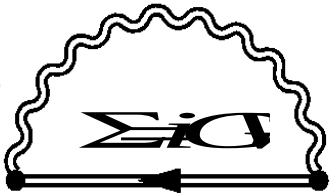
Calculating GW corrections with ABINIT



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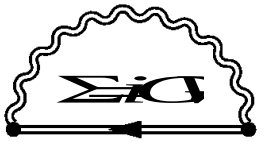
Outline



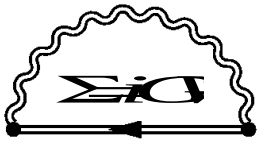
- Introduction, History of the code
- GW Theory
- Structure and Algorithm of the GW code
- Use and Parameters
- Achievements and Future developments
- Conclusions

Motivation:
why to go from DFT to GW

	DFT-LDA		EXP
Silicon	0.55		1.17
Diamond	4.26		5.48
MgO	5.3		7.83

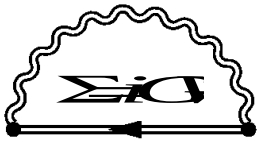
- The Kohn-Sham energies have not an interpretation as removal/addition energies (Kopman Theorem does not hold).
- Nevertheless, the KS energies can be considered as an approximation to the true Quasiparticle energies, but they suffer from some problems (for example, the band gap underestimation).
-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

The ABINIT-GW code
in few words



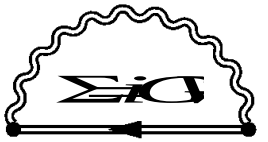
- The thing: GW code in Frequency-Reciprocal space on a PW basis.
- Purpose: Quasiparticle Electronic Structure.
- Systems: Bulk, Surfaces, Clusters.
- Approximations: GW, Plasmon-Pole model and RPA on W, non Self-Consistent G^0W^{RPA}, first step of self-consistency on W and G.

Quality of the code

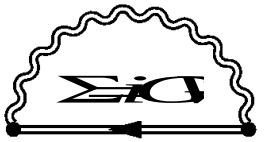


- **Efficacy**: the code gives the desired result. *****
- **Reliability**: the result must be correct and, in case of possible or certain failure, it is signalled in an unambiguous mode. ****
- **Robustness**: the code is without premature or unwished stops, like overflows, divergences… ***
- **Economy**: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

GW Theory



Quasiparticle Energies



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

$$\left[-\frac{\partial_r^2}{2}+v_{ext}(r)+v_H(r)\right]\phi_{nk}(r)+\int dr'\,\Sigma(r,r',\omega=\epsilon_{nk}^{QP})\phi_{nk}(r')=\epsilon_{nk}^{QP}\phi_{nk}(r)$$ QP equation

which is very similar to the Kohn-Sham equation:

$$\left[-\frac{\partial_r^2}{2}+v_{ext}(r)+v_H(r)\right]\phi_{nk}(r)+v_{xc}(r)\phi_{nk}(r)=\epsilon_{nk}^{DFT}\phi_{nk}(r)$$ KS equation

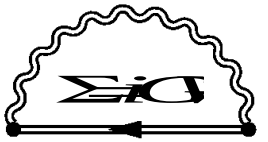
with V_{xc} that replaces Σ, the **self-energy** (a non-local and energy dependent operator).
We can calculate the **QP (GW) corrections** to the DFT KS eigenvalues by 1st order PT:

0-order wavefunctions

$$\epsilon_{nk}^{QP}=\epsilon_{nk}^{DFT}+\langle\phi_{nk}^{DFT}|\Sigma(r,r',\omega)-v_{xc}(r)|\phi_{nk}^{DFT}\rangle$$ Quasiparticle correction

0-order

The Self-Energy in the GW approximation



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

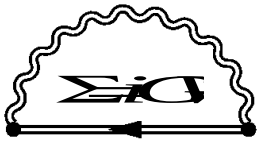
$$\Sigma^{GW}(r,r',\omega)=\frac{i}{2\pi}\int d\omega'\, e^{-i\delta\omega'} G(r,r',\omega-\omega') W(r,r',\omega')$$

GW Self-Energy

Green's Function

Dynamical Screened Interaction

The Green's function G

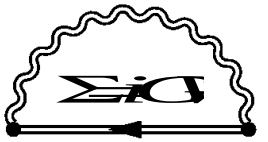


Furthermore, the Green's function G is approximated by the independent particle $G^{(0)}$:

$$G(r,r',\omega)=\sum_{nk}\frac{\phi_{nk}^{DFT}(r)\,\phi_{nk}^{DFT\,*}(r')}{\omega-\epsilon_{nk}^{DFT}+i\,\delta\,\mathrm{sgn}(\epsilon_{nk}^{DFT}-\mu)}$$

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

W and the RPA approximation



and W by its RPA expression:

$$W_{GG'}(q,\omega)=\epsilon^{-1}_{GG'}(q,\omega)\,v_{G'}(q)$$ Dynamically Screened Interaction

