GW in productions: algorithms and approximations

Giacomo Sesti

CNRNANO MODENA

MAX DRIVING THE EXASCALE TRANSITION

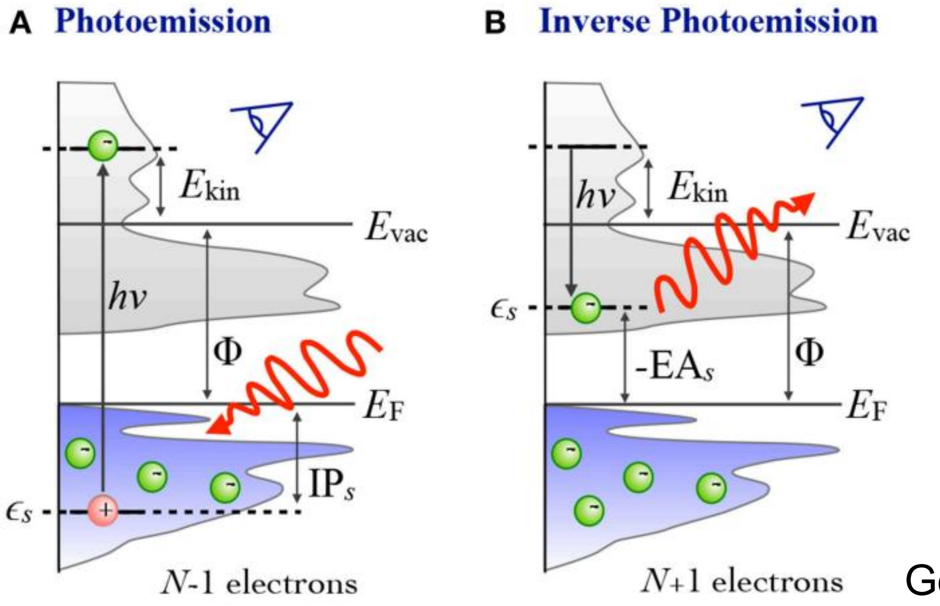
EURO CZECHIA

Why many-body?

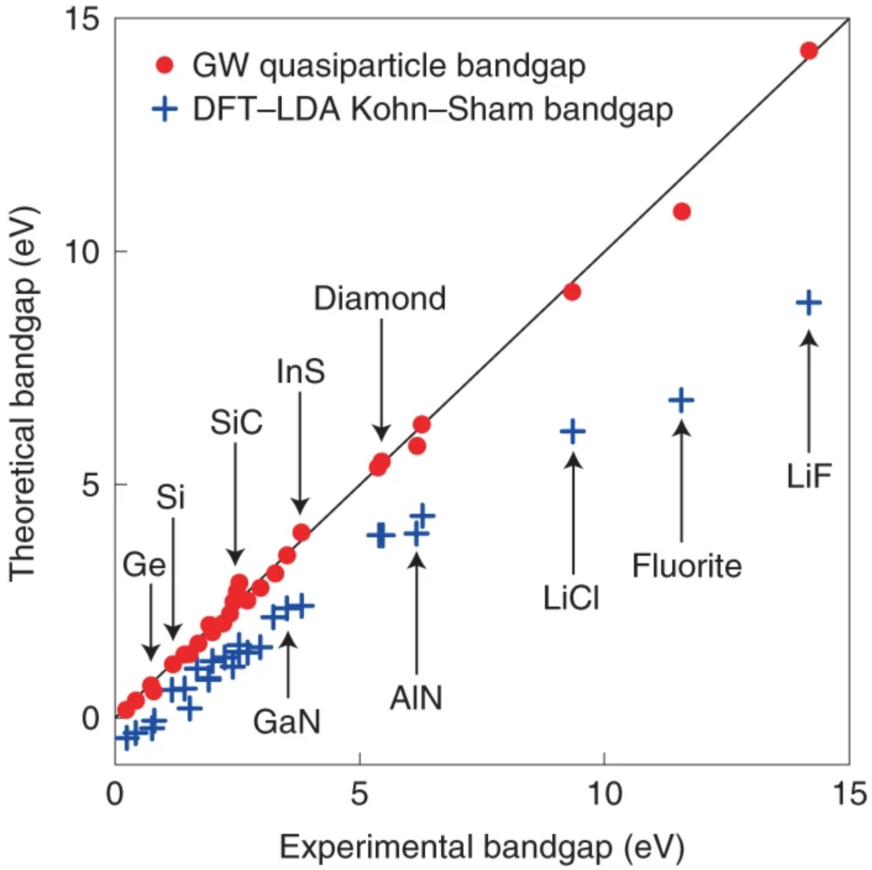
Study of electronic spectroscopy is conceptually limited with DFT:

