Tutorial on dynamical self-energy and spectral functions

Lorenzo Sponza

Dynamical self-energy (GW self-energy)

The QSGW loop passes through a dynamical self-energy: the GW self-energy

$$H^{QSGW}_{ij\mathbf{k}} = H^{LDA}_{ij\mathbf{k}} + \Delta V^{xc}_{ij\mathbf{k}}$$

$$\varepsilon_{i\mathbf{k}} \; ; \; \psi_{i\mathbf{k}}$$

RPA polarizability

$$\chi(\mathbf{r},\mathbf{r}',t) = -iG(\mathbf{r},\mathbf{r}',t)G(\mathbf{r}',\mathbf{r},-t)$$

RPA screened Coulomb

$$W(\mathbf{r},\mathbf{r}',t) = \left(1 - v\chi\right)^{-1} v$$

quasiparticlization

$$\Delta V^{xc}_{ij\mathbf{k}} = V^{xc,LDA}_{ij\mathbf{k}} - \frac{1}{2}\mathrm{Re}\left[\Sigma^{GW}_{ij\mathbf{k}}(\varepsilon_{i\mathbf{k}}) + \Sigma^{GW}_{ij\mathbf{k}}(\varepsilon_{j\mathbf{k}})\right]$$

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

GW self-energy: **exchange term dynamically screened by polarization processes**

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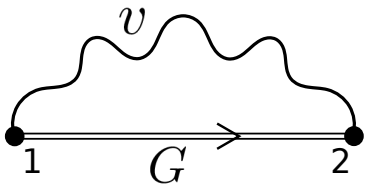
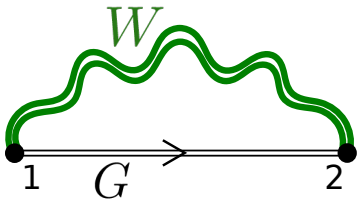
GW self-energy: **exchange term dynamically screened by polarization processes**

Fock operator
Only exchange
bare Coulomb



GW self-energy
Exchange + Correlation
dynamically screened Coulomb



A dynamical theory

Stop at converged QSGW cycle:

$$H_{ij\mathbf{k}} \equiv H^{QSGW}_{ij\mathbf{k}}$$

$$= H^{0}_{ij\mathbf{k}} + V^{xc,LDA}_{ij\mathbf{k}} + \Delta V^{xc}_{ij\mathbf{k}}$$

Static Hamiltonian
Mean-field theory (the best possible)
Independent-particle Green's function

$$\mathcal{E}_{i\mathbf{k}}$$

Energies are independent-particle levels (quasiparticles)
Can be visualized and interpreted as a **band structure**

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Make a step furhter and compute GW self-energy

$$H_{ij\mathbf{k}}(\omega) \equiv H^{0}_{ij\mathbf{k}} + \Sigma^{GW}_{ij\mathbf{k}}(\omega)$$

Dynamical Hamiltonian
Many-body theory (RPA)
Interacting Green's function

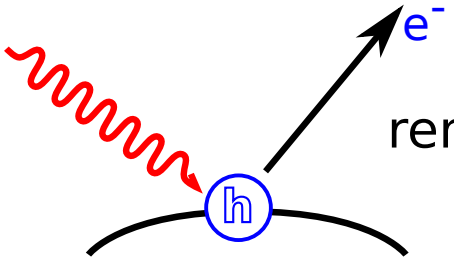
$$E_{i\mathbf{k}}(\omega)$$

What are energies in this case?
How do we visualise them?