Dielectric Matrix

Coulomb Interaction $v_{G'}(q)=\dfrac{4\pi}{|q+G'|^2}$

$$\epsilon^{RPA}_{GG'}(q,\omega)=\delta_{GG'}-v_G(q)\,\chi^{(0)}_{GG'}(q,\omega)$$ **RPA approximation**

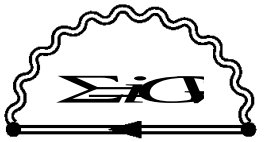
Independent Particle Polarizability

$$\chi^{(0)}_{GG'}(q,\omega)=2\sum_{n,n',k}(f_{nk}-f_{n',k+q})\frac{\langle\phi^{DFT}_{n',k+q}|e^{-i(q+G)r}|\phi^{DFT}_{nk}\rangle\langle\phi^{DFT}_{nk}|e^{i(q+G')r}|\phi^{DFT}_{n',k+q}\rangle}{\epsilon^{DFT}_{nk}-\epsilon^{DFT}_{n',k+q}-\omega-i\delta}$$

ingredients: KS wavefunctions and KS energies

Adler-Wiser expression

Single Plasmon Pole Model for ε



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

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

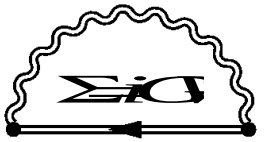
Plasmon Pole Model

this gives Σ_x

this gives Σ_c

To calculate the 2 parameters of the model,
we need to calculate in 2 frequencies (0 and pure imag) (Godby model),
or in 1 frequency (0) and adjust for the asymptotic behaviour (Hybertsen-Louie).

Σ_x (exchange) and Σ_c (correlation)



Defining ρ (calculated through FFT):

$$\rho_{ij}(G)=\langle \phi_i^{DFT}|e^{-i(q+G)r}|\phi_j^{DFT}\rangle=\int dr\, e^{-i(q+G)r}\phi_i^{DFT}(r)\phi_j^{DFT}(r) \qquad q=k_j-k_i$$

We are led to:

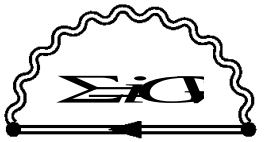
$$\langle \phi_i^{DFT}|\Sigma_x|\phi_j^{DFT}\rangle=-\frac{4\pi}{V_{cryst}}\sum_i^{occ}\sum_G \frac{\rho_{ij}^2(G)}{|q+G|^2}$$

ω-independent, only occupied states

$q=k_j-k_i$

$$\langle \phi_j^{DFT}|\Sigma_c|\phi_j^{DFT}\rangle=\frac{2\pi}{V_{cryst}}\sum_i\sum_{GG'}\frac{\rho_{ij}^*(G)}{|q+G|}\frac{\rho_{ij}(G')}{|q+G'|}\frac{\Omega_{GG'}^2(q)}{\tilde{\omega}_{GG'}(q)[\omega-\epsilon_i^{DFT}+\tilde{\omega}_{GG'}(q)(2f_i-1)]}$$

Dynamic dependence



Σ depends on $\omega=\varepsilon_{nk}$:

$$\epsilon_{nk}^{QP}=\epsilon_{nk}^{DFT}+\langle\phi_{nk}^{DFT}|\Sigma(r,r',\omega=\epsilon_{nk}^{QP})-v_{xc}(r)|\phi_{nk}^{DFT}\rangle$$

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

$$\langle\Sigma(\omega=\epsilon_{nk}^{QP})\rangle=\langle\Sigma(\omega=\epsilon_{nk}^{DFT})\rangle+(\epsilon_{nk}^{QP}-\epsilon_{nk}^{DFT})\left\langle\frac{d\Sigma(\omega)}{d\omega}\right|_{\omega=\epsilon_{nk}^{DFT}}\right\rangle$$

and defining the renormalization constant Z_{nk} (the derivative is calculated numerically):