- band gap problem
- QP underestimated compared to experiments

GW calculations: very close to experiments



Golze et al. Front. Chem. **7** (2019)



Louie *et al. Nat. Mat* 20,728 (2021)

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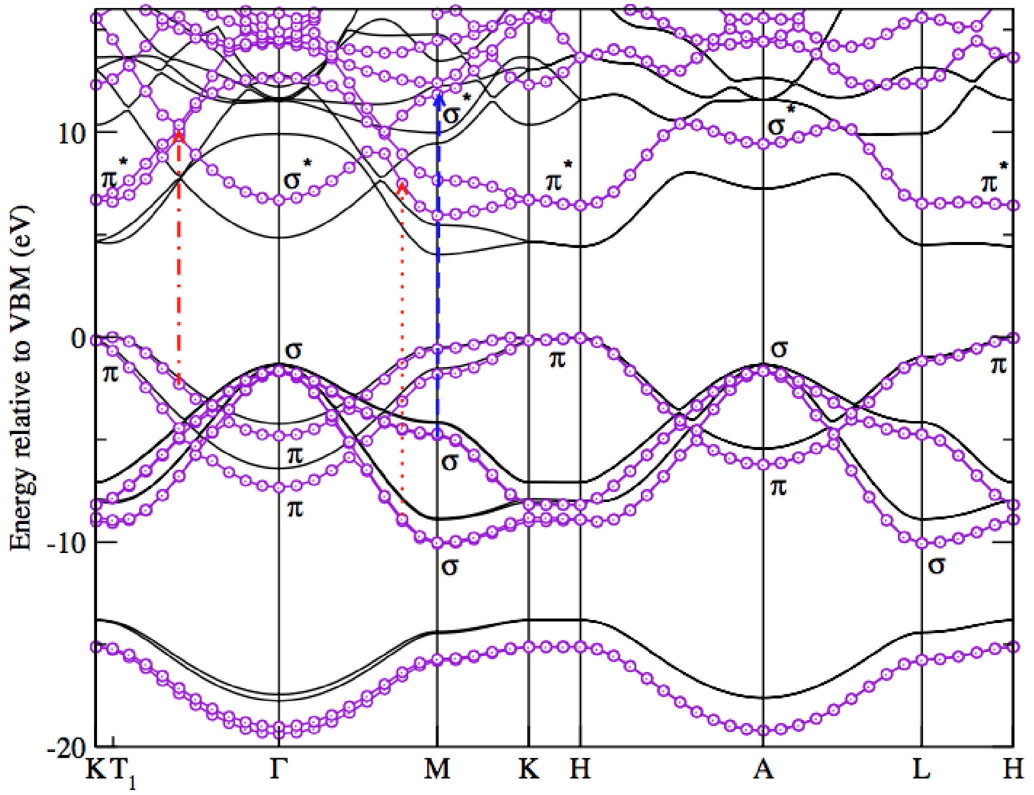

Phys, Rev. Lett. 96, 026402 (2006)

