Practical session I

From ABINIT to EXC

Lecturers: Matteo Gatti, Francesco Sottile

May 17, 2013 ■ 14h00m-18h00m

Introduction

It is your duty now to prepare the ground-state and screening files in order to solve the Bethe-Salpeter equation using EXC.

The EXC code firstly creates the excitonic Hamiltonian

$$H_{exc}^{e-h} = [(\epsilon_c + \Delta_c - \epsilon_v + \Delta_v)\,\delta_{cc'vv'} + 2 << v >> - << W >>]$$

with Δ_n being the GW correction (or a scissor operator shift)
$<< v >>= \int \phi_v(r)\phi_c(r)v(r,r')\phi_{v'}(r')\phi_{c'}(r')$ and $<< W >>= \int \phi_v(r)\phi_{v'}(r)W(r,r')\phi_c(r')\phi_{c'}(r')$ where $W(r,r') = \frac{\varepsilon^{-1}(r,r')}{|r-r'|}$. So EXC needs a KSS file (for ϵ_n and ϕ_n), a GW file (for Δ_n) or simply a scissor shift, and a screening file SCR (for the ε^{-1}).

Tasks

1. Create the "∗_KSS" file containing complete information on the Kohn-Sham bandstructure (use the usual Monkorst-Pack 4x444 k-grid).
2. Create the "∗_SCR" file containing the RPA screening function (this should contain 19 q-points).
3. Create the "∗_GW" file containing the GW corrections to the DFT eigenvalues.
4. Create now another "∗_KSS" file, using these shifts in the abinit input file:

```
nshiftk 4
shiftk
0.6 0.7 0.8
0.6 0.2 0.3
0.1 0.7 0.3
0.1 0.2 0.8
```

Q1. What is the difference between the two KSS files ? (hint: look at the symmetries)

Q2. How many k-points are contained in the two KSS files ?

Comments

Practical session II

EXC

Lecturers: Francesco Sottile, Matteo Gatti

May 17, 2013 ■ 14h00m-18h00m

Introduction

We are ready to use the Bethe-Salpeter equation to calculate the absorption spectra of solids.

Objectives

- Calculate the different kind of spectra (RPA, with and without local fields, GW-RPA, BSE)
- Study the convergence of the spectrum with respect to the number of bands, the number of plane waves in the wavefunctions, the dimension of the dielectric matrix, the set of **k**-points.

  In order to run an exciton calculation, use the same input file as for DP, with the additional variable `exciton`. Again, in the transition framework, you can do `rpa`, `alda` or now `exc`.

Tasks

- Run a RPA calculation, with the EXC code, with and without local fields, and answer the following question.

  Q1. Is there a difference between a RPA calculation with EXC and DP ? Why?

  Q2. What is the difference among the files `outexc.mdf outrpanlf.mdf outgwnlf.mdf`?

- Perform now a GW-RPA calculation (using a scissor for example). Plot the spectra and consider again the three files `outexc.mdf outrpanlf.mdf outgwnlf.mdf`.
- Finally perform an exciton calculation (still using a scissor if you wish). Plot the spectra and consider again the three files `outexc.mdf outrpanlf.mdf outgwnlf.mdf`.
- Perform a calculation including coupling (i.e. using the variable `coupling`).

  Q1. What is the effect of the coupling on the absorption spectrum ?

  Q2. And what the effect on the eels (hint: generate smaller kss and scr files for the evaluation of the eels spectra, for the convergence parameters might imply long calculations)? [If you have no time to generate new kss files, use the ones included in the `/nfs_home/tutoadmin/spectroscopy_lectures/work/Si` directory, but prior to calculation export the variable F_UFMTENDIAN to big].

  In the directories ∼/spectroscopy_lectures/work/"other material" input files for other simple semiconductors and insulators are available. Create the kss and scr with Abinit and try to obtain the absorption spectra (for example, try LiF).

Comments