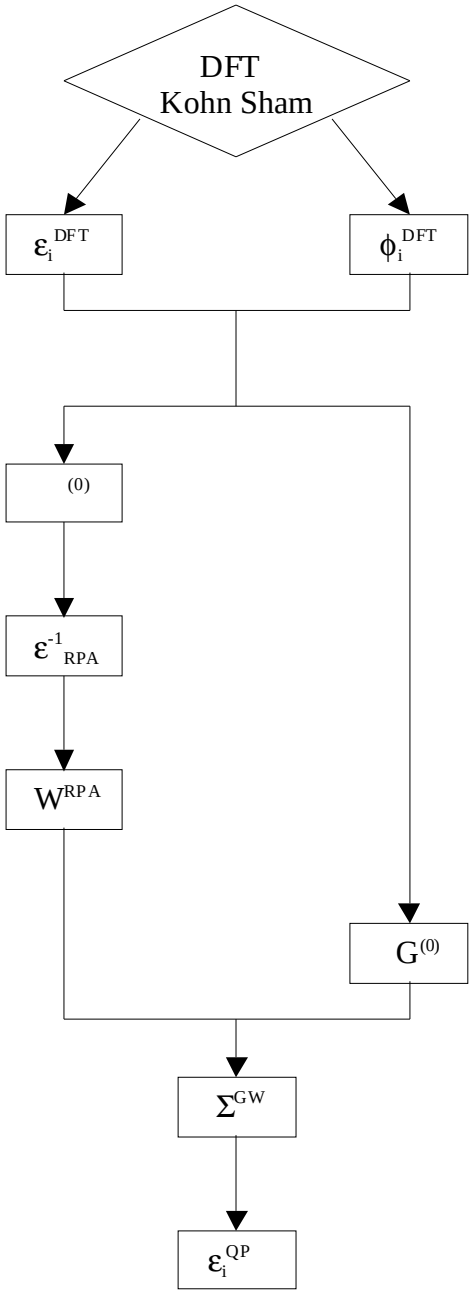
$$Z_{nk}=\left(1-\frac{d\langle\phi_{nk}^{DFT}|\Sigma(\omega)|\phi_{nk}^{DFT}\rangle}{d\omega}\right|_{\omega=\epsilon_{nk}^{DFT}}\Bigg)^{-1}$$

renormalization constant

we finally get at:

$$\epsilon_{nk}^{QP}=\epsilon_{nk}^{DFT}+Z_{nk}\langle\phi_{nk}^{DFT}|\Sigma(r,r',\omega=\epsilon_{nk}^{DFT})-v_{xc}(r)|\phi_{nk}^{DFT}\rangle$$

