws = .true.          !Should we use Wigner-Seitz cell
wannierize = .false.     !Wannierization
fsthick = 6.0            !Fermi surface thickness
degaussw = 0.1           !Gaussian spread (for DOS)
dvscf_dir = './save'     !dvscf directory
nk1 = 6                  !Coarse grid kx
nk2 = 6                  !Coarse grid ky
nk3 = 6                  !Coarse grid kz
nq1 = 3                  !Coarse grid qx
nq2 = 3                  !Coarse grid qy
nq3 = 3                  !Coarse grid qz

!!!!! Parameters of optical absorption !!!!!!

temps = 300.0            !Temperatures
loptabs = .true.         !For optical absorption
omegamin = 0.05          !Photon energy minimum
omegamax = 4.0           !Photon energy maximum
omegastep = 0.05         !Photon energy resolution
nkf1 = 12                !Fine grid kx
```

```
nkf2 = 12                !Fine grid ky
nkf3 = 12                !Fine grid kz
nqf1 = 3                 !Fine grid qx
nqf2 = 3                 !Fine grid qy
nqf3 = 3                 !Fine grid qz
mp_mesh_k = .true.       !Use IBZ
efermi_read = .true.     !Read Fermi level
fermi_energy = 6.2       !Fermi energy
/
```

Next, the calculation for QDPT starts. Here, we are calculating with $12 \times 12 \times 12$ **k** grid and $3 \times 3 \times 3$ **q** grid. The photon energy range is $0 - 4.0$ eV. With this range we cover both the direct and indirect absorption regime for Si.

QDPT outputs the imaginary dielectic constant $\epsilon_2(\omega)$ as a function of photon energy $\hbar\omega$. The relevant equation is

$$
\begin{aligned}
\varepsilon_2(\omega) = & \frac{\pi e^2}{\epsilon_0 \Omega} \frac{1}{\omega^2} \frac{1}{N} \sum_{i_0,p} Z^{-1} \exp\left(-\beta E_{i_0}\right) \\
\times & \left| \mathbf{e} \cdot \sum_{cv\mathbf{k}} \left\{ U^*_{p,i_0-1_{v\mathbf{k}}+1_{c\mathbf{k}}} \mathbf{v}_{cv\mathbf{k}} + \quad N^{-1/2} \sum_{\mathbf{q}\nu\eta} \sqrt{n_{\mathbf{q}\nu} + \frac{1+\eta}{2}} \; U^*_{p,i_0-1_{v\mathbf{k}}+1_{c\mathbf{k}+\mathbf{q}}+\eta 1_{-\eta\mathbf{q}\nu}} \right.\right. \\
\times & \left[\sum_{c'} \frac{g_{cc'\nu}(\mathbf{k},\mathbf{q}) \mathbf{v}_{c'v\mathbf{k}}}{(\bar{E} - E_{i_0}) - (\varepsilon_{c'\mathbf{k}} - \varepsilon_{v\mathbf{k}})} \theta_{c'v\mathbf{k}} + \quad \sum_{v'} \frac{\mathbf{v}_{cv'\mathbf{k}+\mathbf{q}} \, g_{v'v\nu}(\mathbf{k},\mathbf{q})}{(\bar{E} - E_{i_0}) - (\varepsilon_{c\mathbf{k}+\mathbf{q}} - \varepsilon_{v'\mathbf{k}+\mathbf{q}})} \theta_{cv'\mathbf{k}+\mathbf{q}} \right. \\
& \left.\left. + \sum_{c'} \frac{\mathbf{v}_{cc'\mathbf{k}+\mathbf{q}} \, g_{c'v\nu}(\mathbf{k},\mathbf{q})}{\varepsilon_{v\mathbf{k}} - \varepsilon_{c'\mathbf{k}+\mathbf{q}} - \eta\hbar\omega_{-\eta\mathbf{q}\nu}} \sum_{v'} \frac{g_{cv'\nu}(\mathbf{k},\mathbf{q}) \mathbf{v}_{v'v\mathbf{k}}}{\varepsilon_{v'\mathbf{k}} - \varepsilon_{c\mathbf{k}+\mathbf{q}} - \eta\hbar\omega_{-\eta\mathbf{q}\nu}} \right] \right\} \right|^2 \\
\times & \; \delta(E_p - E_{i_0} - \hbar\omega) \; . \qquad (1)
\end{aligned}
$$

In this expression, the energy of the initial state $|i_0\rangle$ is given by $E_{i_0} = E_0 + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu}/2 + \sum_{\mathbf{q}\nu} n_{\mathbf{q}\nu}\hbar\omega_{\mathbf{q}\nu}$, where E_0 is the energy of the electronic ground state. The canonical average must be performed over all possible occupations $n_{\mathbf{q}\nu} = 0, 1, 2, \cdots$. Unlike in second-order perturbation theory, in this case the transition rates are not simple linear functions of $n_{\mathbf{q}\nu}$, therefore the replacement of $n_{\mathbf{q}\nu}$ by the Bose-Einstein occupation is not allowed in principle. In particular, the occupations $n_{\mathbf{q}\nu}$ are implicitly contained in the energies E_{i_0}, in the unitary matrices U_{mp}, and in the eigenvalues E_p. The choice of occupations $n_{\mathbf{q}\nu}$ is determined by flag **nq_init** .

nq_init = -1 (default)→ Bose-Einstein

nq_init = -3 → Monte-Carlo integration of Eq.(1).

From the imaginary dielectric constant, the absorption coefficient and luminescence can be calculated with simple expressions see Phys. Rev. B **109**, 195127 (2024).