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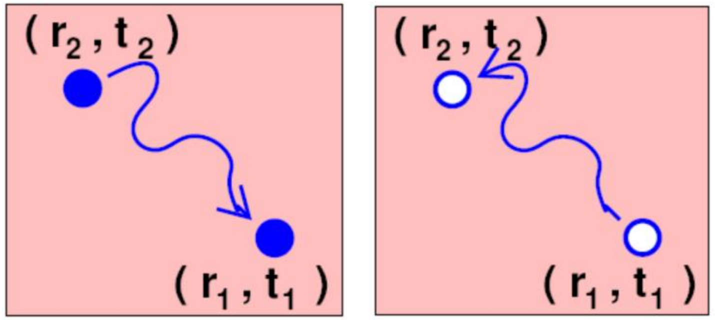

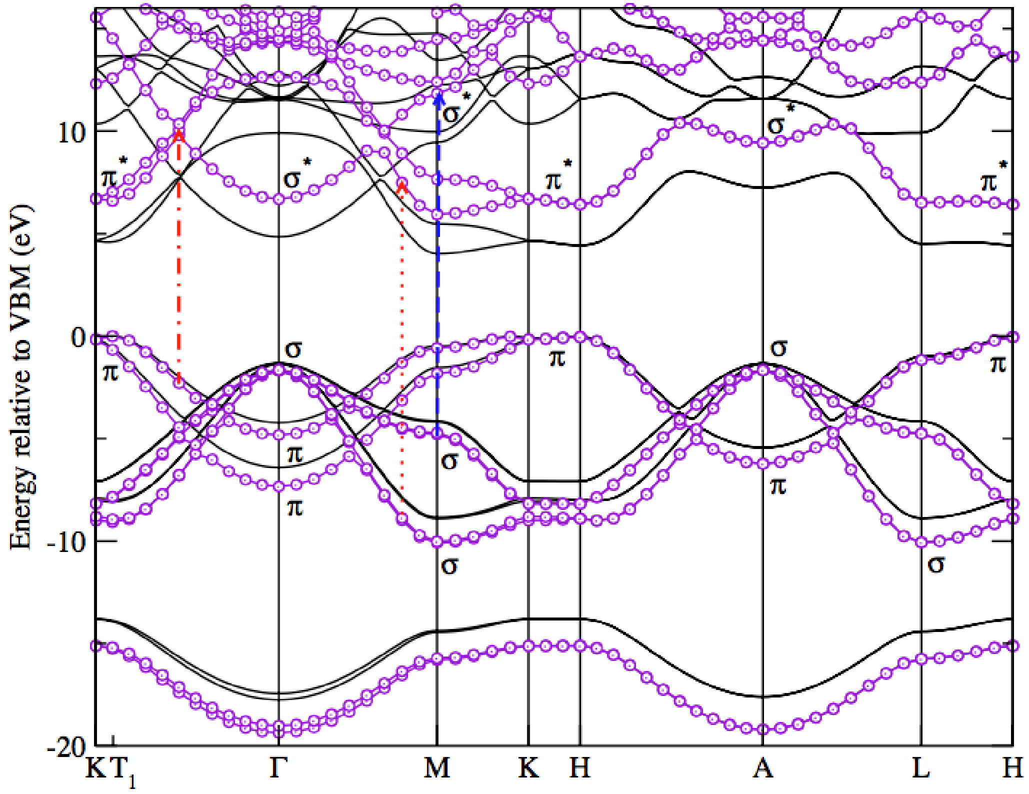

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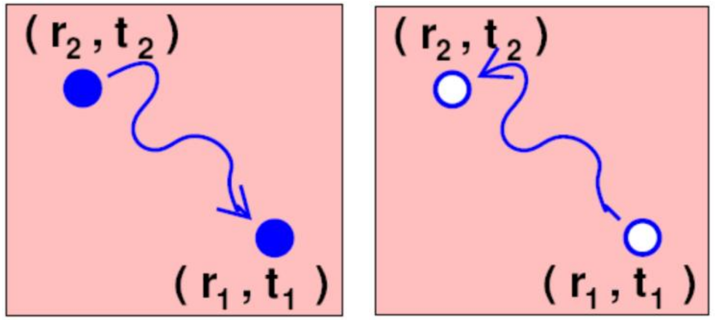

