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

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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.

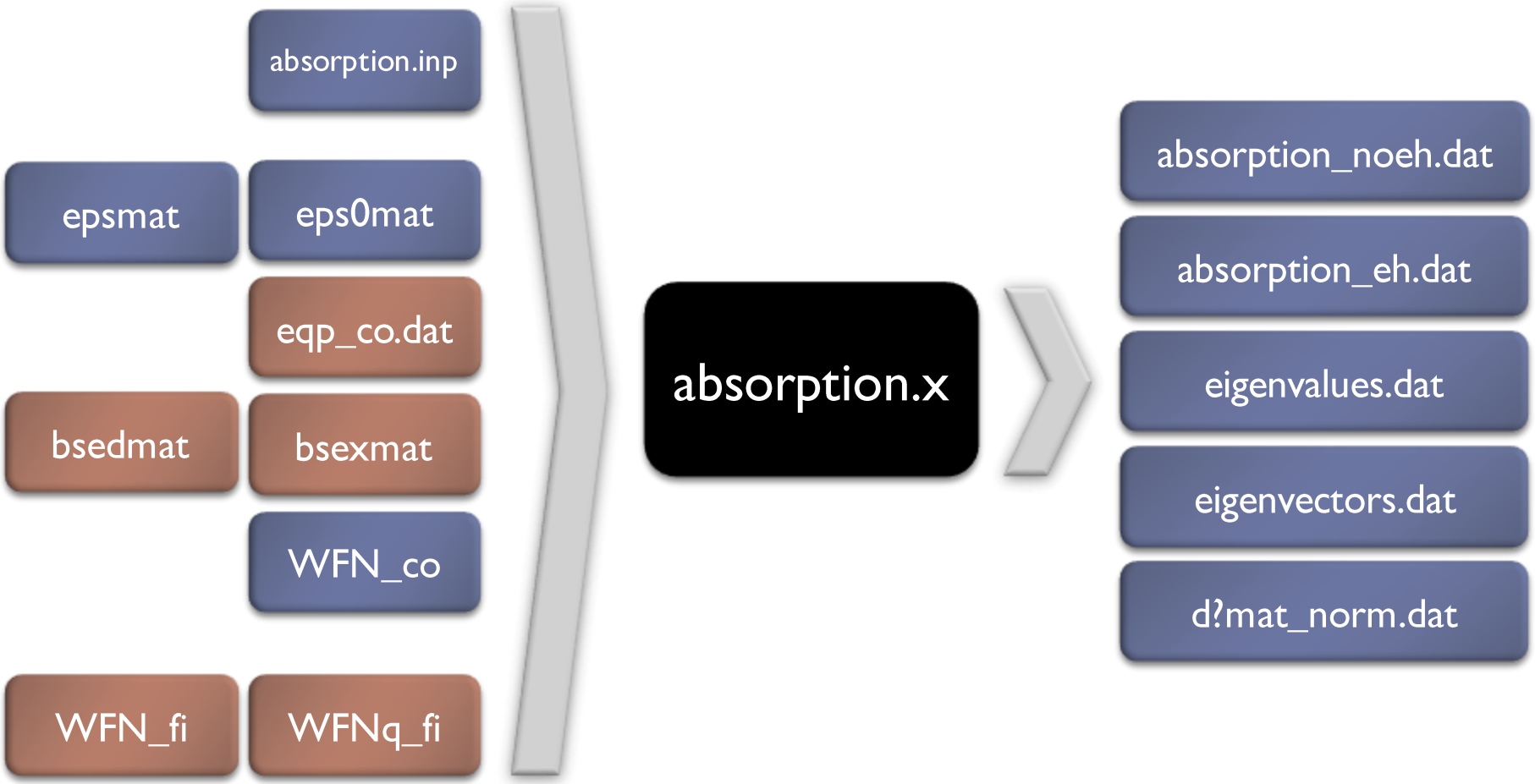
Hands-on Session #4

- 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`.