Spectral functions

Spectral function
structures at poles of G

$$A(\omega) = \frac{1}{\pi} |\mathrm{Im}G(\omega)|$$



Photoemission
removal energy (hole creation)

Static Hamiltonian
IP-like G

$$A^{\mathrm{IP}}(\omega) = 1/\left(\omega - E^{\mathrm{IP}}\right)$$

delta peak

$A(\omega)$

ω

E^{IP}

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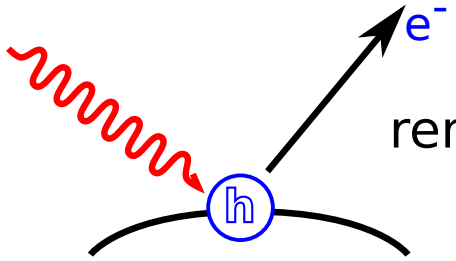

Photoemission
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Dynamic self-energy
Many Body G

$$A^{\mathrm{MB}}(\omega) = 1/\left(\omega - E^{\mathrm{IP}} - \Sigma(\omega)\right)$$

Static Hamiltonian
IP-like G

$$A^{\mathrm{IP}}(\omega) = 1/\left(\omega - E^{\mathrm{IP}}\right)$$

$A(\omega)$

wide structures
satellites
incoherent

delta peak

ω

redistribution of spectral weight
from the QP peak to the satellites
RENORMALIZATION of the IP peak

E^{QP} E^{IP}

quasiparticle correction
to the IP-energy

Spectral functions

Spectral function
structures at poles of G

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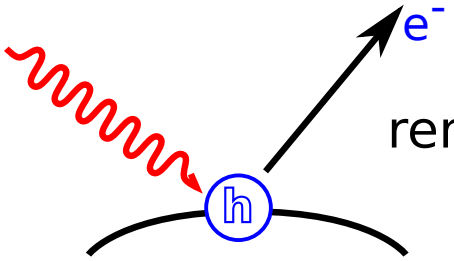

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IP-like G

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$A(\omega)$

wide structures
satellites
incoherent

broadened peak
quasiparticle peak
coherent

delta peak

ω

E^{QP} E^{IP}

redistribution of spectral weight
from the QP peak to the satellites
RENORMALIZATION of the IP peak

quasiparticle correction
to the IP-energy

About renormalization of the IP peak

Independent particle Hamiltonian

$$[H^0 + V^{xc,LDA} + \Delta V^{xc}]\psi^{IP} = \varepsilon\psi^{IP}$$

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Fully interacting Hamiltonian (non-hermitian and dynamical)

$$[H^0 + \Sigma(\omega)]\phi^R(\omega) = E(\omega)\phi^R(\omega)$$

$$\phi^L(\omega)[H^0 + \Sigma(\omega)] = E^*(\omega)\phi^L(\omega)$$

and $G(\omega) = \dfrac{\phi^L\phi^R}{\omega - E(\omega)}$

The Green's function can still be written in Lehman representation, but how to deal with it?

The main contributions from the Green's function come from its poles

$$E(E^{QP}) - E^{QP} = 0$$

quasipartilce approximation

About renormalization of the IP peak

Independent particle Hamiltonian

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quasipartilce approximation

Quasiparticle Hamiltonian

$$[H^0 + \Sigma(E^{QP})]\phi^{QP} = E^{QP}\phi^{QP}$$

Its structure is very similar to an IP Hamiltonian,
but it is a more complicated problem, since the self-energy is computed
at the eigenvalues of the Hamiltonian itself.

About renormalization of the IP peak

$$[H^0 + V^{xc,LDA} + \Delta V^{xc}]\psi^{IP} = \varepsilon\psi^{IP}$$ Independent particle Hamiltonian

$$[H^0 + \Sigma(E^{QP})]\phi^{QP} = E^{QP}\phi^{QP}$$ Quasiparticle Hamiltonian

Perturbative approach:

$$\psi^{IP} = \phi^{QP} \Rightarrow E^{QP} - \varepsilon = \Sigma(E^{QP}) - V^{xc,LDA} - \Delta V^{xc}$$

Non-linear equation!