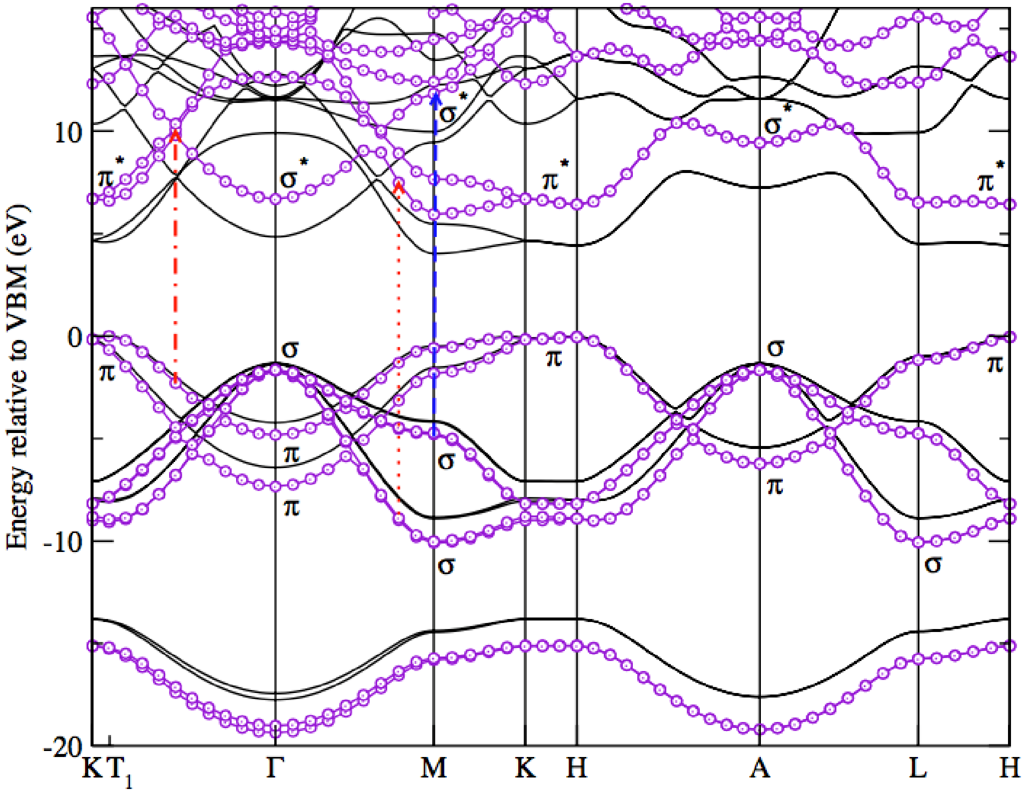

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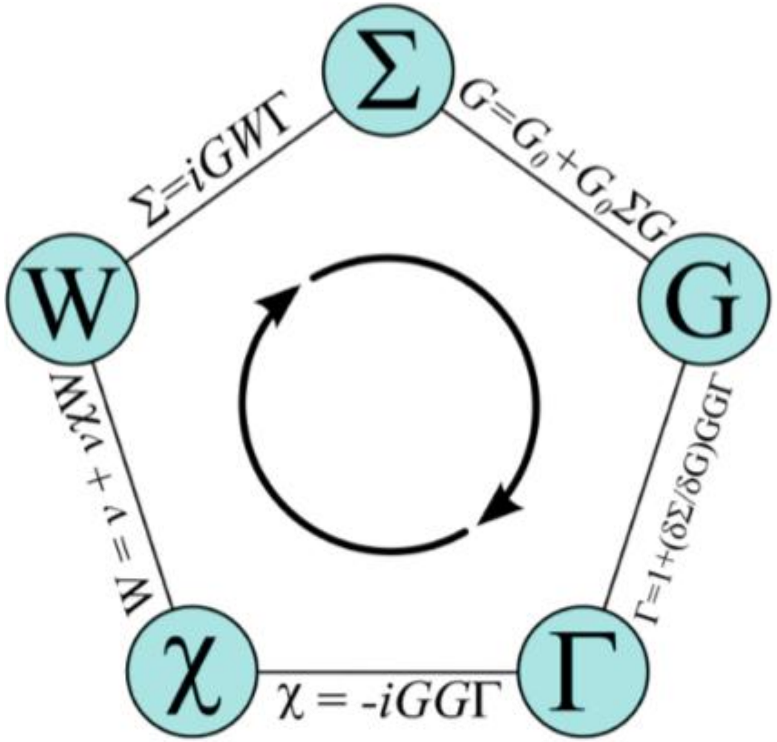
