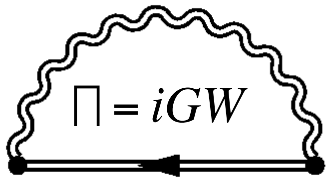
Calculating GW corrections with ABINIT



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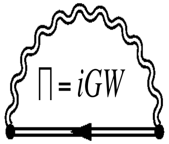
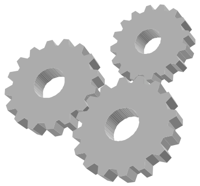
Outline

Introduction



GW Theory



Structure and Algorithm of the GW code

Practical use in ABINIT

Future developments

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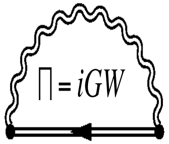

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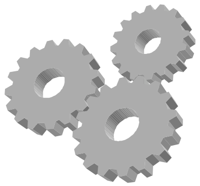

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Motivation:

Why to go from DFT to GW?

- The Kohn-Sham energies have not an interpretation as removal/addition energies (Koopman Theorem does not hold).
- Even though, the KS energies can be considered as an approximation to the true Quasiparticle energies, but they suffer of some problems (for example, the band gap underestimation).
- Need to correct these inaccuracies ➞ calculation of the GW corrections.

The ABINIT-GW code

(in few words)

- **The thing**: GW code in Frequency-Reciprocal space on a PW basis.
- **Purpose**: Quasiparticle Electronic Structure.
- **Systems**: Bulk, Surfaces, Clusters.
- **Approximations**: non Self-Consistent G^0W^{RPA}, Plasmon Pole model.

Quality of the code

- **Efficacy**: the code gives the desired result. *****
- **Reliability**: the result must be correct and, in case of possible or certain failure, it is signalled in an unambiguous mode. ****
- **Robustness**: the code is without premature or unwished stops, like overflows, divergences… ***
- **Economy**: the code saves, as much as possible, hardware and software resources. ***

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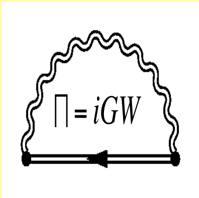

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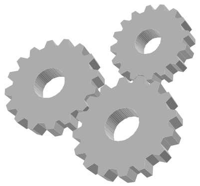

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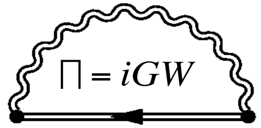
Quasiparticle energies



In the **quasiparticle (QP) formalism**, the energies and wavefunctions are obtained by the **Dyson equation**:

$$\left[-\frac{\nabla^2}{2} + V_{ext}(\mathbf{r}) + V_H(\mathbf{r})\right]\psi_{n\mathbf{k}}(\mathbf{r}) + \int d\mathbf{r}'\,\Sigma\left(\mathbf{r},\mathbf{r}',\omega = \varepsilon_{n\mathbf{k}}^{\mathrm{QP}}\right)\psi_{n\mathbf{k}}(\mathbf{r}') = \varepsilon_{n\mathbf{k}}^{\mathrm{QP}}\psi_{n\mathbf{k}}(\mathbf{r}) \quad \text{QP equation}$$

which is very similar to the Kohn-Sham equation:

$$\left[-\frac{\nabla^2}{2} + V_{ext}(\mathbf{r}) + V_H(\mathbf{r})\right]\psi_{n\mathbf{k}}(\mathbf{r}) + V_{xc}(\mathbf{r})\psi_{n\mathbf{k}}(\mathbf{r}) = \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}}\psi_{n\mathbf{k}}(\mathbf{r}) \quad \text{KS equation}$$

with V_{xc} that replaces Σ, the **self-energy** (a non-local and energy dependent operator).
We can calculate the **QP (GW) corrections** to the DFT KS eigenvalues by 1st order PT:

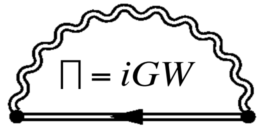
0-order wavefunctions

$$\varepsilon_{n\mathbf{k}}^{\mathrm{QP}} = \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} + \left\langle \psi_{n\mathbf{k}}^{\mathrm{DFT}} \right| \Sigma(\mathbf{r},\mathbf{r}',\omega) - V_{xc}(\mathbf{r}) \left| \psi_{n\mathbf{k}}^{\mathrm{DFT}} \right\rangle$$

0-order

Quasiparticle correction

The Self-Energy
in the GW approximation



Within the **GW approximation**, Σ is given by:

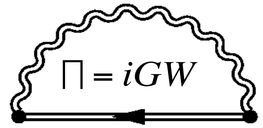
$$\Sigma^{\mathrm{GW}}(\mathbf{r},\mathbf{r}',\omega) = \frac{i}{2\pi}\int d\omega' \, e^{i\omega'\eta} \, G(\mathbf{r},\mathbf{r}',\omega+\omega') \, W(\mathbf{r},\mathbf{r}',\omega')$$