About renormalization of the IP peak

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⇩

Linearization of the self-energy $\Sigma(E^{QP}) \approx \Sigma(\varepsilon) + \frac{d\Sigma}{d\omega}\Big|_{\omega=\varepsilon}(E^{QP} - \varepsilon)$

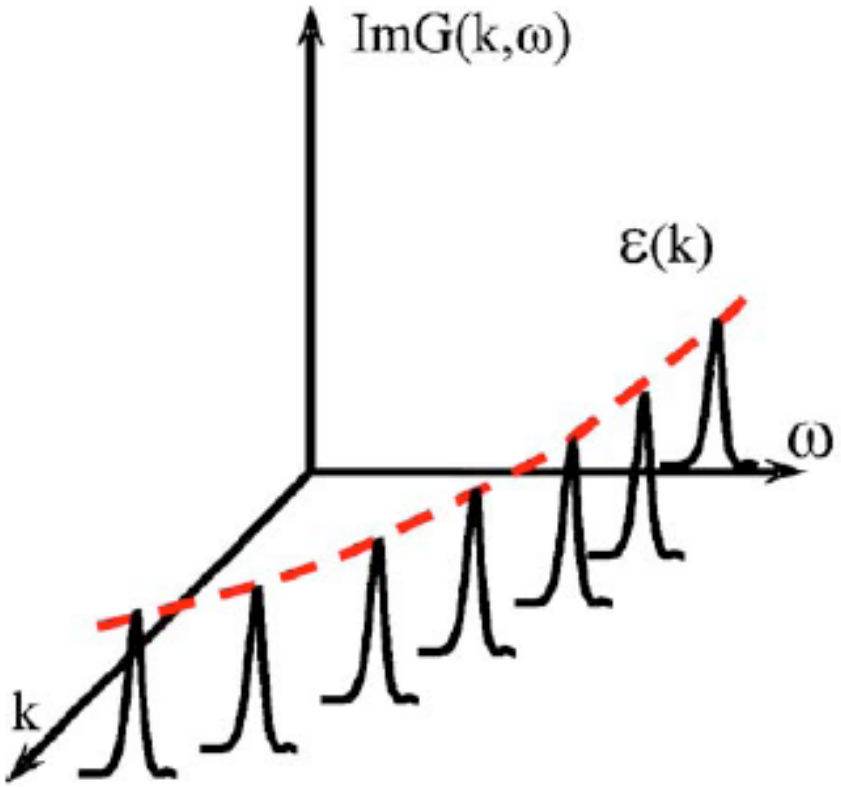
$$E^{QP} = \varepsilon + \mathcal{Z}\left(\Sigma(\varepsilon) - V^{xc,LDA} - \Delta V^{xc}\right)$$ Quasiparticle energies

$$\mathcal{Z} = \frac{1}{1 - d\Sigma/d\omega|_{\omega=\varepsilon}}$$ Renormalization factor

Independent particle energies: band structure

Static Hamiltonian (LDA and QSGW)

In the case of a static Hamiltonian H_{ijk}
(as in DFT or QSGW),
the independent-particle eigenvalues ε_{ik}
are no energy-dependend.
Their dispersion in k gives the **band structure**.



From a Green's function perspective,
one looks at the **spectral function**

$$A(\omega) = \frac{1}{\pi} |\mathrm{Im}G(\omega)|$$

whose poles are related to
addition or removal energies.

Theory	**Spectral function**	**Physical interpretation**
static	poles at ω-ε_{ik} **delta-like peaks**	Addition and removal energies are just the IP-energies. **No additional process** induced.