GW: scheme of the calculation



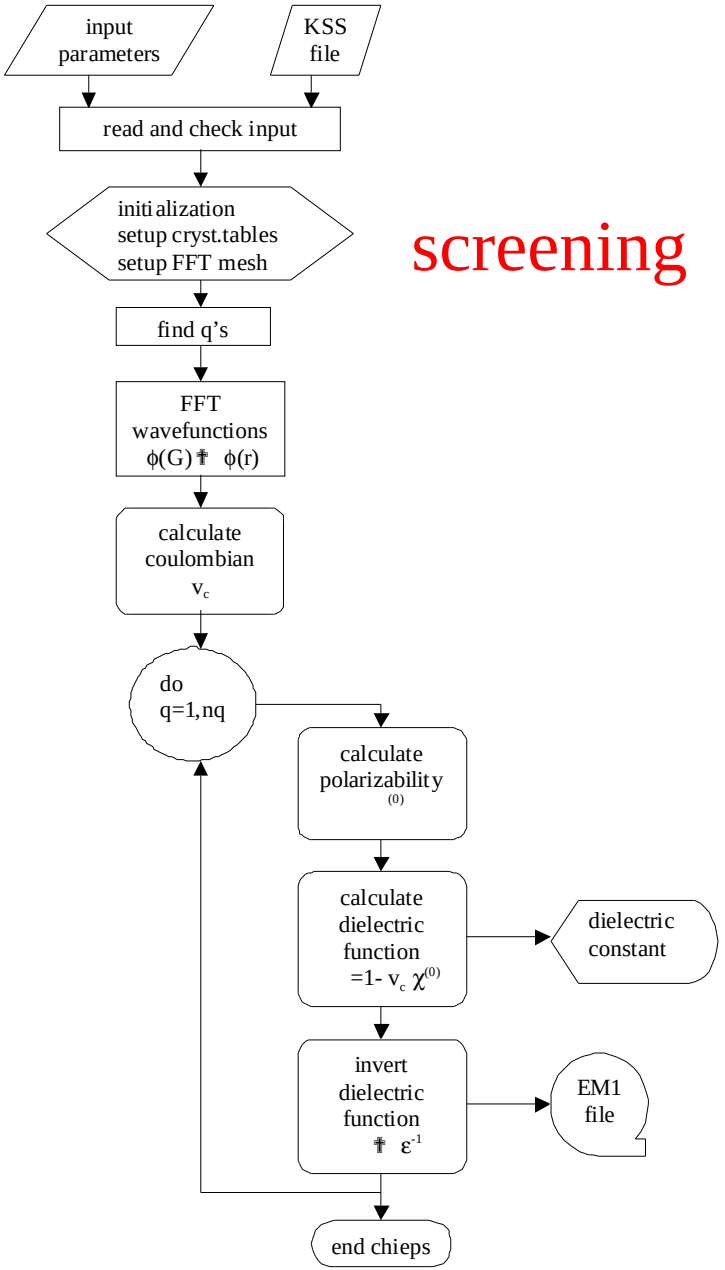
GW calculation scheme

calculation of the
KS ELECTRONIC STRUCTURE
ε

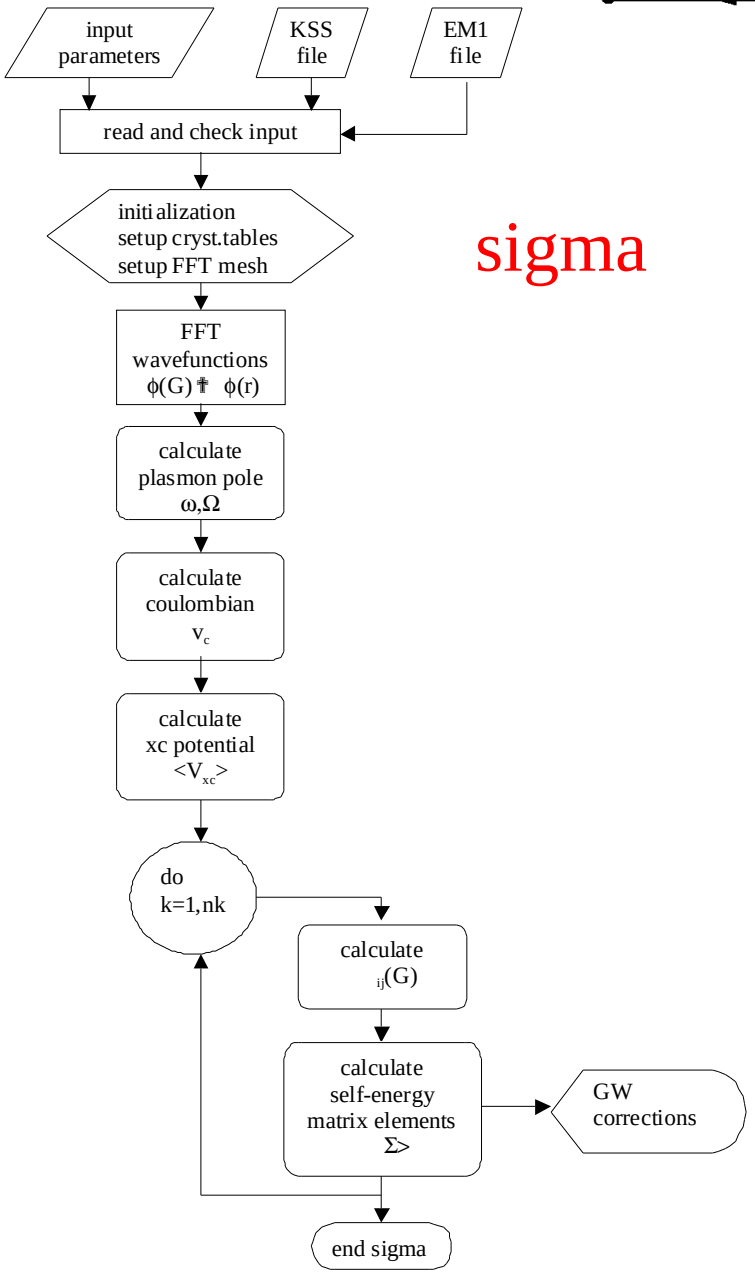
calculation of the
RPA SCREENING
W

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

GW: code flow diagram

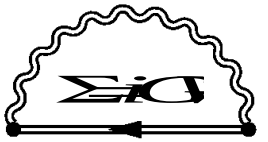


screening



sigma

Practical use in ABINIT



- Three step process:
  1. DFT-KS wavefunctions and eigenvalues ($\phi^{DFT\text{-}KS}$,$\varepsilon^{DFT\text{-}KS}$);
  2. Dielectric Matrix (ε) and Screening (W);
  3. Self-Energy (Σ) and GW corrections.

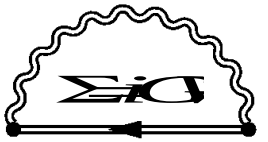
Ground State calculation and common part

```
# 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
 ntypat  1
 typat   1 1
 xred    0.000  0.000  0.000
         0.250  0.250  0.250
 zatnum  14.0

 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

 ecut    8.0
 nstep   10
 toldfe  0.001
```

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

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

Kohn-Sham electronic structure and KSS file



```
# Kohn-Sham electronic
# Structure 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

 kssform         1
 nbandkss        -1
 npwkss          0
```

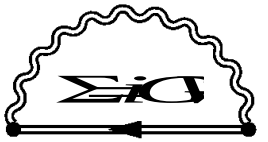
nbandkss

Mnemonics: Number of BANDs for KSS file

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

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

Kohn-Sham electronic structure and KSS file



```
# Kohn-Sham electronic
# Structure 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

 kssform         1
 nbandkss        -1
 npwkss          0
```

npwkss

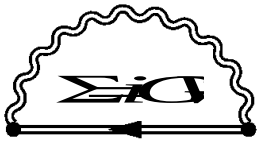
Mnemonics: Number of PlaneWave for KSS file

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

If **npwkss**=-1, the maximal number of components is stored.

The planewave basis is the same for all k-points (Gamma centered planewaves).