```
================================================================
Phonon-assisted absorption with quasidegenerate perturbation
================================================================


Fermi surface thickness =   5.000000 eV

The following temperatures are calculated:
```

```
Temperature T =   0.025852 eV

size for cell = 275.717717 per A

nqtotf =         27

nktotf =         72

*************************************************************************

            QDPT calculation accelerated with ELPA Library

Refer: https://elpa.mpcdf.mpg.de/ELPA_PUBLICATIONS.html for citation

*************************************************************************

*****************************************************

*****  Automatic generation of QDPT meshgrids  *****

 Number of QDPT meshgrids to be performed:         17

*****************************************************
Size of QD bins    237.50meV
Finished building matrix
```

The key items to notice here are

- (1) The Fermi surface thickness which dictates upto what range the states are included for perturbation.
- (2) The temperature (300.0 K/ 25.852 meV)
- (3) QD bin size (automatically determined to 237.5 meV (ensures convergence))
- (4) Number of QD bins inside the photon energy range is 17

Further down the output,

```
Performing mesh =        12
Finished sorting, Entering eigenvalue calculation

QD matrix rank =        78

Building Hamiltonian with total elements:       496

Starting diagonalization

LAPACK diagonalization complete

Used LAPACK for diagonalization

Performing epsilon summation
```

As stated, QDPT is a two-step rocess,

- In step 1: (starting diagonalization) we diagonalize the QD Hamiltoian in the QD bin
- In step 2: (performing epsilon summation) we perform the summation to obtain the ϵ_2 in Eq. (1)

After the calculation ends:

```
python ../py_codes/plot_contributions.py
```

You will get Si.png that shows.:

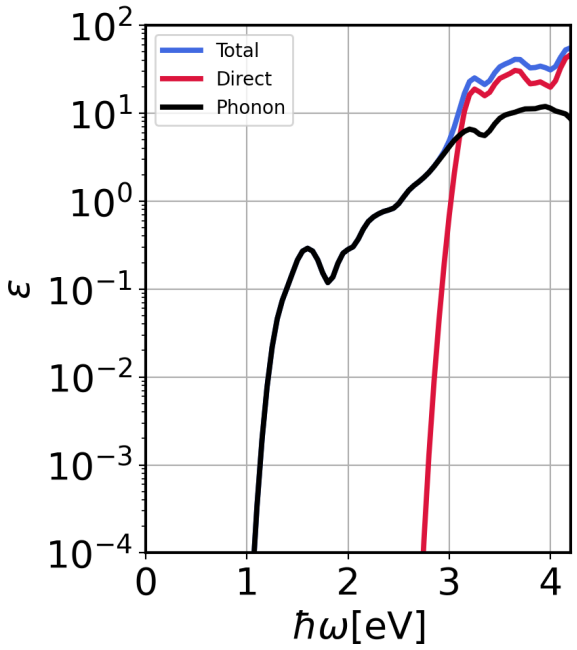

Fig. 2 Silicon imaginary dielectric constant. Controbuutions from direct and phonon-assisted processes.

Here, we plot the silicon imaginary dielectric coefficient and its spectral decomposition in phonon and direct part. We see that below 3 eV (below direct gap) phonon-assisted process dominates, while after 3 eV, the direct contribution dominates.

These calculations are unconverged and a denser grid of 60X60X60 $\mathbf{k}$-grid would converge the calculation. After convergence the results would appear like,

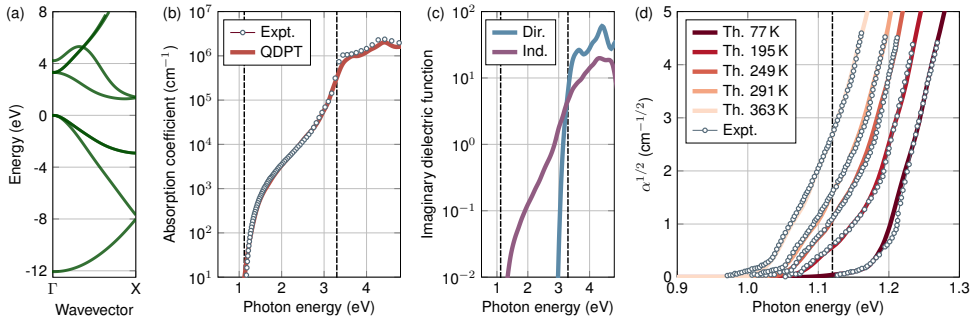

Fig. Si Silicon bandstructure(a), absorption coefficient (b), contributions from direct and phonon-assisted processes (c), absorption coefficient near the absorption edge (d). Taken verbatim fromPhys. Rev. B **109**, 195127 (2024)

▶ We now save the calculation files,

