Calculation of Optical Properties with YAMBO

In this tutorial we are going to learn how to calculate the absorption spectra for 2D MoS_2 using the GW-BSE method implemented in YAMBO. This calculation depends on previously calculated QP energies; therefore, we are going to run this calculation in the same directory as the GW calculation.

In order to generate the input file for the GW-BSE calculation, apply the following command inside the "MoS2.save" directory.

```
$ ./yambo -o b -k sex -b -y h
```

Options:

-o b: the option -o is to select the type of optics calculation. Available options are b (optical properties in the eh-space with Bethe Salpeter equation), c (optical properties in G-space and results are similar to DFT level).

-k sex: the option -k is to select the type of correlation in the BSE calculation. The standard one is the Screened EXchange (SEX). Other options are Hartree-Fock (HF), Hartree, TD-LDA, and independent particles (IP).

-b: the option -b is to ask the code to construct the BSE kernel which is the second term of the two-particle Hamiltonian matrix elements. The kernel includes the sum of the electron-hole exchange part and the electron-hole attraction. The kernel both shifts and couples the quasiparticle energy differences.

-y h: the option -y is to select the Bethe-Salpeter equation solver to derive the macroscopic dielectric function including excitonic effects. The available options are h (Haydock recursive algorithm), d (diagonalization), and i (inversion solver).

The command above will generate the following input file (yambo.in) for a GW-BSE calculation and will immediately open the following input file in vi editor. The only modification to the input will be the line marked in red. To include the quasi-particle correction, copy this line to your input and save your input file.

```
#  **    **    **     ****     ****  ******     *******
# //**  **    ****   /**/**   **/** /*////**   **/////**
#  //****    **//**  /**//** ** /** /*   /**  **     //**
#   //**    **  //** /** //***  /** /******  /**      /**
#    /**   **********/**  //*   /** /*//// **/**      /**
#    /**  /**//////**/**   /    /** /*    /**//**     **
#    /**  /**     /**/**        /** /*******  //*******
#    //   //      // //         //  ///////    ///////
```

```
# GPL Version 4.2.1 Revision 110. (Based on r.14778 h.7b4dc3
#                        MPI Build
#                http://www.yambo-code.org
optics                         # [R OPT] Optics
em1s                           # [R Xs] Static Inverse Dielectric Matrix
bss                            # [R BSS] Bethe Salpeter Equation solver
bse                            # [R BSE] Bethe Salpeter Equation.
bsk                            # [R BSK] Bethe Salpeter Equation kernel
em1d                           # [R Xd] Dynamical Inverse Dielectric Matrix
ppa                            # [R Xp] Plasmon Pole Approximation
Chimod= "hartree"              # [X] IP/Hartree/ALDA/LRC/BSfxc
BSEmod= "retarded"             # [BSE] resonant/retarded/coupling
BSKmod= "SEX"                  # [BSE] IP/Hartree/HF/ALDA/SEX
BSSmod= "h"    # [BSS] (h)aydock/(d)iagonalization/(i)nversion/(t)ddft`
BSENGexx=  4985             RL # [BSK] Exchange components
BSENGBlk= 1005              RL # [BSK] Screened interaction block size
#WehCpl                     # [BSK] eh interaction included also in coupling
KfnQPdb= "E < SAVE/ndb.QP"      # [EXTQP BSK BSS] Database
% BEnRange
  0.00000 | 10.00000 | eV       # [BSS] Energy range
%
% BDmRange
  0.10000 |  0.10000 | eV       # [BSS] Damping range
%
BEnSteps= 100                   # [BSS] Energy steps
% BLongDir
 1.000000 | 0.000000 | 0.000000 |         # [BSS] [cc] Electric Field
%
% BSEBands
   1 |  50 |                    # [BSK] Bands range
%
BSHayTrs= -0.02000              # [BSS] Relative [o/o] Haydock treshold.
% BndsRnXs
   1 |  50 |                    # [Xs] Polarization function bands
%
NGsBlkXs= 1                 RL      # [Xs] Response block size
% DmRngeXs
  0.10000 |  0.10000 | eV       # [Xs] Damping range
%
% LongDrXs
 1.000000 | 0.000000 | 0.000000 |         # [Xs] [cc] Electric Field
%
% BndsRnXp
   1 |  50 |                    # [Xp] Polarization function bands
%
NGsBlkXp= 1005              RL      # [Xp] Response block size
% LongDrXp
0.1000E-4 | 0.000    | 0.000    |         # [Xp] [cc] Electric Field
```

```
%
PPAPntXp= 27.21138     eV      # [Xp] PPA imaginary energy
```

The following is a sample job submission file for the GW-BSE calculation. This will submit your job to the parallel queue by the qsub/sbatch command (this is a long job compared to Quantum Espresso calculations and it will take a while to finish)

```
#!/bin/bash -l
#SBATCH --job-name=job-gw
#SBATCH --time=24:00:00
#SBATCH --partition=parallel
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=24
mpirun -np 96 yambo -F yambo.in > yambo.out
```