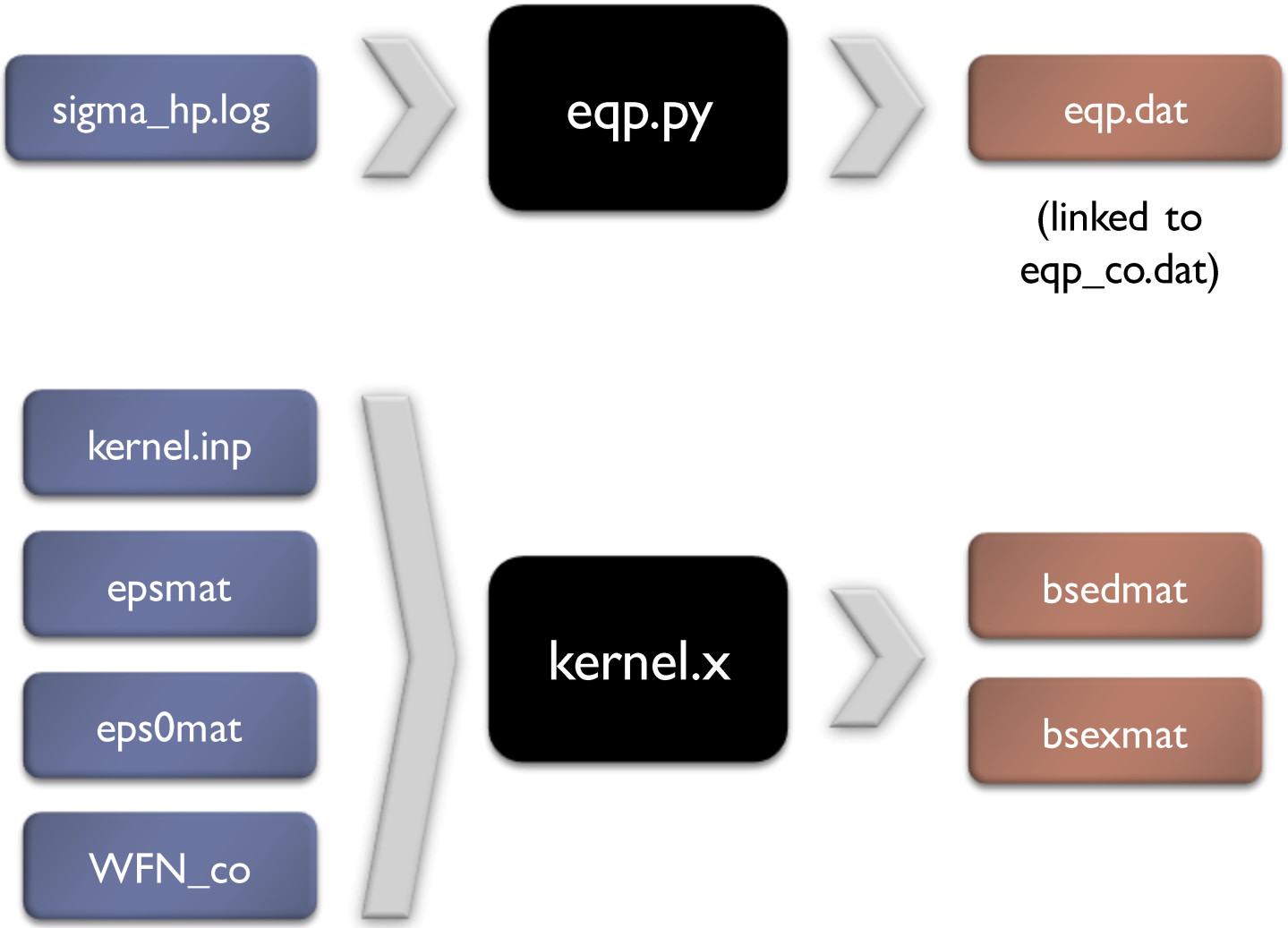
- From the sigma side, you'll only have to run `eqp.py` (with eqp1) to get eqp.dat

- You'll have to generate:
  - WFN_fi and WFNq_fi (for absorption.x)
  - bsedmat and bsexmat

Absorption – Workflow



Sigma and Kernel – Workflow



Let's Put the Donkey to Work!