Kohn-Sham electronic structure and KSS file



```
# Kohn-Sham electronic
# Structure 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

 kssform         1
 nbandkss        -1
 npwkss          0
```

kssform

Mnemonics: KSS file FORmat

kssform=1

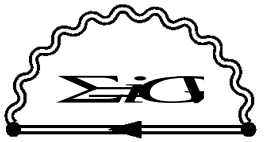
By default kssform=1 (full or partial diago of the Kohn-Sham hamiltonian)

kssform=3

Avoid diago.

If kssform=3, take Kohn-Sham eigenvalues and eigenfunctions from CG minimization algorithm -> choose an appropriate value for tolwfr < 1.0d-3

Screening calculation and the SCR file



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

optdriver

case=3 : susceptibility and dielectric matrix calculation (screening), routine "screening"

npwwfn

Mnemonics: Number of PlaneWaves for WaveFunctioNs

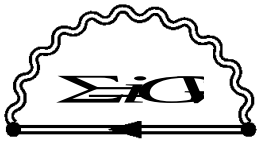
npweps

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

plasfrq

Mnemonics: PLASmon pole FReQuency

Screening calculation



- Informations in the ABINIT output file:

The calculated dielectric constant is printed:

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

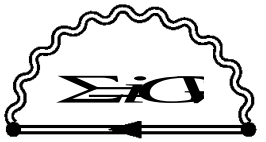
Note that the convergence in the dielectric constant DOES NOT GUARANTEE the convergence in the GW correction values at the end of the calculation.

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 Σ.

Recipe:

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

Self-Energy calculation and GW corrections




```
# 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, routine "sigma"

npwmat

Mnemonics: Number of PlaneWaves for the exchange term MATrix Sigma_x

zcut

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

Parameters and Formulas

- Three step process:

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

2. Dielectric matrix:

$$\epsilon_{\mathrm{G\,G'}}^{\mathrm{RPA}}(\mathrm{q},\omega)=\delta_{\mathrm{G\,G'}}-\mathrm{v}_{\mathrm{G}}(\mathrm{q})\chi_{\mathrm{G\,G'}}^{(0)}(\mathrm{q},\omega)$$

$$\chi_{\mathrm{G\,G'}}^{(0)}(\mathrm{q},\omega)=2\sum_{\mathrm{n,n',k}}(\mathrm{f_{nk}}-\mathrm{f_{n',k+q}})\frac{\langle\phi_{\mathrm{n',k+q}}^{\mathrm{DFT}}|\mathrm{e}^{-\mathrm{i}(\mathrm{q}+\mathrm{G})\mathrm{r}}|\phi_{\mathrm{nk}}^{\mathrm{DFT}}\rangle\langle\phi_{\mathrm{nk}}^{\mathrm{DFT}}|\mathrm{e}^{\mathrm{i}(\mathrm{q}+\mathrm{G'})\mathrm{r}}|\phi_{\mathrm{n',k+q}}^{\mathrm{DFT}}\rangle}{\epsilon_{\mathrm{nk}}^{\mathrm{DFT}}-\epsilon_{\mathrm{n',k+q}}^{\mathrm{DFT}}-\omega-\mathrm{i}\,\delta}$$

3. GW corrections:

$$\epsilon_{\mathrm{nk}}^{\mathrm{QP}}-\epsilon_{\mathrm{nk}}^{\mathrm{DFT}}=\langle\phi_{\mathrm{nk}}^{\mathrm{DFT}}|\Sigma(\mathrm{r},\mathrm{r'},\omega)-\mathrm{v}_{\mathrm{xc}}(\mathrm{r})|\phi_{\mathrm{nk}}^{\mathrm{DFT}}\rangle$$

$$\langle\phi_{\mathrm{i}}^{\mathrm{DFT}}|\Sigma_{\mathrm{x}}|\phi_{\mathrm{j}}^{\mathrm{DFT}}\rangle=-\frac{4\pi}{\mathrm{V_{cryst}}}\sum_{\mathrm{i}}^{\mathrm{occ}}\sum_{\mathrm{G}}\frac{\rho_{\mathrm{ij}}^{2}(\mathrm{G})}{|\mathrm{q}+\mathrm{G}|^{2}}$$ ω-independent, only occupied states

$$\langle\phi_{\mathrm{j}}^{\mathrm{DFT}}|\Sigma_{\mathrm{c}}|\phi_{\mathrm{j}}^{\mathrm{DFT}}\rangle=\frac{2\pi}{\mathrm{V_{cryst}}}\sum_{\mathrm{i}}\sum_{\mathrm{G\,G'}}\frac{\rho_{\mathrm{ij}}^{*}(\mathrm{G})}{|\mathrm{q}+\mathrm{G}|}\frac{\rho_{\mathrm{ij}}(\mathrm{G'})}{|\mathrm{q}+\mathrm{G'}|}\frac{\Omega_{\mathrm{G\,G'}}^{2}(\mathrm{q})}{\tilde{\omega}_{\mathrm{G\,G'}}(\mathrm{q})[\omega-\epsilon_{\mathrm{i}}^{\mathrm{DFT}}+\tilde{\omega}_{\mathrm{G\,G'}}(\mathrm{q})(2\mathrm{f_i}-1)]}$$

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

Action of Convergence Parameters into Formulas

k-point grid through $\mathbf{q}=\mathbf{k}_j-\mathbf{k}_i$ in all the following equations

$$\phi_{nk}^{DFT}(r) \overset{FFT}{\Leftarrow} \phi_{nk}^{DFT}(G)$$

npwwfn

$$\epsilon_{GG'}^{RPA}(q,\omega)=\delta_{GG'}-v_G(q)\chi_{GG'}^{(0)}(q,\omega)$$

npweps

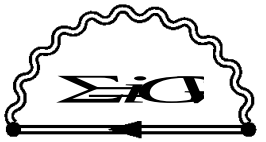
$$\chi_{GG'}^{(0)}(q,\omega)=2\sum_{n,n',k}(f_{nk}-f_{n',k+q})\frac{\langle\phi_{n',k+q}^{DFT}|e^{-i(q+G)r}|\phi_{nk}^{DFT}\rangle\langle\phi_{nk}^{DFT}|e^{i(q+G')r}|\phi_{n',k+q}^{DFT}\rangle}{\epsilon_{nk}^{DFT}-\epsilon_{n',k+q}^{DFT}-\omega-i\delta}$$

nband

$$\langle\phi_j^{DFT}|\Sigma_c|\phi_j^{DFT}\rangle=\frac{2\pi}{V_{cryst}}\sum_i\sum_{GG'}\frac{\rho_{ij}^*(G)}{|q+G|}\frac{\rho_{ij}(G')}{|q+G'|}\frac{\Omega_{GG'}^2(q)}{\tilde{\omega}_{GG'}(q)[\omega-\epsilon_i^{DFT}+\tilde{\omega}_{GG'}(q)(2f_i-1)]}$$

npwmat

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



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

All in one input