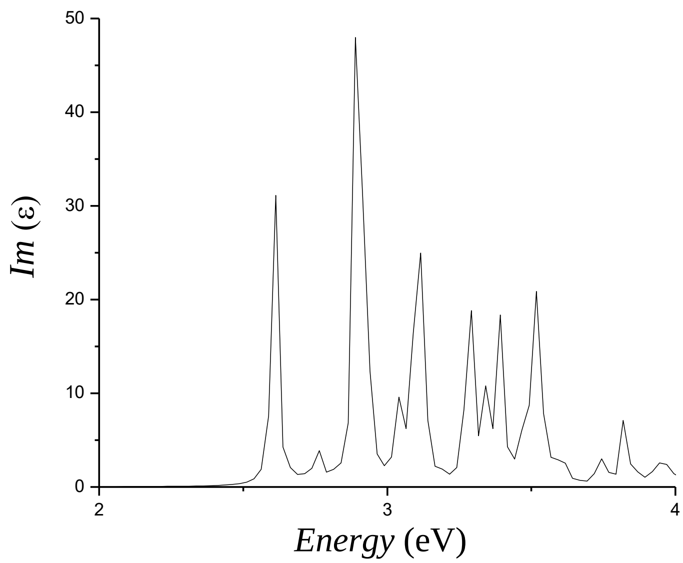
After you finish the GW-BSE calculation with the above job script, the system will generate the output file, “o.eps_q1_haydock_bse”. See below for a sample output file. You can extract the data points for the GW-BSE spectrum from this output.

```
#  **    **    **     ****     ****  ******     *******
# //**  **    ****   /**/**   **/** /*////**   **/////**
#  //****    **//**  /**//** ** /** /*   /**  **     //**
#   //**    **  //** /** //***  /** /******  /**      /**
#    /**   **********/**  //*   /** /*//// **/**      /**
#    /**  /**//////**/**   /    /** /*    /**//**     **
#    /**  /**     /**/**        /** /*******  //*******
#    //   //      // //         //  ///////    ///////
#
# GPL Version 4.2.1 Revision 110. (Based on r.14778 h.7b4dc3
#                          MPI Build
#                  http://www.yambo-code.org
#
# Absorption @ Q(1) [q->0 direction] :0.1000E-4  0.000     0.000
#
#
# - Energies      are  E < SAVE/ndb.QP + E Fit
# - Wavefunctions are Perdew, Burke & Ernzerhof(X)+Perdew, Burke & Ernz
erhof(C)
#
# - The Green`s function is Retarded -
# - Using the Length Gauge -
# - [r,Vnl] *is* included -
#
#   BSK|Identifier              :8262
#      |Dimension               :24379
#      |Bands                   :1 - 26
```

```
#       |Exchange           [res]: yes
#       |Correlation        [res]: yes
#       |Kernel`s coupling       : no
#       |Exchange           [cpl]: no
#       |Correlation        [cpl]: no
#       |W interaction is bare   : no
#       |ALDA kernel in R-space  : no
#       |RL vectors    [exchange]:4627
#       |RL vectors [correlation]:1005
#       |E/h energy range    [ev]:-1.000000 - -1.000000
#       |Coupling range     [o/o]: 100.0000 -  100.0000
#     W |Interaction is diagonal : no
#       |Matrix size             :1005
#       |Bands                   :1 - 26
#       |e/h energy range    [ev]:-1.000000 - -1.000000
#       |Poles              [o/o]: 100.0000
#       |RL vectors in the sum   :4459
#       |[r,Vnl] included        : yes
#       |Field direction         :0.1000E-4  0.000000  0.000000
#       |Coulomb Cutoff          :none
#       |xc-Kernel               :none
#    RIM|RL components      [col]:0
#       |Random points      [col]:0
#
#   Haydock|Accuracy (requested) [o/o]: -0.02000
#          |Accuracy (reached)   [o/o]:  0.01943
#          |Iteration                  :974
#
#    E/ev[1]      EPS-Im[2]    EPS-Re[3]    EPSo-Im[4]   EPSo-Re[5]   E
PS`-Im[6]   EPS`-Re[7]
#
    0.000000     0.000000     4.900739     0.000000     4.286737     0.
000000     4.900739
   0.2513E-1    0.1398E-3     4.901       0.7966E-4     4.287       0.1
398E-3     4.901
   0.5025E-1    0.2798E-3     4.901       0.1594E-3     4.287       0.2
798E-3     4.901
   0.7538E-1    0.4199E-3     4.902       0.2391E-3     4.288       0.4
199E-3     4.902
   0.1005       0.5603E-3     4.904       0.3190E-3     4.288       0.5
603E-3     4.904
   0.1256       0.7012E-3     4.905       0.3991E-3     4.289       0.7
012E-3     4.905
   0.1508       0.8426E-3     4.907       0.4794E-3     4.290       0.8
426E-3     4.907
   0.1759       0.9846E-3     4.909       0.5599E-3     4.292       0.9
846E-3     4.909
```

```
   0.2010       0.1127E-2     4.912        0.6407E-3     4.293        0.1
127E-2     4.912
   0.2261       0.1271E-2     4.915        0.7218E-3     4.295        0.1
271E-2     4.915
   0.2513       0.1415E-2     4.918        0.8034E-3     4.297        0.1
415E-2     4.918
   0.2764       0.1561E-2     4.922        0.8853E-3     4.299        0.1
561E-2     4.922
   0.3015       0.1708E-2     4.926        0.9677E-3     4.301        0.1
708E-2     4.926
   0.3266       0.1856E-2     4.931        0.1051E-2     4.304        0.1
856E-2     4.931
   0.3518       0.2006E-2     4.936        0.1134E-2     4.307        0.2
006E-2     4.936
--More--(16%)
```

Now you can plot “EPS-Im[2] vs E/ev[1]” using any preferred graphing tool such as excel, origin, etc…, to generate the spectrum as follows,



Absorption spectra for 2D MoS_2, obtained with GW-BSE

If you are interested in further details on the convergence parameters for MoS_2 for publication quality work, please refer to: Molina-Sánchez *et* al, Phys. Rev. **B 88**, 045412 (2013), https://arxiv.org/abs/1306.4257.