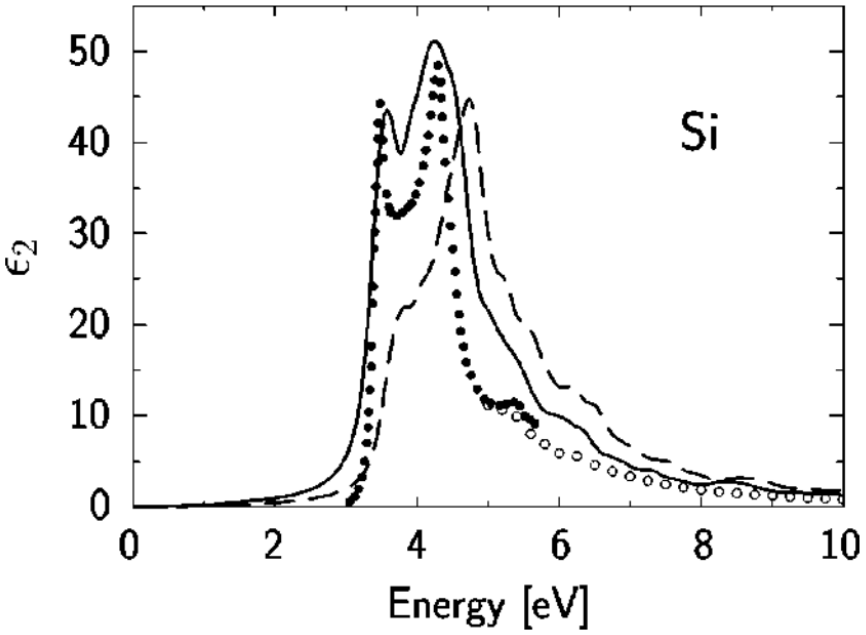
BerkeleyGW

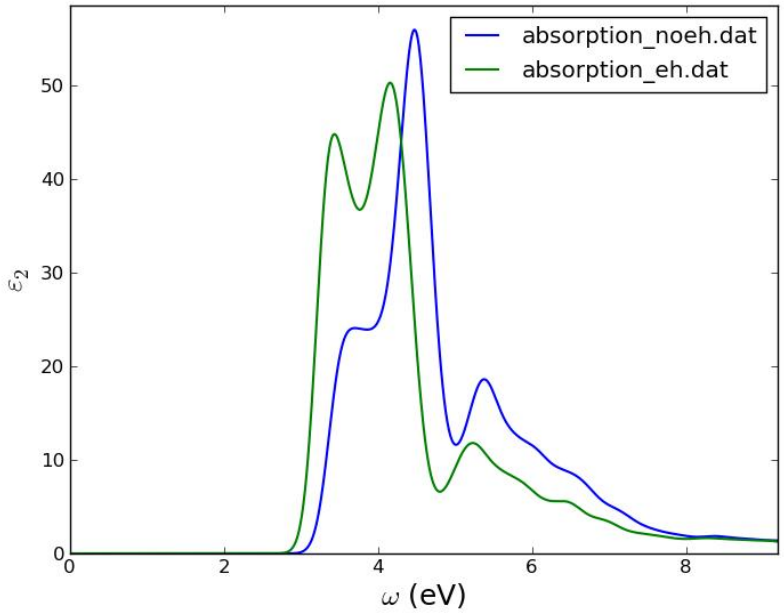
Predicting quasiparticle band structures since 1985.