From Hedin's equations to GW

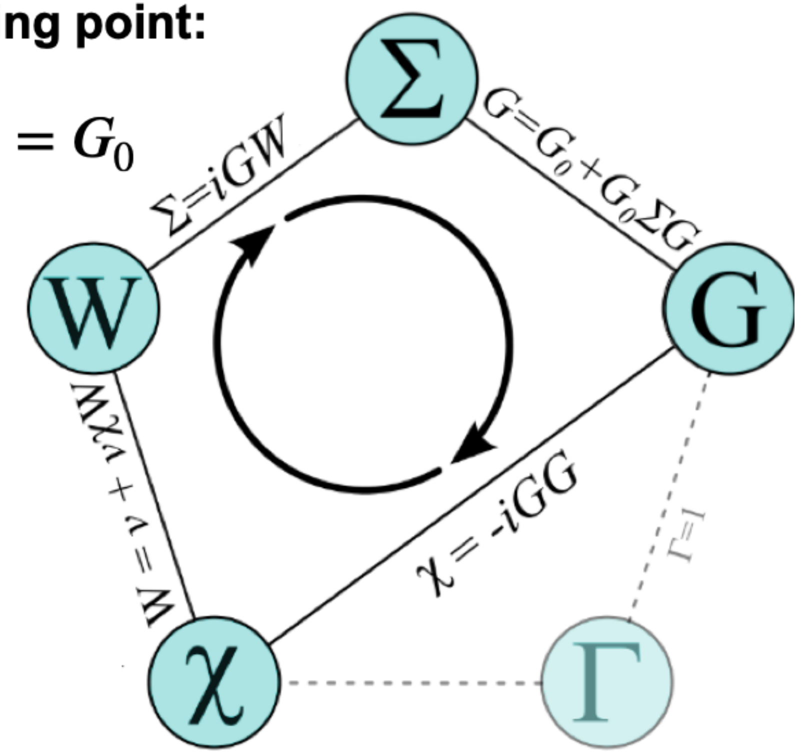
Hedin's



The GW approximation

Starting point:

