Hands-On Session #4
Optical Absorption Spectra of Si and LiCl

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BerkeleyGW Workshop – Nov. 23rd, 2013
Hands-on Session #4

4.1 - Calculate optical absorption spectrum of Si
   - Goals:
     - Plot the optical absorption spectrum of Silicon with and without e-h interactions.
   - Stretch Goals:
     - Use scissors corrections with the absorption code.
     - Compare results with RPA spectrum with local fields.

4.2 – Optical absorption spectrum of LiCl
   - Goals:
     - Plot optical absorption spectrum of LiCl with and without e-h interactions.
     - Calculate exciton binding energy
   - Stretch goals:
     - Analyze where the exciton is coming from.
     - Rerun with Haydock iterative scheme.
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- **General remarks**
  - Si: we’ll reuse `sigma_hp.log` from the first tutorial session.
  - LiCl: you’ll be given a pre-calculated `sigma_hp.log`.

- From the sigma side, you’ll only have to run `eqp.py` (with `eqpl`) to get `eqp.dat`

- You’ll have to generate:
  - `WFN_fi` and `WFNq_fi` (for `absorption.x`)
  - `bsedmat` and `bsexmat`
Absorption – Workflow

absorption.inp

epsmat
eps0mat
eqp_co.dat
bsedmat
bsexmat
WFN_co

WFN_fi
WFNq_fi

absorption_noeh.dat
absorption_eh.dat
eigenvalues.dat
eigenvectors.dat
d?mat_norm.dat
Sigma and Kernel – Workflow

- sigma_hp.log
- eqp.py
- eqp.dat (linked to eqp_co.dat)

- kernel.inp
- epsmat
- eps0mat
- WFN_co

- kernel.x
- bsepmat
- bsexmat
Let’s Put the Donkey to Work!

BerkeleyGW

Predicting quasiparticle band structures since 1985.

cd $SCRATCH2
cp -r /project/projectdirs/m1694/BGW-2013/4.1-Si
cp -r /project/projectdirs/m1694/BGW-2013/4.2-LiCl

4.1 - Si

[Graph showing the energy and ε₂ for Si]

[Graph showing additional data with markers labeled as absorption_noeh.dat and absorption_eh.dat]
4.1 - Si

GW-RPA: effect of local fields

Scissors v.s eqp
4.2 - LiCl

GW-BSE v.s GW-RPA

Diagonalization v.s Haydock

Binding energy $\sim 0.6$ eV
(unconverged!)