GW Self-Energy

Green Function

Dynamical Screened Interaction

The Green function G

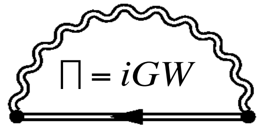


Furthermore, the Green function G is approximated by the independent particle $G^{(0)}$:

$$G^{(0)}(\mathbf{r},\mathbf{r}',\omega) = \sum_{n\mathbf{k}} \frac{\psi_{n\mathbf{k}}^{\mathrm{DFT}}(\mathbf{r})\psi_{n\mathbf{k}}^{\mathrm{DFT}*}(\mathbf{r}')}{\omega - \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} + i\eta\,\mathrm{sgn}(\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} - \mu)}$$

The basic ingredient of $G^{(0)}$ is the **Kohn-Sham electronic structure**:

W and the RPA approximation



W is approximated by its RPA expression:

$$W_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \varepsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)\, v_{\mathbf{G}'}(\mathbf{q})$$

Dynamical Screened Interaction

Dielectric Matrix

Coulomb Interaction

$$v_{\mathbf{G}'}(\mathbf{q}) = \frac{4\pi}{|\mathbf{q}+\mathbf{G}'|^2}$$

$$\varepsilon^{\mathrm{RPA}}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \delta_{\mathbf{G},\mathbf{G}'} - v_{\mathbf{G}}(\mathbf{q})\,\chi^{(0)}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$$

RPA approximation

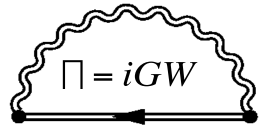
Independent Particle Polarizability

$$\chi^{(0)}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = 2\sum_{n,n',\mathbf{k}} \left(f_{n,\mathbf{k}} - f_{n',\mathbf{k}+\mathbf{q}}\right) \frac{\left\langle \phi^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}} \left| e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \right| \phi^{\mathrm{DFT}}_{n,\mathbf{k}} \right\rangle \left\langle \phi^{\mathrm{DFT}}_{n,\mathbf{k}} \left| e^{i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}} \right| \phi^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}} \right\rangle}{\varepsilon^{\mathrm{DFT}}_{n,\mathbf{k}} - \varepsilon^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}} - \omega - i\eta}$$

Adler-Wiser expression

ingredients: KS wavefunctions and KS energies

Single Plasmon Pole Model for Σ



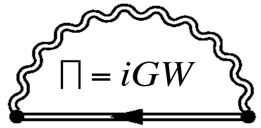
The dynamic (ω) dependence of the Dielectric Matrix is modeled with a Plasmon Pole model:

$$\varepsilon^{-1}(\omega) = 1 + \frac{\Omega^2}{\omega^2 - \tilde{\omega}^2}$$

this gives Σ_x this gives Σ_c

To calculate the 2 parameters of the model, we need to calculate ε in 2 frequencies.

Σ_x (exchange) and Σ_c (correlation)



Defining ρ (calculated through FFT):

$$\rho_{ij}(\mathbf{q}+\mathbf{G}) = \left\langle \phi_i^{\mathrm{DFT}} \left| e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \right| \phi_j^{\mathrm{DFT}} \right\rangle = \int d\mathbf{r}\, e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \phi_i^{\mathrm{DFT}*}(\mathbf{r}) \phi_j^{\mathrm{DFT}}(\mathbf{r}) \qquad \mathbf{q} = \mathbf{k}_j - \mathbf{k}_i$$

We arrive at:

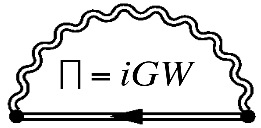
$$\left\langle \phi_j^{\mathrm{DFT}} \left| \Sigma_x \right| \phi_j^{\mathrm{DFT}} \right\rangle = -\frac{4\pi}{V_{cryst}} \sum_i^{occ} \sum_{\mathbf{G}} \frac{\rho_{ij}^2(\mathbf{q}+\mathbf{G})}{|\mathbf{q}+\mathbf{G}|^2}$$

ω-independent, only occupied states

$$\mathbf{q} = \mathbf{k}_j - \mathbf{k}_i$$

$$\left\langle \phi_j^{\mathrm{DFT}} \left| \Sigma_c(\omega) \right| \phi_j^{\mathrm{DFT}} \right\rangle = \frac{2\pi}{V_{cryst}} \sum_i \sum_{\mathbf{G},\mathbf{G}'} \frac{\rho_{ij}^*(\mathbf{q}+\mathbf{G})\rho_{ij}(\mathbf{q}+\mathbf{G}')}{|\mathbf{q}+\mathbf{G}||\mathbf{q}+\mathbf{G}'|} \frac{\Omega_{\mathbf{G}\mathbf{G}'}^2(\mathbf{q})}{\tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\left(\omega - \varepsilon_i^{\mathrm{DFT}} + \tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})(2f_i - 1)\right)}$$