```
cp epsilon2_indabs_300.0K_17.dat epsilon2_indabs_300.0K_all.dat
```

While for coarser grids, it is possible to run in one calculation, for denser grids, one has to perfrom restart calculations. In QDPT, the calculations are independent of the QD bin. Therefore, we can submit calculations independently for each QD bin.

We will perform two such calculations, first using epw2_15.in where we calculate upto QD bin 15. Next using epw2_17.in where we start from QD bin 16 and go upto 17 (2 bins). Finally, we sum the output using "py_eps_sum.py"

▶ 5th step: Run the EPW restart calculation using submit3.sh for QD bins 15 and 17.

epw2_15.in

```
--
&inputepw
prefix = 'si'            !Prefix used
amass(1) = 28.08         !Atomic mass
outdir = './'            !Ourput directory
elph = .true.            !Perform electron-phonon calculations
epwwrite = .false.       !Write epmatwp for restart
epwread = .true.         !Read epmatwp file and few others for restart
etf_mem = 1              !Optimization
nbndsub = 8              !Number of bands
asr_typ = 'crystal'      !Acoustic sum-rule
use_ws = .true.          !Should we use Wigner-Seitz cell
wannierize = .false.     !Wannierization
fsthick = 6.0            !Fermi surface thickness
degaussw = 0.1           !Gaussian spread (for DOS)
dvscf_dir = './save'     !dvscf directory
nk1 = 6                  !Coarse grid kx
nk2 = 6                  !Coarse grid ky
nk3 = 6                  !Coarse grid kz
nq1 = 3                  !Coarse grid qx
nq2 = 3                  !Coarse grid qy
nq3 = 3                  !Coarse grid qz

!!!!! Parameters of optical absorption !!!!!!

temps = 300.0            !Temperatures
loptabs = .true.         !For optical absorption
len_mesh = 18            !Number of QD bins
meshnum = 15             !Last QD bin
omegamin = 0.05          !Photon energy minimum
omegamax = 4.0           !Photon energy maximum
omegastep = 0.05         !Photon energy resolution
nkf1 = 12                !Fine grid kx
```

```
nkf2 = 12                !Fine grid ky
nkf3 = 12                !Fine grid kz
nqf1 = 3                 !Fine grid qx
nqf2 = 3                 !Fine grid qy
nqf3 = 3                 !Fine grid qz
mp_mesh_k = .true.       !Use IBZ
efermi_read = .true.     !Read Fermi level
fermi_energy = 6.2       !Fermi energy
/
```

```
--                                                                                epw2_17.in
&inputepw
prefix = 'si'            !Prefix used
amass(1) = 28.08         !Atomic mass
outdir = './'            !Ourput directory
elph = .true.            !Perform electron-phonon calculations
epwwrite = .false.       !Write epmatwp for restart
epwread = .true.         !Read epmatwp file and few others for restart
etf_mem = 1              !Optimization
nbndsub = 8              !Number of bands
asr_typ = 'crystal'      !Acoustic sum-rule
use_ws = .true.          !Should we use Wigner-Seitz cell
wannierize = .false.     !Wannierization
fsthick = 6.0            !Fermi surface thickness
degaussw = 0.1           !Gaussian spread (for DOS)
dvscf_dir = './save'     !dvscf directory
nk1 = 6                  !Coarse grid kx
nk2 = 6                  !Coarse grid ky
nk3 = 6                  !Coarse grid kz
nq1 = 3                  !Coarse grid qx
nq2 = 3                  !Coarse grid qy
nq3 = 3                  !Coarse grid qz

!!!!! Parameters of optical absorption !!!!!!

temps = 300.0            !Temperatures
loptabs = .true.         !For optical absorption
len_mesh = 18             !Number of QD bins
meshnum = 17             !Last QD bin
meshnum = 16             !First QD bin
omegamin = 0.05          !Photon energy minimum
omegamax = 4.0           !Photon energy maximum
omegastep = 0.05         !Photon energy resolution
nkf1 = 12                !Fine grid kx
nkf2 = 12                !Fine grid ky
nkf3 = 12                !Fine grid kz
nqf1 = 3                 !Fine grid qx
nqf2 = 3                 !Fine grid qy
nqf3 = 3                 !Fine grid qz
mp_mesh_k = .true.       !Use IBZ
efermi_read = .true.     !Read Fermi level
fermi_energy = 6.2       !Fermi energy
/
```

We submit both calculations using submit3.sh.

```
$ sbatch submit3.sh
```

```
--                                                                          submit3.sh
#!/bin/bash
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out
#SBATCH -e qe.%j.err
#SBATCH -N 1
#SBATCH -n 48
```

```
#SBATCH -t 00:30:00
#SBATCH -A DMR23030
#SBATCH -p skx
#SBATCH --reservation=NSF_Summer_School_Sat

## QE bin directory #############
QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/
#################################

### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
MPIRUN="ibrun "
#################################

######## Commands ###############
$MPIRUN $EPW -nk 48 -input epw2_15.in > epw2_15.out
$MPIRUN $EPW -nk 48 -input epw2_17.in > epw2_17.out
#################################
```

After these calculations finish, they produce two epsilon2 files with *_15.dat and *_17.dat. These files contain the imaginary dielectric constant. We sum them using a python code (py_sum_eps.py).