$G = G_0$



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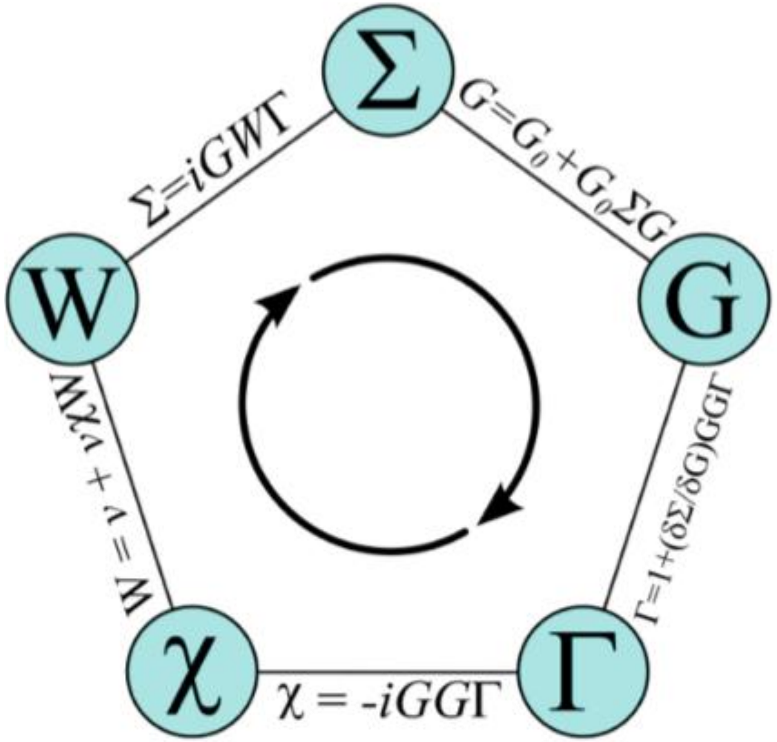

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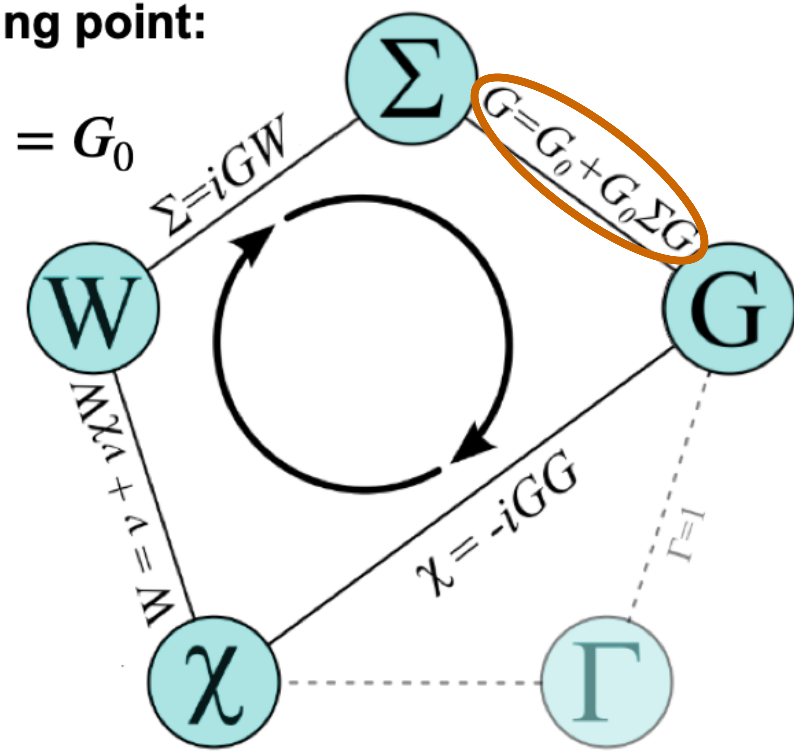

Quasiparticles

DFT :

$$G = G_0 + G_0 \Sigma G$$

The self-energy can be seen as a frequency-dependent potential.
The QP satisfy a pseudo-KS Hamiltonian:

$$\hat{\mathcal{H}}^{\mathrm{KS}} \psi_{n\mathbf{k}} + (\Sigma_{n\mathbf{k}}(E_{n\mathbf{k}}) - v_{xc}) \psi_{n\mathbf{k}} = E_{n\mathbf{k}} \psi_{n\mathbf{k}}$$