Dynamic dependence



Σ depends on $\omega=\varepsilon_{n\mathbf{k}}$:

$$\varepsilon_{n\mathbf{k}}^{\mathrm{QP}} = \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} + \left\langle \psi_{n\mathbf{k}}^{\mathrm{DFT}} \left| \Sigma(\mathbf{r},\mathbf{r}',\omega = \varepsilon_{n\mathbf{k}}^{\mathrm{QP}}) - V_{xc}(\mathbf{r}) \right| \psi_{n\mathbf{k}}^{\mathrm{DFT}} \right\rangle$$

in principle the non-linear equation should be solved self-consistently.
but we linearize:

$$\left\langle \Sigma(\omega = \varepsilon_{n\mathbf{k}}^{\mathrm{QP}}) \right\rangle = \left\langle \Sigma(\omega = \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}}) \right\rangle + \left(\varepsilon_{n\mathbf{k}}^{\mathrm{QP}} - \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} \right) \left\langle \left. \frac{d\Sigma(\omega)}{d\omega} \right|_{\omega=\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}}} \right\rangle$$

and defining the renormalization constant $Z_{n\mathbf{k}}$ (the derivative is calculated numerically):

$$Z_{n\mathbf{k}} = \left[1 - \left. \frac{d\left\langle \psi_{n\mathbf{k}}^{\mathrm{DFT}} \left| \Sigma(\omega) \right| \psi_{n\mathbf{k}}^{\mathrm{DFT}} \right\rangle}{d\omega} \right|_{\omega=\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}}} \right]^{-1}$$

renormalization constant

we finally arrive at:

$$\varepsilon_{n\mathbf{k}}^{\mathrm{QP}} = \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}} + Z_{n\mathbf{k}} \left\langle \psi_{n\mathbf{k}}^{\mathrm{DFT}} \left| \Sigma(\mathbf{r},\mathbf{r}',\omega = \varepsilon_{n\mathbf{k}}^{\mathrm{DFT}}) - V_{xc}(\mathbf{r}) \right| \psi_{n\mathbf{k}}^{\mathrm{DFT}} \right\rangle$$

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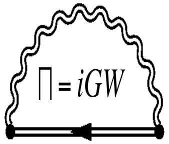

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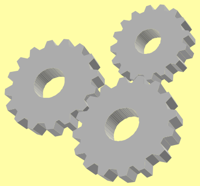

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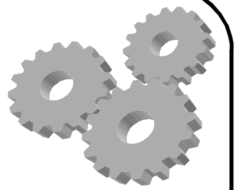
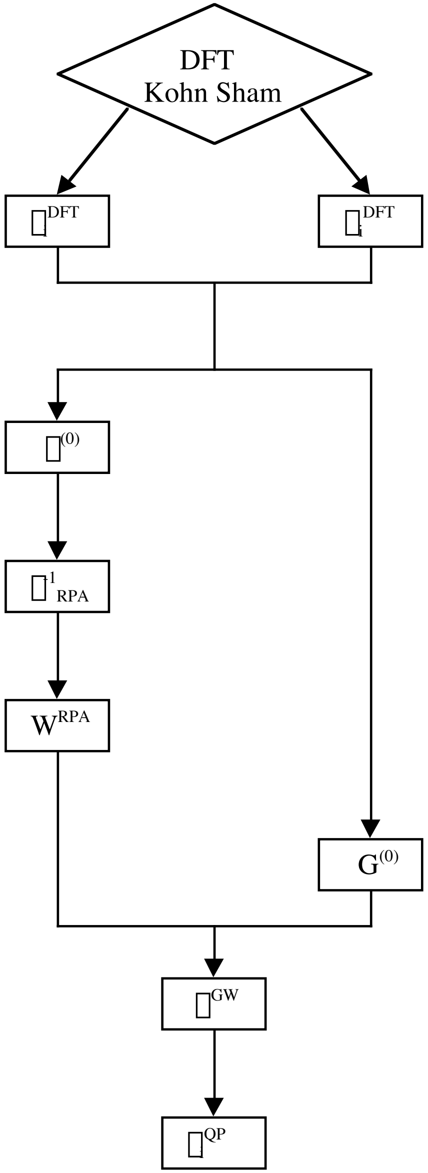
GW: scheme of the calculation