```
python ../py_codes/py_sum_eps.py
```

Now, plot all four using plot_all.py

```
python ../py_codes/plot_epsilon_all.py
```

You will get Si.png that shows.:

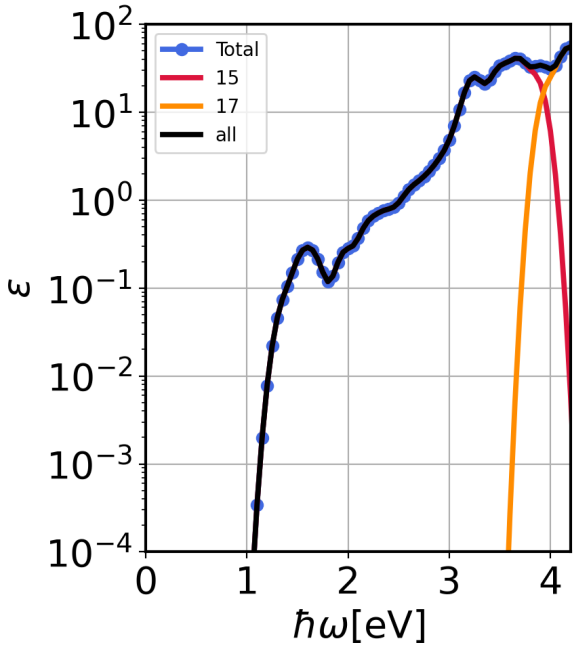

Fig. 3 Silicon imaginary dielectric constant for sum of QD bins 15 and 17 (blue), individual, (red and orange) and the single calculation with both bins. (black).

In the above figure, you see the silicon imaginary dielectric constant for sum of QD bins 15 and 17 (blue), individual, (red and orange) and the single calculation with both bins. (black). As you can see, adding the imaginary dielectric constant from both the bins amounts to calculating them in one single calculation.

▶ bonus task: plot the direction-dependent imaginary dielectric constant.

```
python plot_epsilon_xyz.py
```

The columns (6,7,8) of epsilon2_indabs_300.0K file contain the direction dependent ϵ_2 along three crystallographic directions.

You will get Si_xyz.png that shows.:

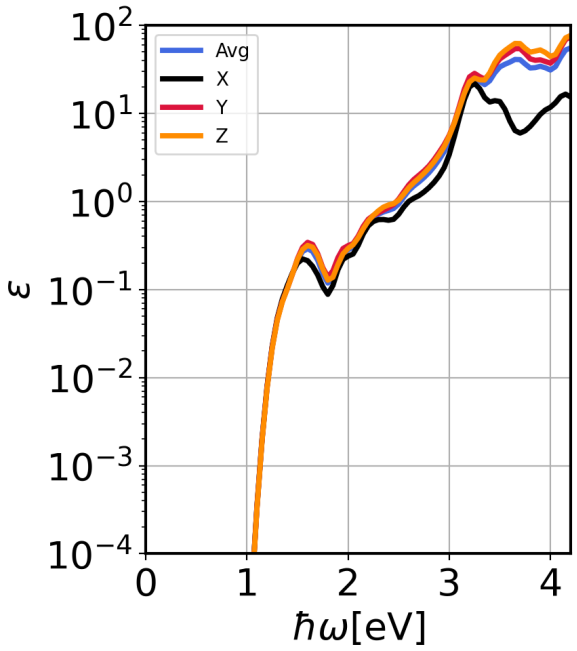

Fig. 4 Silicon imaginary dielectric constant average and crystal-direction dependent (X, Y, Z).

Since silicon is anisotropic, its velocity matrix elements are different in different crystallographic directions. Which leads to anisotropy in its imaginary dielectric constant.

Exercise 2

In this example we are going to calculate the optical absorption in GaAs (a direct gap material) for full photon spectra Phys. Rev. B **109**, 195127 (2024).

```
$ cd Sat.7.Tiwari/exercise2
```

▶ 1st step: Run a self-consistent calculation on a homogeneous 6X6X6 **k**-point grid and a phonon calculation on a homogeneous 3x3x3 **q**-point grid, and a uniform **k**-grid calculation on a grid of 6X6X6 using the following jobscript (`submit1.sh`) and input files (`scf.in`, `ph.in`, and `nscf.in`):

Note 1: The homogeneous **k** grid for the non self-consistent calculations can be generated using the script `kmesh.pl`
`$ /work2/06868/giustino/EP-SCHOOL/q-e/wannier90-3.1.0/utility/kmesh.pl 6 6 6`

Note 2: EPW calculations with `ephwrite = .true.` require that the fine **k** or **q** grids are commensurate, i.e., `nkf1, nkf2, nkf3` to be multiple of `nqf1, nqf2, nqf3`.