```
 ndtset      3

# KSS calculation
 nbandkss1   -1       npwkss1    0


# SCR calculation
 optdriver2  3        getkss2    -1                          → _KSS file
 nband2     10        npweps2    27        npwwfn2    27       generated
                                                               by previous
                                                               data set

# sigma and GW corrections calculation
 optdriver3  4        getkss3    -2        geteps3    -1 → _SCR file
 nband3      10       npwmat3    27        npwwfn3    27       generated
 ngwpt3      1                                                 by previous
 kptgw3      0.250  0.750  0.250                               data set
 bdgw3       4  5
```

The result

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
```

DFT eigenvalues

Exchange term

Correlation term

Self-Energy Interaction

XC potential from DFT

GW corrections

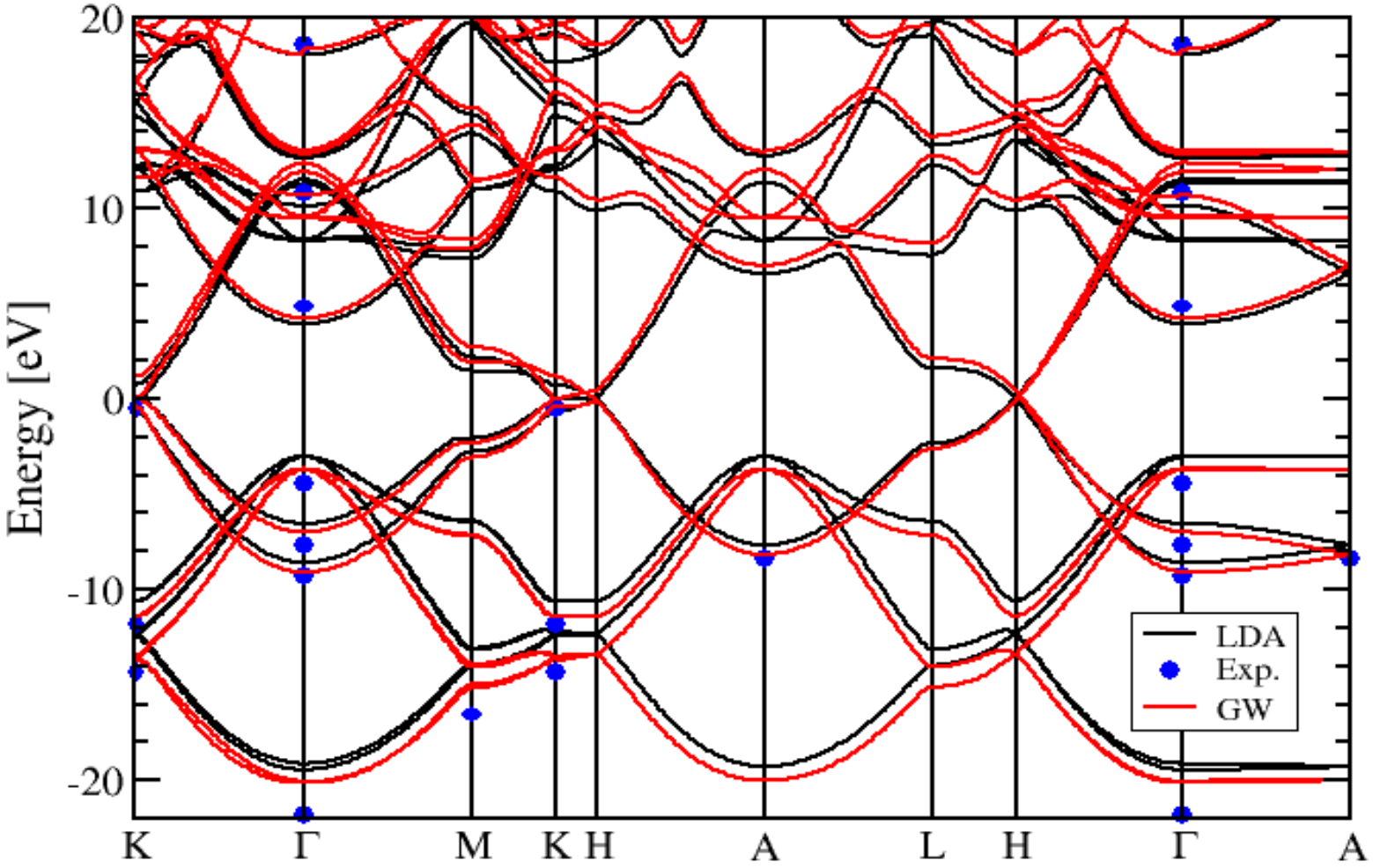
GW and the Photoemission Gap

	DFT-LDA	GW	EXP
Silicon	0.55	1.19	1.17
Diamond	4.26	5.64	5.48
MgO	5.3	7.8	7.83

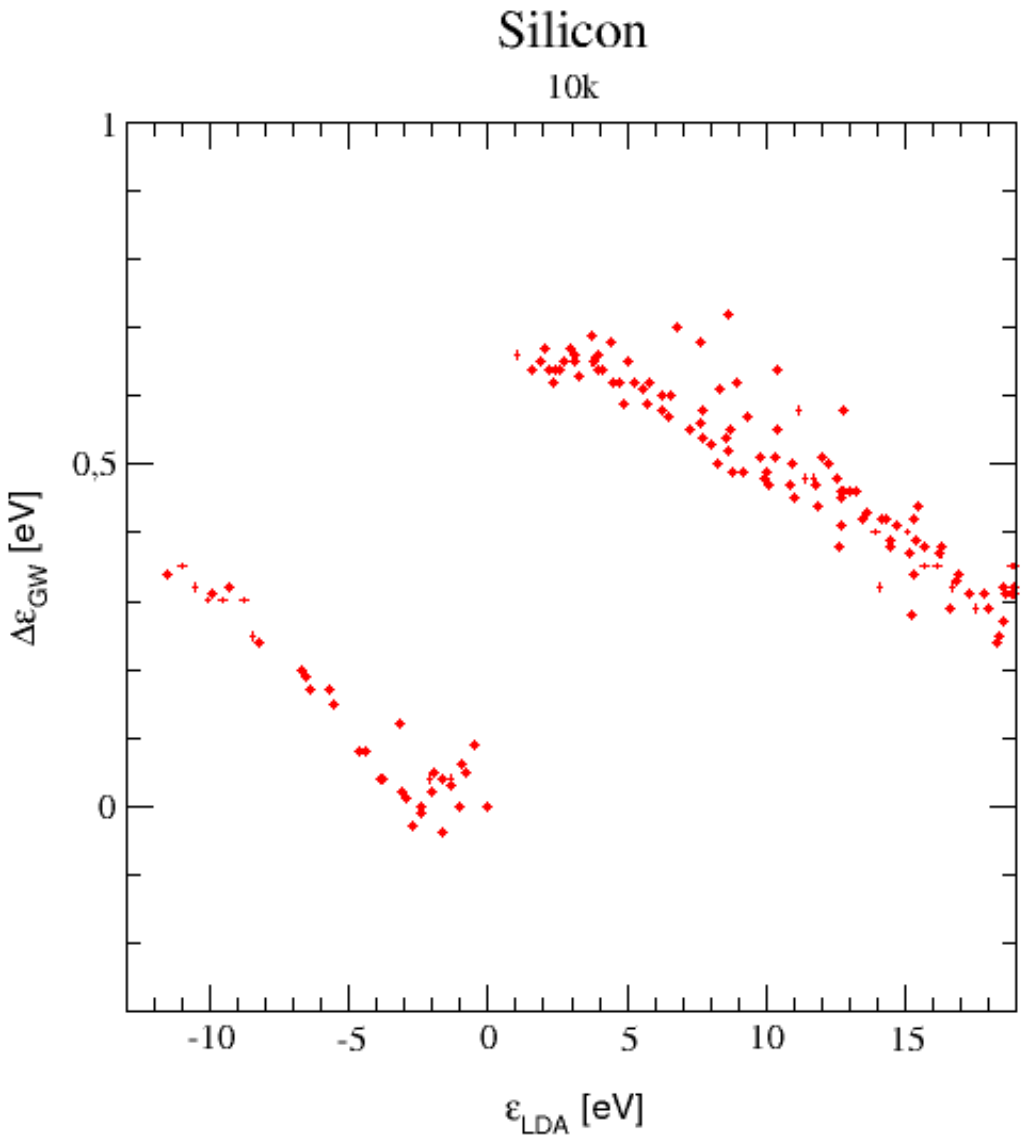
- The GW Approximation corrects the LDA band-gap problem (underestimation) and it is in good agreement with the Experiment.
- The GW Approximation correctly predicts electron Addition/Removal excitations (Photoemission Spectroscopy).