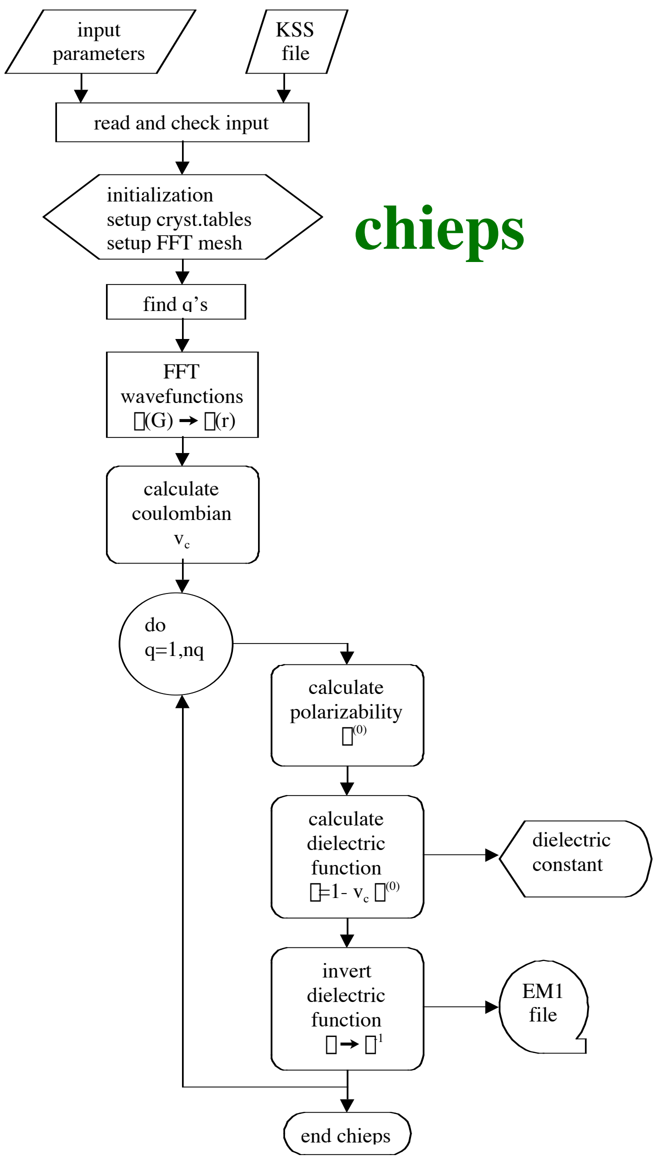
GW calculation scheme

calculation of the
KS ELECTRONIC STRUCTURE
,

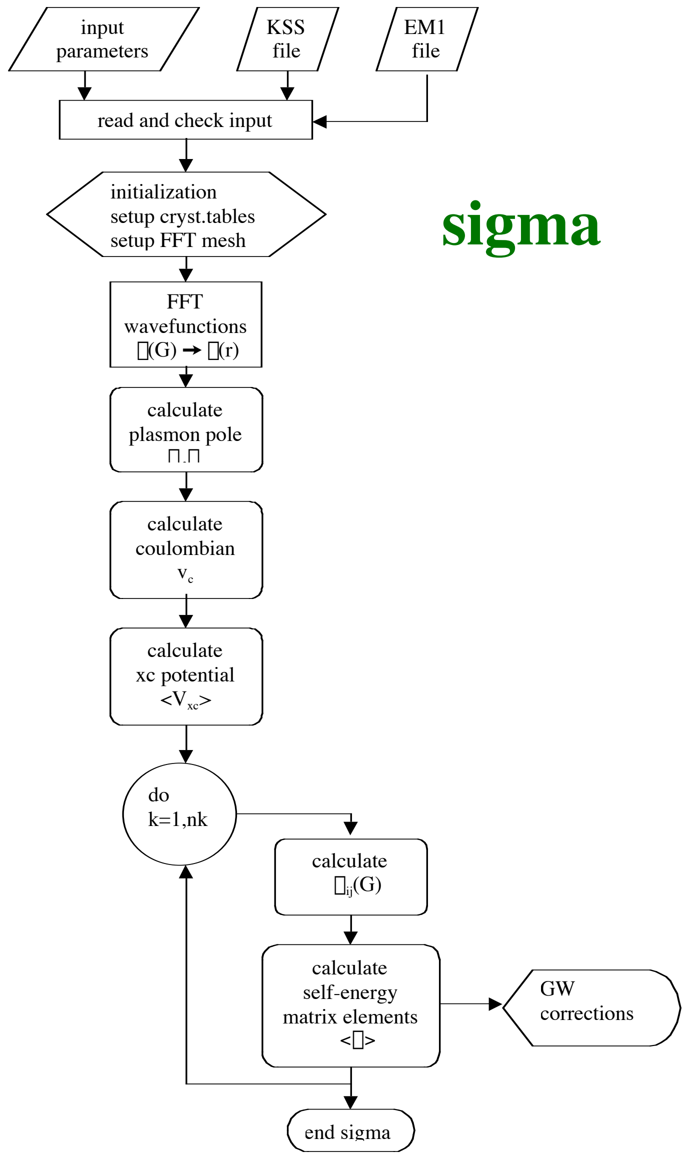
calculation of the
RPA SCREENING
W

calculation of the
GW CORRECTIONS
(SELF-ENERGY MATRIX ELEMENTS
<-V>

GW: code flow diagram



chieps



sigma

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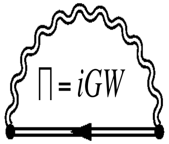

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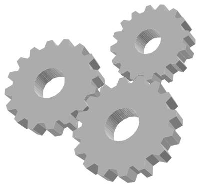

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Three steps process

1. DFT wavefunctions and eigenvalues: $\psi_{n\mathbf{k}}^{\mathrm{DFT}}$ and $\varepsilon_{n\mathbf{k}}^{\mathrm{DFT}}$

2. Dielectric matrix:

$$\varepsilon^{\mathrm{RPA}}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)=\delta_{\mathbf{G},\mathbf{G}'}-v_{\mathbf{G}}(\mathbf{q})\chi^{(0)}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) \quad \text{with} \quad \mathbf{q}=\mathbf{k}_j-\mathbf{k}_i$$

$$\chi^{(0)}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)=2\sum_{n,n',\mathbf{k}}\left(f_{n,\mathbf{k}}-f_{n',\mathbf{k}+\mathbf{q}}\right)\frac{\left\langle\psi^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}}\middle|e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}\middle|\psi^{\mathrm{DFT}}_{n,\mathbf{k}}\right\rangle\left\langle\psi^{\mathrm{DFT}}_{n,\mathbf{k}}\middle|e^{i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}}\middle|\psi^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}}\right\rangle}{\varepsilon^{\mathrm{DFT}}_{n,\mathbf{k}}-\varepsilon^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}}-\omega-i\eta}$$