```
$ sbatch submit1.sh
```

submit1.sh

```
#!/bin/bash
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out
#SBATCH -e qe.%j.err
#SBATCH -N 1
#SBATCH -n 48
#SBATCH -t 00:30:00
#SBATCH -A DMR23030
#SBATCH -p skx
##SBATCH --reservation=NSF_Summer_School_Sat


## QE bin directory #############
QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/
###################################


### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
MPIRUN="ibrun "
###################################

######## Commands ###############
$MPIRUN $PW .true. -nk 4 -nt 4 -in scf.in > scf.out
$MPIRUN $QE_BIN_DIR/ph.x -nk 4 -nt 4 -pd .true. -input ph.in > ph.out
$MPIRUN $PW .true. -nk 4 -nt 4 -in scf.in > scf.out
$MPIRUN $PW .true. -nk 4 -nt 4 -in nscf.in > nscf.out
###################################
```

scf.in

```
--
&CONTROL
calculation = 'scf'
verbosity = 'high'
restart_mode = 'from_scratch'
outdir = './'
pseudo_dir = './pseudos'
prefix = 'GaAs'
/
&SYSTEM
ibrav = 0
nat = 2
```

```
ntyp = 2
ecutwfc = 60
ecutrho = 240
/
&ELECTRONS
conv_thr = 1E-11
diagonalization = 'david'
/
ATOMIC_SPECIES
Ga 95.95 Ga.upf
As 32.06 As.upf
ATOMIC_POSITIONS crystal
Ga 0.25 0.25 0.25
As 0.0 0.0 0.0

K_POINTS automatic
6 6 6 0 0 0

CELL_PARAMETERS angstrom
0.0  2.86759328207563  2.86759328207563
2.86759328207563  0.0  2.86759328207563
2.86759328207563  2.86759328207563  0.0
```

```
 --                                                                                    ph.in
&inputph
prefix = 'GaAs'
fildyn = 'GaAs.dyn'
ldisp = .true.
fildvscf = 'dvscf'
nq1 = 3
nq2 = 3
nq3 = 3
tr2_ph = 1.0d-14
/
```

```
--                                                                                    nscf.in
&CONTROL
calculation = bands
verbosity = 'high'
restart_mode = 'from_scratch'
outdir = './'
pseudo_dir = './pseudos'
prefix = 'GaAs'
/
&SYSTEM
ibrav = 0
nat = 2
ntyp = 2
ecutwfc = 60
ecutrho = 240
nbnd = 36
/
&ELECTRONS
conv_thr = 1E-11
diagonalization = 'david'
/
ATOMIC_SPECIES
Ga 95.95 Ga.upf
As 32.06 As.upf
ATOMIC_POSITIONS crystal
Ga 0.25 0.25 0.25
As 0.0 0.0 0.0

K_POINTS crystal
 216
0.000 0.000 0.000 0.00463
0.000 0.000 0.167  0.00463
  ...
```

▶ 2nd step: Gather the `.dyn`, `.dvscf`, and `patterns` files into a new `save` directory using the pp.py python script.

```
$ python /work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/EPW/bin/pp.py
```

The script will ask you to provide the `prefix` of your calculation (here "GaAs").

▶ 3rd step: Run the epw calculation to obtain the electron-phonon matrix in Wannier representation using epw1.in.

```
$ sbatch submit2.sh
```

submit2.sh

```
#!/bin/bash
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out
#SBATCH -e qe.%j.err
#SBATCH -N 1
#SBATCH -n 48
#SBATCH -t 00:30:00
#SBATCH -A DMR23030
#SBATCH -p skx
##SBATCH --reservation=NSF_Summer_School_Sat

## QE bin directory #############
QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/
#################################


### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
MPIRUN="ibrun "
#################################

######## Commands ###############
$MPIRUN $EPW -nk 48 -input epw1.in > epw1.out
$MPIRUN $EPW -nk 48 -input epw2.in > epw2.out
#################################
```

epw1.in

```
--
&inputepw
prefix = 'GaAs'
amass(1) = 95.95
amass(2) = 32.06
outdir = './'
elph = .true.
epbwrite = .false.
epbread = .false.
epwwrite = .true.
epwread = .false.
etf_mem = 1
nbndsub = 8
asr_typ = 'crystal'
use_ws = .true.
wannierize = .true.
num_iter = 5000
iprint = 2
dis_win_max = 20
dis_froz_max = 10
fsthick = 1.2
temps = 1
degaussw = 0.005
dvscf_dir = './save'
```

```
band_plot = .true.
nk1 = 6
nk2 = 6
nk3 = 6
nq1 = 3
nq2 = 3
nq3 = 3
wdata(1) = 'guiding_centres = .true.'
wdata(2) = 'dis_num_iter = 500'
wdata(3) = 'num_print_cycles  = 10'
wdata(4) = 'dis_mix_ratio = 1'
wdata(5) = 'use_ws_distance = T'
dis_froz_min = -7
dis_win_min = -10
proj(1) = 'Ga : sp3'
proj(2) = 'As: sp3'
filkf = 'LGX.txt'
filqf = 'LGX.txt'
eig_read = false
/
```

With the above input, we are instructing EPW to:

- Representing electron-phonon coupling in Wannier representation. Notice the starting Wannier orbitals.

  After the epw1.out calculation is finished, perform these commands to download bandstructure in your local machine,

  ```
  $ scp <userid>@frontera.tacc.utexas.edu:$pwd/band.eig .
  ```

  Next, plot using the python codes provided in pycodes