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

Manual: http://www.berkeleygw.org/releases/manual_v1.0.6.html

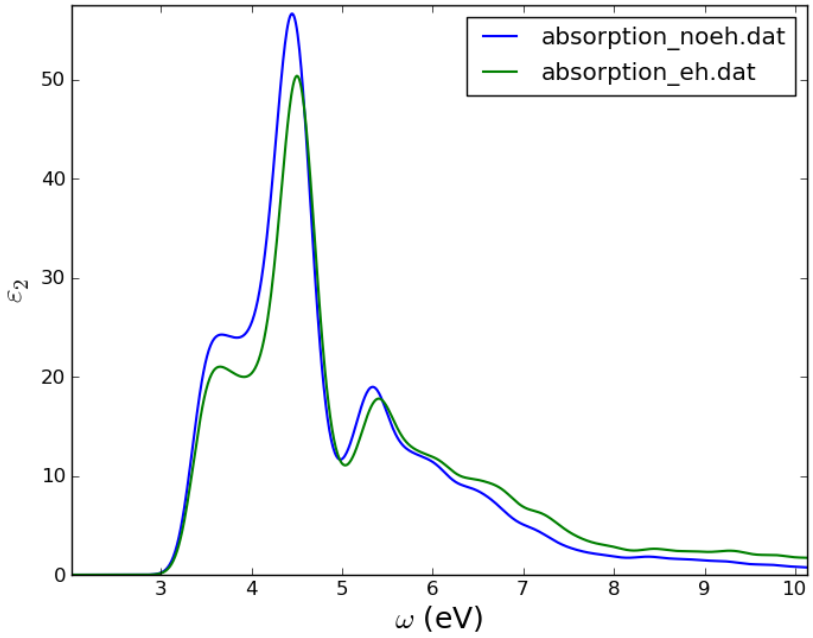
4.1 - Si


Si
ϵ_2
Energy [eV]
0
10
20
30
40
50
0
2
4
6
8
10

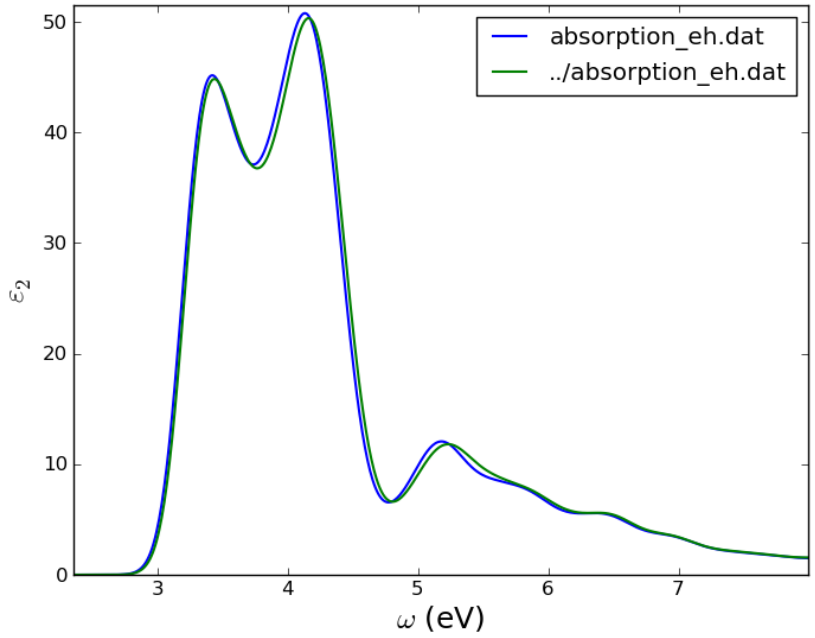

absorption_noeh.dat
absorption_eh.dat