3. GW corrections:

$$E^{\mathrm{QP}}_{n\mathbf{k}}-\varepsilon^{\mathrm{DFT}}_{n\mathbf{k}}=\left\langle\psi^{\mathrm{DFT}}_{n\mathbf{k}}\middle|\Sigma(\mathbf{r},\mathbf{r}',E)-V_{xc}(\mathbf{r})\middle|\psi^{\mathrm{DFT}}_{n\mathbf{k}}\right\rangle$$

$$\left\langle\psi^{\mathrm{DFT}}_{j}\middle|\Sigma_x\middle|\psi^{\mathrm{DFT}}_{j}\right\rangle=-\frac{4\pi}{V_{cryst}}\sum_{i}^{occ}\sum_{\mathbf{q},\mathbf{G}}\frac{\rho^2_{ij}(\mathbf{q}+\mathbf{G})}{|\mathbf{q}+\mathbf{G}|^2}$$

$$\left\langle\psi^{\mathrm{DFT}}_{j}\middle|\Sigma_c(E)\middle|\psi^{\mathrm{DFT}}_{j}\right\rangle=\frac{2\pi}{V_{cryst}}\sum_{i}\sum_{\mathbf{q},\mathbf{G},\mathbf{G}'}\frac{\rho^*_{ij}(\mathbf{q}+\mathbf{G})\rho_{ij}(\mathbf{q}+\mathbf{G}')}{|\mathbf{q}+\mathbf{G}||\mathbf{q}+\mathbf{G}'|}\frac{\Omega^2_{\mathbf{G}\mathbf{G}'}(\mathbf{q})}{\tilde\omega_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\left(E-\varepsilon^{\mathrm{DFT}}_i+\tilde\omega_{\mathbf{G}\mathbf{G}'}(\mathbf{q})(2f_i-1)\right)}$$

$$\varepsilon^{-1}(\omega)=1+\frac{\Omega^2}{\omega^2-\tilde\omega^2}$$ $\Rightarrow$ plasmon pole model

Input file

- Common part

```
# Si in diamond structure
 acell 3*10.25
 rprim  0.000  0.500  0.500
        0.500  0.000  0.500
        0.500  0.500  0.000
 natom  2
 ntype  1
 type  2*1
 xred   0.000  0.000  0.000
        0.250  0.250  0.250
 zatnum 14.0
 ecut  6

 enunit 2
 intxc  1
```

Avoid the use of **non-symmorphic symmetry operations** (not yet implemented) if possible.