  ```
  $ python py_codes/plot_band_GaAs.py
  ```

  You will notice the bandstructure file pop out which would look something like,

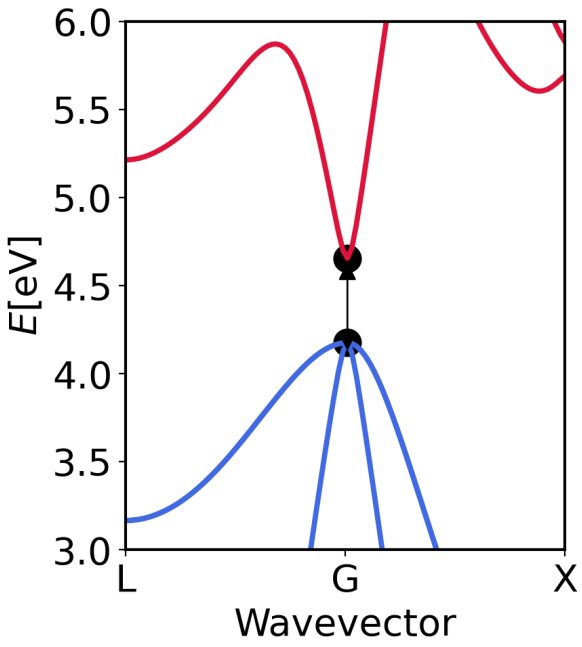

Fig. 5 GaAs bandstructure. The arrow shows the minima of conduction band and maxima of valence band. We see that the gap is about 0.6 eV at the same k-point.

We see that the gap is about 0.6 eV which is lower than experimental gap of (1.4 eV). The reason is that PBE (GGA) underestimates the gap. It can be corrected by using GW eigenvalues as you must have learnt in indabs tutorial. We will correct the gap at the end using a rigid scissor shift.

- We have written on disk the `GaAs.epmatwp` file, hence, we restart the QDPT calculation with the ep matrix files. Comment the first line and uncomment the second line in submit2.sh (commands). ▶ 4th step: Run the EPW restart calculation using submit2.sh.

```
$ sbatch submit2.sh
```

submit2.sh

```
#!/bin/bash
#SBATCH --mail-type=END,FAIL
#SBATCH --mail-user=sxt174030@utdallas.edu
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out                          # define stdout & stderr output files
#SBATCH -e qe.%j.err
#SBATCH -N 1
#SBATCH -n 48
#SBATCH -p development
#SBATCH -t 00:30:00
#SBATCH -A DMR21002

## QE bin directory #############
QE_BIN_DIR=/scratch1/05193/sabyadk/tutorials/EPW_code/q-e/bin/
#################################

### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
MPIRUN="ibrun "
#################################

######## Commands ###############
#$MPIRUN $EPW -nk 48 -input epw1.in > epw1.out
$MPIRUN $EPW -nk 48 -input epw2.in > epw2.out
#################################
```

epw2.in

```
--
&inputepw
prefix = 'GaAs'
amass(1) = 95.95
amass(2) = 32.06
outdir = './'
elph = .true.
epwwrite = .false.
epwread = .true.
etf_mem = 1
nbndsub = 8
asr_typ = 'crystal'
use_ws = .true.
wannierize = .false.
fsthick = 6.0
degaussw = 0.12
dvscf_dir = './save'
nk1 = 6
nk2 = 6
nk3 = 6
nq1 = 3
nq2 = 3
nq3 = 3
eig_read = .false.
```

```
loptabs = .true.

omegamin = 0.05         !Photon energy minimum
omegamax = 2.6          !Photon energy maximum
omegastep = 0.05        !Photon energy resolution
nkf1 = 36               !Fine grid kx
nkf2 = 36               !Fine grid ky
nkf3 = 36               !Fine grid kz
nqf1 = 3                !Fine grid qx
nqf2 = 3                !Fine grid qy
nqf3 = 3                !Fine grid qz
mp_mesh_k = .true.      !Use IBZ
efermi_read = .true.    !Read Fermi level
fermi_energy = 4.5      !Fermi energy
mode_res = 6            !Number of modes over which epsilon2 is decomposed
/
```

Notice, we have added an extra tag, **mode_res**. This tag controls among how many modes we spectrally decompose the imaginary dielectric constant. The maximum number of modes a system can have is $3N$ where N is the number of atoms. Hence, for GaAs we have maximum number of modes $= 6$.

After the calculation finishes, perform

```
$python ../py_codes/plot_epsilon_GaAs.py
```

You will get GaAs.png that shows.:

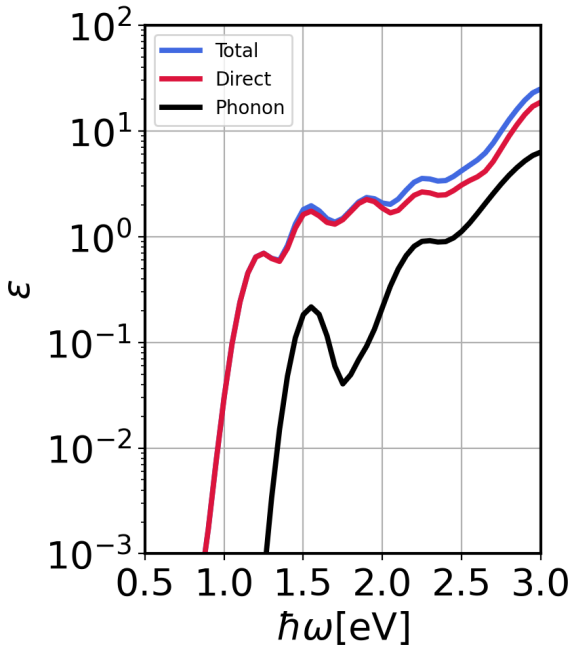

Fig. 6 GaAs imaginary dielectric constant. Contribuutions from direct and phonon-assisted processes.

We see that the phonon-assisted contribution remains below direct contribution since GaAs is direct gap material. However, with increasing photon energy, we see an increase in phonon contribution. This happens because the phase-space increases for phonon assisted processes.

We next plot the mode resolved imaginary dielectric constant. To do so