GW band plot

Graphite

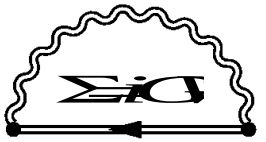


GW corrections interpolation



To calculate a full band plot one can use interpolatation.

New Features



nomegasrd maxomegasrd

Mnemonics: Number of OMEGAs to evaluate Sigma Real axis Derivatives, MAX OMEGA to evaluate Sigma Real axis Derivatives.
Fine tuning of the parameters related to the calculation of the renormalization factor Z.

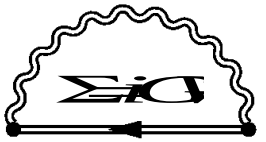
soenergy

Mnemonics: Scissor Operator ENERGY
first step of self-consistency on W (use SO corrected eigenvalues).
One can also use an out.gw file got from a previous GW calculation
by renaming it in.gw.

gwcalctype

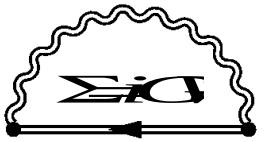
Mnemonics: GW CALCulation TYPE
switch between Godby and Hybertsen-Louie Plasmon-Pole-Models

Future Developments



- full treatment of non-symmorphic operations: done but to be integrated!
- parallelization (at least on q-points for screening, and on kptgw for sigma)
- other XC functionals (already implemented in ABINIT): done!
- allow the use of non-diagonalized KS eigenfunctions: done!
- Allow different PP models: done!
- NetCDF: to be integrated.

Future Developments



- introduction of the spin degree of freedom
- calculation of the GW total energy: done but never integrated.
- calculation of a real GW band plot through automatic generation of the needed k-grids: waiting for improvements in the KS part.
- full screening (beyond plasmon-pole) and lifetimes
- vertex corrections and GWGamma
- update of the eigenvalues (self-consistency): done!
- update of the wavefunctions (1^{st} order) and of the energy (2^{nd} order): off-diagonal elements of Σ

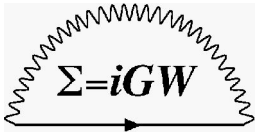
Know problems, bugs, or limitations

- allow higher angular momentum projectors (mproj/=1)
- proper treatment of the case lim q→0, G=0 in screening for space groups other than FCC

Conclusions

- The use of the GW part is still quite limited.
- The GW part still needs much work to be really user-friendly (example: automatic band-plot).
- New complex features, which require beyond a x.3 ABINIT version time to be developed, present difficulties to be integrated.

GW theory: Off-diagonal Elements



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

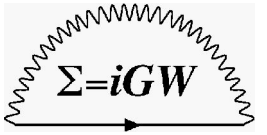
$$\psi^{QP}_{n,\sigma,\mathbf{k}} = \psi^{DFT}_{n,\sigma,\mathbf{k}} + \sum_{n' \neq n} \alpha_{n,n',\sigma,\mathbf{k}} \psi^{DFT}_{n',\sigma,\mathbf{k}} \quad \xrightarrow{\text{usually}} \quad \psi^{QP}_{n,\sigma,\mathbf{k}} \approx \psi^{DFT}_{n,\sigma,\mathbf{k}}$$

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

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

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

GW Theory



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

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

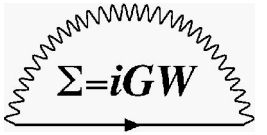
where $\Sigma^{\sigma,\sigma'}$ is the self energy operator $\left(\sigma,\sigma'=\uparrow \text{ or } \downarrow\right)$

Within the GW approximation, it is given by:

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

(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

$$\varepsilon_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega=0) = \delta_{\mathbf{G},\mathbf{G}'} - v(\mathbf{q}+\mathbf{G}')\,\chi^{\uparrow}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega=0) - v(\mathbf{q}+\mathbf{G}')\,\chi^{\downarrow}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega=0)$$

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

Dynamic Dielectric Matrix ← Generalized Plasmon Pole model

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