If not, specify by hand (nsym, symrel) only symmorphic symmetry operations

Ground state calculation

- To generate the _KSS file

```
# wavefunctions calculation
 kptopt          1
 ngkpt           2 2 2
 nshiftk         4
 shiftk          0.5 0.5 0.5
                 0.5 0.0 0.0
                 0.0 0.5 0.0
                 0.0 0.0 0.5
 mkmem           0

 nstep          10
 tolwfr          1.0d-16

 occopt          1
 nbndsto        -1
 ncomsto         0
```

nbndsto

Mnemonics: Number of BaNDs for eigenSTate Output

If **nbndsto**=-1, all the available eigenstates (energies and eigenfunctions) are stored in the _KSS file at the end of the ground state calculation complete diagonalization

If **nbndsto** is greater than 0, abinit stores (about) **nbndsto** eigenstates in the _KSS file partial diagonalization

The number of states is forced to be the same for all k-points.

Ground state calculation

- To generate the _KSS file

```
# wavefunctions calculation
 kptopt             1
 ngkpt              2  2  2
 nshiftk            4
 shiftk             0.5  0.5  0.5
                    0.5  0.0  0.0
                    0.0  0.5  0.0
                    0.0  0.0  0.5
 mkmem              0

 nstep             10
 tolwfr             1.0d-16

 occopt             1
 nbndsto           -1
 ncomsto            0
```

ncomsto

Mnemonics: Number of planewave COMponents for eigenSTate Output

If nbndsto/=0, **ncomsto** defines the number of planewave components of the Kohn-Sham states to be stored in the _KSS file.

If **ncomsto**=0, the maximal number of components is stored.

The planewave basis is the same for all k-points.

Screening calculation

- To generate the _EM1 file

```
# screening calculation
 optdriver   3
 nband      10
 npweps     27
 npwwfn     27
 plasfrq    16.5 eV
```

optdriver
case=3 : susceptibility and dielectric matrix calculation (CHI), routine "chieps"

npwwfn
Mnemonics: Number of PlaneWaves for WaveFunctioNs

npweps
Mnemonics: Number of PlaneWaves for EPSilon (the dielectric matrix)

plasfrq
Mnemonics: PLASmon pole FReQuency

Screening calculation

- The output file

The calculated dielectric constant is printed:

```
dielectric constant =  13.7985
dielectric constant without local fields =  15.3693
```

Note that the convergence in the dielectric constant DOES NOT GUARANTEE the convergence in the GW correction values at the end of the calculation.

In fact, the dielectric constant is representative of only one element, the **head** of ϵ^{-1} .
In a GW calculation, **all the elements** of the ϵ^{-1} matrix are used to build W.

Recipe:
A reasonable starting point for input parameters can be found in EELS calculations existing in literature. Indeed, Energy Loss Function (-Im ϵ^{-1}_{00}) spectra converge with similar parameters as screening calculations.

Self-energy calculation

```
# sigma calculation
 optdriver   4
 nband      10
 npwmat     27
 npwwfn     27
 ngwpt       1
 kptgw     0.250  0.750  0.250
 bdgw     4  5
 zcut        0.1 eV
```

optdriver

case=4 : self-energy calculation (SIG), routine "sigma"

npwmat

Mnemonics: Number of PlaneWaves for the exchange term MATrix elements

zcut

parameter used to avoid some divergencies that might occur in the calculation due to integrable poles along the integration path

Convergence parameters

k-point grid through **q=k**$_j$**-k**$_i$ in all following equations

npwwfn: in the FFTs $\psi^{\mathrm{DFT}}_{n\mathbf{k}}(\mathbf{r}) \leftrightarrow \psi^{\mathrm{DFT}}_{n\mathbf{k}}(\mathbf{G})$

npweps:

$$\varepsilon^{\mathrm{RPA}}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \delta_{\mathbf{G},\mathbf{G}'} - v_{\mathbf{G}}(\mathbf{q})\chi^{(0)}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$$

$$\chi^{(0)}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = 2\sum_{n,n',\mathbf{k}} \left(f_{n,\mathbf{k}} - f_{n',\mathbf{k}+\mathbf{q}}\right) \frac{\langle \psi^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}}|e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|\psi^{\mathrm{DFT}}_{n,\mathbf{k}}\rangle\langle\psi^{\mathrm{DFT}}_{n,\mathbf{k}}|e^{i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}}|\psi^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}}\rangle}{\varepsilon^{\mathrm{DFT}}_{n,\mathbf{k}} - \varepsilon^{\mathrm{DFT}}_{n',\mathbf{k}+\mathbf{q}} - \omega - i\eta}$$