```
python ../py_codes/plot_epsilon_GaAs_cont.py
```

You will get GaAs_contribution.png that shows.:

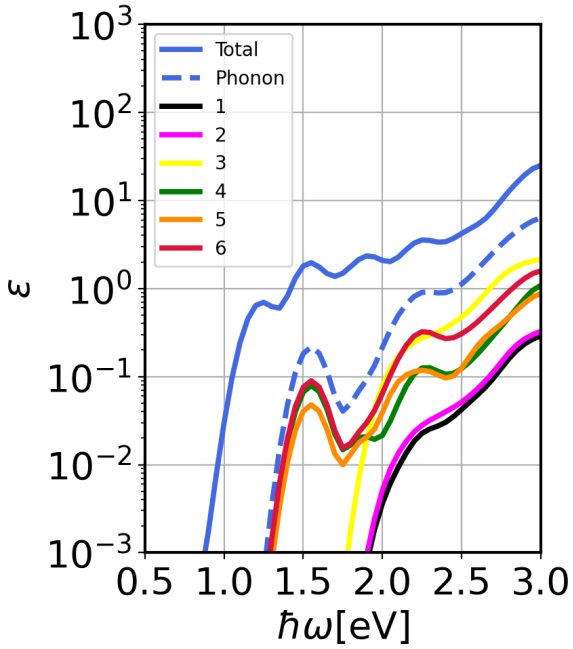

Fig. 7 GaAs imaginary dielectric constant. Contribuutions from direct and phonon-assisted processes.

With this we can see the contribution from each of the phonon modes to the imaginary dielectric constant.

Exercise 3

This is a bonus exercise. In this exercise we are going to understand the convergence of QDPT calculation with respect to QD bin size.

```
$cp exercise3/*.in exercise1/
$cp exercise3/*.sh exercise1/
$cd exercise1
```

Notice, inside exercise3 you will find 4 .in files, **epw2_0.35.in**, **epw2_0.45.in**, **epw2_2.80.in**, and **epw2_all.in**. Here the number after _ corresponds to respective QD bin size.

```
--                                                                              epw2_0.35.in
&inputepw
prefix = 'si'           !Prefix used
amass(1) = 28.08         !Atomic mass
outdir = './'            !Ourput directory
elph = .true.            !Perform electron-phonon calculations
epwwrite = .false.       !Write epmatwp for restart
epwread = .true.         !Read epmatwp file and few others for restart
etf_mem = 1              !Optimization
nbndsub = 8              !Number of bands
asr_typ = 'crystal'      !Acoustic sum-rule
use_ws = .true.          !Should we use Wigner-Seitz cell
wannierize = .false.     !Wannierization
fsthick = 6.0            !Fermi surface thickness
degaussw = 0.1           !Gaussian spread (for DOS)
dvscf_dir = './save'     !dvscf directory
nk1 = 6                  !Coarse grid kx
nk2 = 6                  !Coarse grid ky
nk3 = 6                  !Coarse grid kz
nq1 = 3                  !Coarse grid qx
nq2 = 3                  !Coarse grid qy
nq3 = 3                  !Coarse grid qz

!!!!! Parameters of optical absorption !!!!!!

temps = 300.0            !Temperatures
loptabs = .true.         !For optical absorption
QD_bin = 0.35            !QD bin size
QD_min = 0.6             !QD bin starting energy
omegamin = 0.05          !Photon energy minimum
omegamax = 4.0           !Photon energy maximum
omegastep = 0.05         !Photon energy resolution
nkf1 = 12                !Fine grid kx
nkf2 = 12                !Fine grid ky
nkf3 = 12                !Fine grid kz
nqf1 = 3                 !Fine grid qx
nqf2 = 3                 !Fine grid qy
nqf3 = 3                 !Fine grid qz
mp_mesh_k = .true.       !Use IBZ
efermi_read = .true.     !Read Fermi level
fermi_energy = 6.2       !Fermi energy
/
```

Notice, the tag **QD_bin** which dictates the size of QD bin in eV. Here it is 350 meV.

```
$cd exercise1/
```

▶ Now we perform the QDPT calculation for two of the three input files.