Interacting many-body self-energy

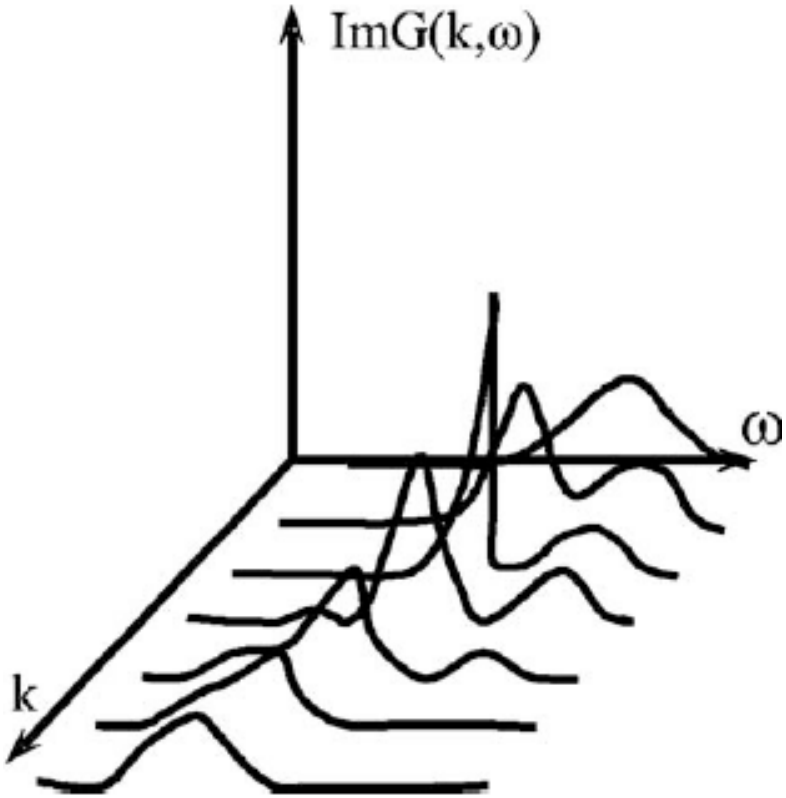
Dynamic Hamiltonian (GW self-energy)

In the case of a dynamic Hamiltonian $H_{ijk}(\omega)$ the eigenvalues $\varepsilon_{ik}(\omega)$ are energy-dependentend. No representation in a band structure scheme is possible.

The **spectral function** has poles where

$$\omega - \varepsilon_{i\mathbf{k}}(\omega) = 0$$

This gives a structured spectral function, depending on the functional form of $\varepsilon_{ik}(\omega)$.



Theory	Spectral function	Physical interpretation
dynamical	poles at ω-$\varepsilon_{ik}(\omega)$ **structured peaks**	Addition and removal energies depends on the many-body interactions. **Additional process** (e.g. plasmons).

Structure of the tutorial: programs and scripts

Be sure to correctly locate the following executables:
hsfp0_om
spectral
lmfgws
and add them in your path!

input files

QSGW loop (Fe)

step 1) Generate the GW self-energy
- text editor (nano, vi ...)
- program hsfp0_om (part of the gw routines in foder code2)

previously computed IP-DOS

step 2) Compare the interacting spectral function with IP-DOS
- spectral
- lmfgws
- text editor + gnuplot or fplot

Step 1: Compute the GW self-energy

Specify the frequency grid

Edit **GWinput** to define the frequency grid where $\Sigma(\omega)$ is to be computed

a) change line

--- Specify qp and band indices at which to evaluate Sigma

into lines

****** ---Specify the q and band indices for which we evaluate the omega dependence of self-energy ---*
0.01 2 (Ry) ! dwplot omegamaxin(optional) : dwplot is mesh for plotting.
: this omegamaxin is range of plotting -omegamaxin to omegamaxin.
: If omegamaxin is too large or not exist, the omegarange of W by hx0fp0 is used.

b) change lines

**** Sigma at all q -->1; to specify q -->0. Second arg : up only -->1, otherwise 0*
0 0

into lines

**** Sigma at all q -->1; to specify q -->0. Second arg : up only -->1, otherwise 0*
1 0

Generate the GW self-energy

run the GW routine hsfp0_om to generate self-energy files

echo '4' | hsfp0_om > out.hsfp0_om (parallel run recommended)

output files: SEComg.UP and **SEComg.DN**

Step 2: Compare spectral function and IP-DOS

1) Correct formatting of the output files

run spectral to set up the information in the right format

spectral --ws --nw=1

mv se se.fe

2) Generate the spectral function

use lmfgws to edit the output files and generate plottable output

```
lmfgws fe --sfuned
  units eV
  readsek
  eps 0.030
  dos isp=1  range=-10,10  nq=32  nw=30
  savesea
  q
```

output file: **sdos.fe**

3) Visualize the spectral function and the IP-DOS

- copy **dosp.fe** (from lm/gwd/test/fe or provided)
- use fplot as described in the web site to plot the content of sdos.fe
  OR edit **sdos.fe** changing 'D' into 'E' and '%' into '#', then plot with gnuplot