$$\langle\psi^{\mathrm{DFT}}_j|\Sigma_c(\omega)|\psi^{\mathrm{DFT}}_j\rangle = \frac{2\pi}{V_{cryst}}\sum_i\sum_{\mathbf{q},\mathbf{G},\mathbf{G}'}\frac{\rho^*_{ij}(\mathbf{q}+\mathbf{G})\rho_{ij}(\mathbf{q}+\mathbf{G}')}{|\mathbf{q}+\mathbf{G}||\mathbf{q}+\mathbf{G}'|}\frac{\Omega^2_{\mathbf{GG}'}(\mathbf{q})}{\tilde\omega_{\mathbf{GG}'}(\mathbf{q})\left(\omega-\varepsilon^{\mathrm{DFT}}_i+\tilde\omega_{\mathbf{GG}'}(\mathbf{q})(2f_i-1)\right)}$$

npwmat:

$$\langle\psi^{\mathrm{DFT}}_j|\Sigma_x|\psi^{\mathrm{DFT}}_j\rangle = -\frac{4\pi}{V_{cryst}}\sum_i^{occ}\sum_{\mathbf{q},\mathbf{G}}\frac{\rho^2_{ij}(\mathbf{q}+\mathbf{G})}{|\mathbf{q}+\mathbf{G}|^2}$$

nband: in previous equations

Convergence parameters

npwwfn npweps npwmat

Mnemonics: Number of PlaneWaves

MUST BE numbers corresponding to closed G-shells

alternatively use:

nshwfn nsheps nshmat

Mnemonics: Number of Shells

ecutwfn ecuteps ecutmat

Mnemonics: Energy CUT-off

GW Corrections

The GW corrections are presented in the output file:

```
 k =    -0.125    0.000    0.000
  Band    E0      SigX    SigC(E0) dSigC/dE  Sig(E)  <VxcLDA>   E-E0
     4  5.6163  -12.3340   0.9073  -0.2986 -11.3590 -11.1322  -0.2268
     5  8.3569   -5.9512  -3.7032  -0.2922  -9.7681 -10.1571   0.3889
```

- E0: DFT eigenvalues
- SigX: Exchange term
- SigC(E0): Correlation term
- Sig(E): Self-Energy Interaction
- <VxcLDA>: XC potential from DFT
- E-E0: GW corrections

Vxc is calculated using Perdew-Zunger functional
Other XC functionals should be implemented

All in one input

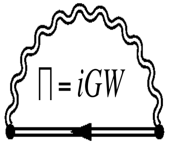
```
 ndtset       3
# wavefunctions calculation
 nbndsto1    -1    ncomsto1    0

# chieps calculation
 optdriver2   3    getkss2     -1
 nband2      10    npweps2     27    npwwfn2     27
 plasfrq2 16.5 eV

# sigma calculation
 optdriver3   4    getkss3     -2    geteps3     -1
 nband3      10    npwmat3     27    npwwfn3     27
 ngwpt3       1
 kptgw3    0.250  0.750  0.250
 bdgw3     4  5
 zcut3        0.1 eV
```

→ _KSS file generated by previous data set

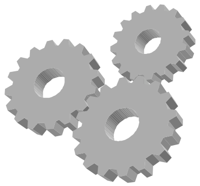
→ _EM1 file generated by previous data set

Outline

Introduction



GW Theory



Structure and Algorithm of the GW code

Practical use in ABINIT

Future developments

Wish list

- full treatment of non-symmorphic operations
- allow to perform chieps calculations for a limited number of q-points and then merge _EM1 files
- parallelization (at least on q-points for chieps, and on kptgw for sigma)
- other XC functionals (already implemented in ABINIT)
- allow to use non-diagonalized KS eigenfunctions (basically those that are in the _WFK file)

Wish list

- introduction of the spin degree of freedom
- calculation of the GW total energy
- calculation of a real GW band plot through automatic generation of the needed k-grids
- possibility to set □(G,G´)≈□(G,G´) beyond ecuteps
- full screening (beyond plasmon-pole) and lifetimes
- update of the eigenvalues (self-consistency)
- update of the wavefunctions (1st order) and of the energy (2nd order): off-diagonal elements of □

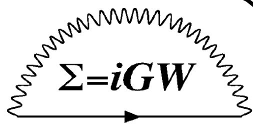
Known bugs and limitations

- allow higher angular momentum projectors (mproj/=1) → reintroduction in the header of lmax and lref removed in v3.4
- proper treatment of the case lim q→ 0, G=0 in chieps for space groups other than FCC

Conclusion

We want you for GW !