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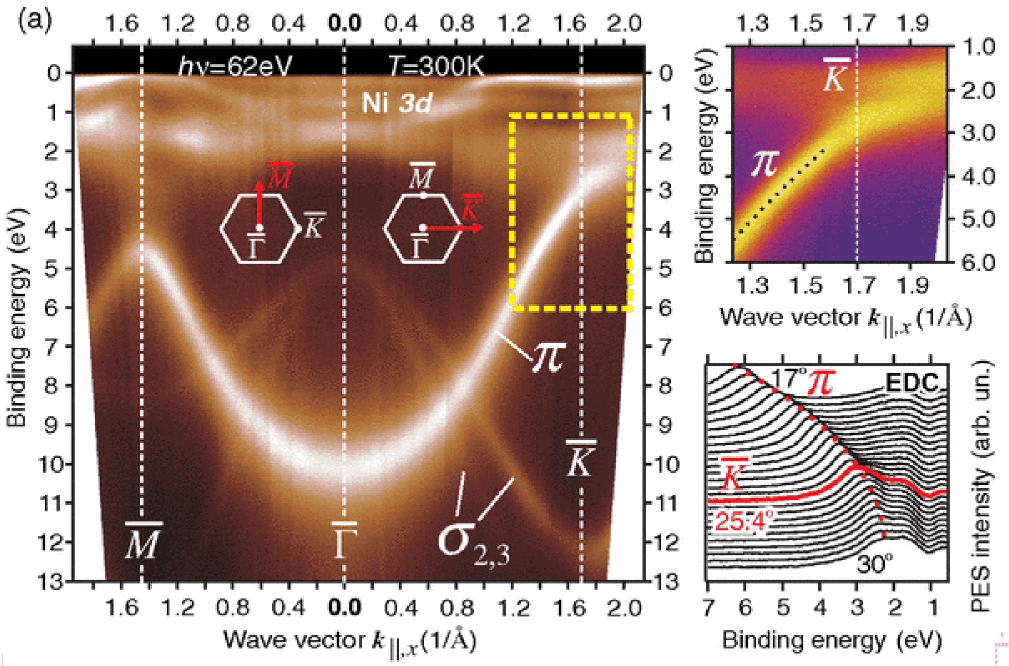
G_0W_0 :

The QP and KS wavefunctions are taken the same:

$$\psi_{n,\mathbf{k}}(\mathbf{r}) \simeq \varphi^{KS}_{n,\mathbf{k}}(\mathbf{r})$$

$$E_{n\mathbf{k}} = \varepsilon^{KS}_{n\mathbf{k}} + \langle \varphi^{KS}_{n\mathbf{k}} | \Sigma(E_{n\mathbf{k}}) - v_{xc} | \varphi^{KS}_{n\mathbf{k}} \rangle$$

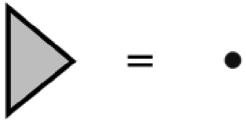
Graphene@Ni



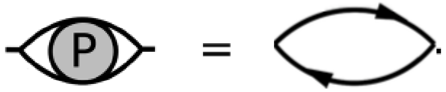
A. Varykhalov, PRX 2, 041017 (2012)

G_0W_0 in a nutshell

$$(1)\quad \Gamma = 1$$

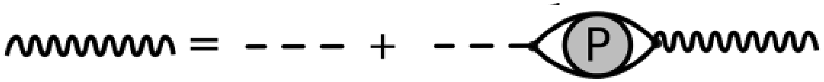


$$(2)\quad \chi_0 = -iG_0G_0$$

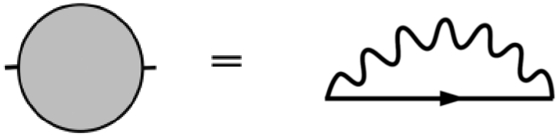


(RPA approximation)