ε_2
ω (eV)
0
10
20
30
40
50
0
2
4
6
8

4.1 - Si

GW-RPA: effect of local fields

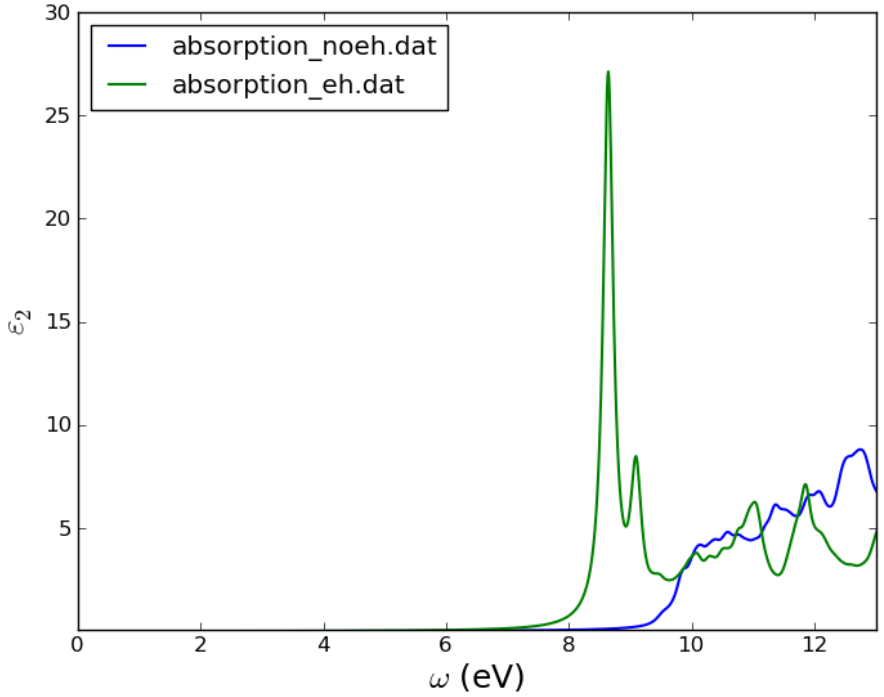


Scissors v.s eqp

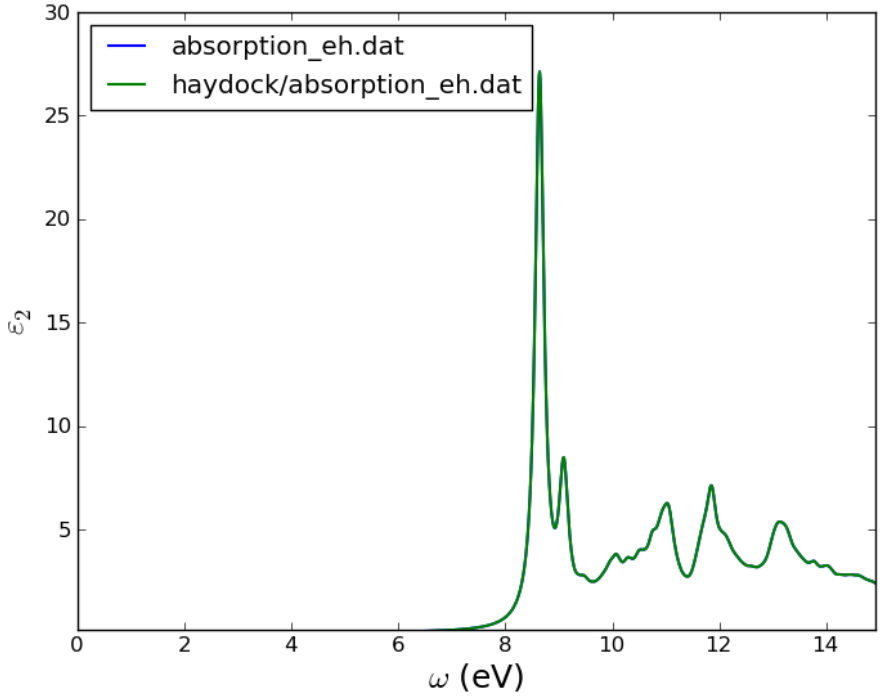


4.2 - LiCl

GW-BSE v.s GW-RPA



Diagonalization v.s Haydock



Binding energy ~ 0.6 eV
(unconverged!)