GW theory: Off-diagonal Elements



QP wave functions expanded in terms of DFT (LDA or GGA) wave functions:

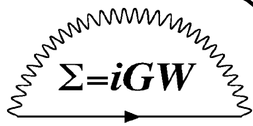
$$\psi^{QP}_{n,\sigma,\mathbf{k}} = \psi^{DFT}_{n,\sigma,\mathbf{k}} + \sum_{n'\neq n} \alpha_{n,n',\sigma,\mathbf{k}} \psi^{DFT}_{n',\sigma,\mathbf{k}} \quad \xrightarrow{\text{usually}} \quad \psi^{QP}_{n,\sigma,\mathbf{k}} \approx \psi^{DFT}_{n,\sigma,\mathbf{k}}$$

$$E^{QP}_{n,\sigma,\mathbf{k}} = E^{DFT}_{n,\sigma,\mathbf{k}} + \overbrace{\left\langle n,\sigma,\mathbf{k} \middle| \Sigma^{\sigma,\sigma}(E^{QP}_{n,\sigma,\mathbf{k}}) - V^{\sigma,\sigma}_{XC} \middle| n,\sigma,\mathbf{k} \right\rangle}^{\text{diagonal element}}$$

$$\underbrace{+ \sum_{n'\neq n} \frac{\left| \left\langle n,\sigma,\mathbf{k} \middle| \Sigma^{\sigma,\sigma}(E^{QP}_{n,\sigma,\mathbf{k}}) - V^{\sigma,\sigma}_{XC} \middle| n',\sigma,\mathbf{k} \right\rangle \right|^2}{E^{DFT}_{n,\sigma,\mathbf{k}} - E^{DFT}_{n',\sigma,\mathbf{k}}}}_{\text{off-diagonal elements}}$$

$$\alpha_{n,n',\sigma,\mathbf{k}} = \frac{\left\langle n',\sigma,\mathbf{k} \middle| \Sigma^{\sigma,\sigma}(E^{QP}_{n,\sigma,\mathbf{k}}) - V^{\sigma,\sigma}_{XC} \middle| n,\sigma,\mathbf{k} \right\rangle}{E^{DFT}_{n,\sigma,\mathbf{k}} - E^{DFT}_{n',\sigma,\mathbf{k}}}$$

GW Theory



In the quasiparticle (QP) formalism, the energies and wave functions are obtained by the Dyson equation:

$$(T + V_{ext} + V_H)\psi_{n,\sigma,\mathbf{k}}(\mathbf{r}) + \sum_{\sigma'}\int \Sigma^{\sigma,\sigma'}\left(\mathbf{r},\mathbf{r}';E^{QP}_{n,\sigma,\mathbf{k}}\right)\psi_{n,\sigma',\mathbf{k}}(\mathbf{r}')\,d\mathbf{r}' = E^{QP}_{n,\sigma,\mathbf{k}}\psi_{n,\sigma,\mathbf{k}}(\mathbf{r})$$

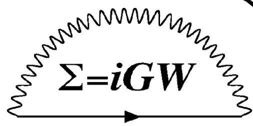
where $\Sigma^{\sigma,\sigma'}$ is the self energy operator $\left(\sigma,\sigma' = \uparrow \text{ or } \downarrow\right)$

Within the GW approximation, it is given by:

$$\begin{cases} \Sigma^{\sigma,\sigma}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \dfrac{i}{2\pi}\displaystyle\int G^{\sigma,\sigma}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega+\omega')W_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega')e^{-i\delta\omega'}d\omega' \\ \Sigma^{\sigma,\sigma'}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = 0 \quad \text{for } \sigma' \neq \sigma \end{cases}$$

(no spin-flip, no spin-orbit coupling)

RPA approximation for W



Dynamical Screened Interaction

$$W_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \varepsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)\, v(\mathbf{q}+\mathbf{G}')$$

Coulomb Interaction

$$v(\mathbf{q}+\mathbf{G}') = \frac{4\pi}{|\mathbf{q}+\mathbf{G}'|^2}$$

Static Dielectric Matrix → Random Phase Approximation

$$\varepsilon_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega=0) = \delta_{\mathbf{G},\mathbf{G}'} - V(\mathbf{q}+\mathbf{G})\left[\chi^{\uparrow\uparrow}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega=0) + \chi^{\downarrow\downarrow}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega=0)\right]$$

$$\chi^{\sigma,\sigma'}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega=0) = \delta_{\sigma,\sigma'} \sum_{n,n',\mathbf{k}} \frac{\langle n,\sigma,\mathbf{k}|e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|n',\sigma',\mathbf{k}+\mathbf{q}\rangle\langle n',\sigma',\mathbf{k}+\mathbf{q}|e^{i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}}|n,\sigma,\mathbf{k}\rangle}{E^{DFT}_{n',\sigma',\mathbf{k}+\mathbf{q}} - E^{DFT}_{n,\sigma,\mathbf{k}}}$$

Dynamic Dielectric Matrix → Generalized Plasmon Pole model

[M.S. Hybertsen and S. G. Louie, PRB **34**, 5390 (1986)]