```
$sbatch submit4.sh
```

submit4.sh

```
#!/bin/bash
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out
#SBATCH -e qe.%j.err
#SBATCH -N 1
#SBATCH -n 48
#SBATCH -t 00:30:00
#SBATCH -A DMR23030
#SBATCH -p skx
#SBATCH --reservation=NSF_Summer_School_Sat


## QE bin directory #############
QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/
#################################

### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
MPIRUN="ibrun "
#################################

######## Commands ###############
$MPIRUN $EPW -nk 48 -input epw2_0.45.in > epw2_0.45.out
$MPIRUN $EPW -nk 48 -input epw2_0.35.in > epw2_0.35.out
#################################
```

After this calculation finishes, there will be two extra epsilon2_indabs files with subscript 8 and 10. We now plot the imaginary dielectric constant from these calculations and compare with automatic QD bin generation (epsilon2_indabs_300.0K_all.dat).

```
$python ../py_codes/plot_convergence.py
```

You will get a file Si_conv.png.

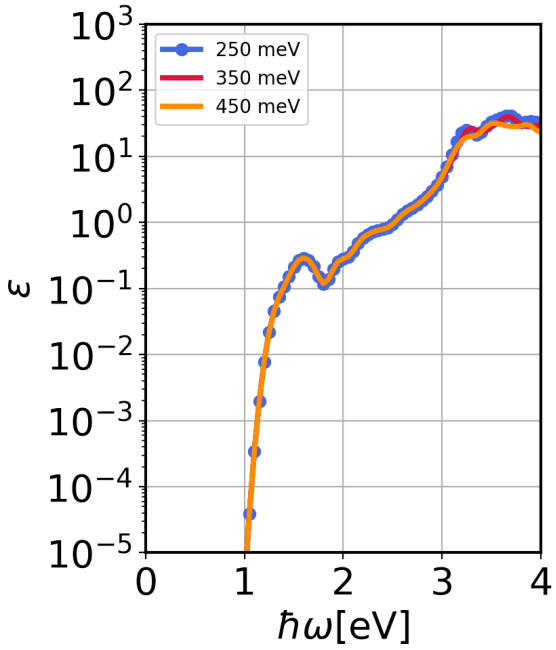

Fig. 8 Si imaginary dielectric constant calculated using QDPT for three QD bins.

We see the QD bin generated automatically ensures covergence. However, for each material, this convergence should be checked for production level calculations.

Somehing you can try in free time after school.

▶ Now perform the same calculations with file epw2_2.80.in

Note: For this calculation you need to submit over 4 nodes. Also, this calculation will take longer (about 40 minutes), so try at home!

`$sbatch submit5.sh`

submit5.sh

```
#!/bin/bash
#SBATCH -J Si_absorption
#SBATCH -o qe.%j.out
#SBATCH -e qe.%j.err
#SBATCH -N 4
#SBATCH -n 48
#SBATCH -t 01:00:00
#SBATCH -A DMR23030
#SBATCH -p skx
#SBATCH --reservation=NSF_Summer_School_Sat


## QE bin directory #############
QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e/bin/
#################################

### Executables #################
PW="${QE_BIN_DIR}/pw.x"
PH="${QE_BIN_DIR}/ph.x"
EPW="${QE_BIN_DIR}/epw.x"
MPIRUN="ibrun "
#################################

######## Commands ###############
$MPIRUN $EPW -nk 48 -input epw2_2.80.in > epw2_2.80.out
```

```
$MPIRUN $EPW -nk 48 -input epw2_all.in > epw2_all.out
################################
```

After these calculations finish, they produce two epsilon2 files *_2.dat and *_17.dat.

The epw2_all.in file is a simple QDPT calculation with automatic QD bin but with a denser $\mathbf{q}$-grid of 6X6X6. While the epw2_2.80.in is a QDPT calculation with a QD bin of size 2800 meV. This large size ensures we are performing full-diagonalization (almost).

Plot them using

```
$python ../py_codes/plot_convergence2.py
```

You will get a file Si_conv2.png.

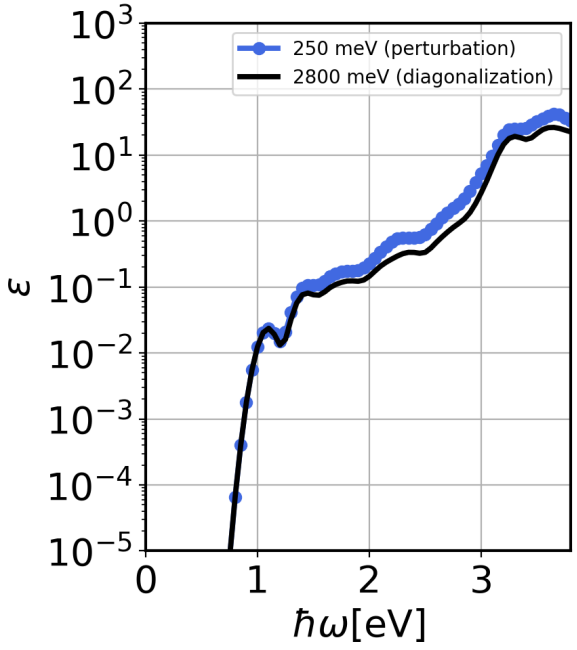

Fig. 9 Si imaginary dielectric constant calculated using QDPT for two QD bins. Here, at size 2800 meV, we almost reach full diagonalization.

As you can see, the perturbation and exact diagonalization give almost the same result. Slight difference is due to small grid sizes used and denser grids ensure exact comparison.