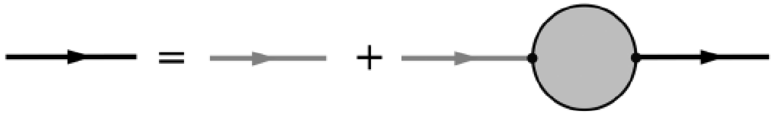
$$(3)\quad W = v + v\chi_0 W$$



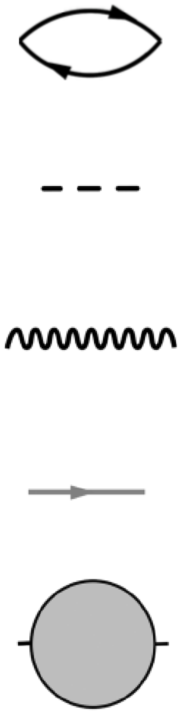
$$(4)\quad \Sigma = iGW$$



$$(5)\quad G = G_0 + G_0\Sigma G$$



Basis set representation



	Plane waves $\{e^{i\mathbf{G}\cdot\mathbf{r}}\}$	Kohn-Sham states $\{\varphi_i\}$
χ_0	$\chi_{0,\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$	$\chi_{0,i,j}(\omega)$
v	$v(\mathbf{q}+\mathbf{G})$	$v_{i,j}^{k,l}$
W	$W_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$	$W_{i,j}^{k,l}(\omega)$
G_0	$G_{0,\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$	$G_{0,i}(\omega)\delta_{i,j}$
Σ	$\Sigma_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$	$\Sigma_{i,j}(\omega)$

N.B. crystal $\rightarrow i = n\mathbf{k}$

Change of base: $\rho_{i,j}(\mathbf{q},\mathbf{G}) = \langle \varphi_{n\mathbf{k}} | e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} | \varphi_{m\mathbf{k}'} \rangle$

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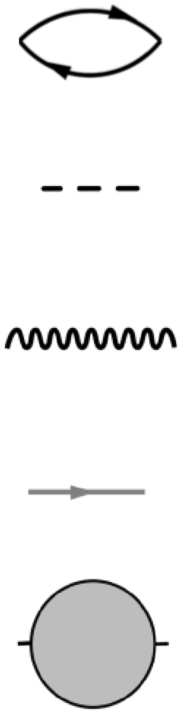

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N.B. crystal → $i = n\mathbf{k}$

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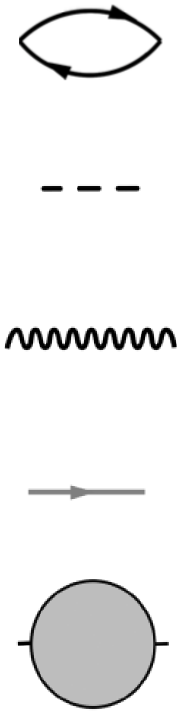

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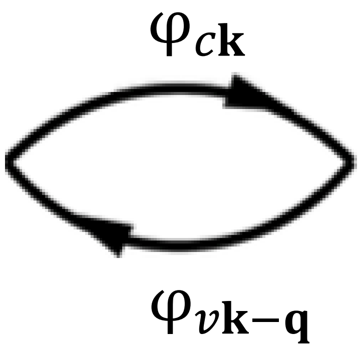
Σ		$\Sigma_i(\omega)\delta_{i,j}$

Convergence of E_{cut}, N_{bnds} is interconnected!

Irreducible polarizability



$$\chi_0 = -iG_0G_0$$

$$\chi_{0,\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = 2\sum_{v,c}\int_{BZ}\frac{d\mathbf{k}}{(2\pi)^3}\rho_{cv\mathbf{k}}(\mathbf{q},\mathbf{G})\rho^*_{cv\mathbf{k}}(\mathbf{q},\mathbf{G}')\left[\frac{1}{\omega+\varepsilon_{v\mathbf{k-q}}-\varepsilon_{c\mathbf{k}}+i\eta}-\frac{1}{\omega+\varepsilon_{c\mathbf{k}}-\varepsilon_{v\mathbf{k+q}}-i\eta}\right]$$

Irreducible polarizability

$\varphi_{c\mathbf{k}}$

$\varphi_{v\mathbf{k}-\mathbf{q}}$

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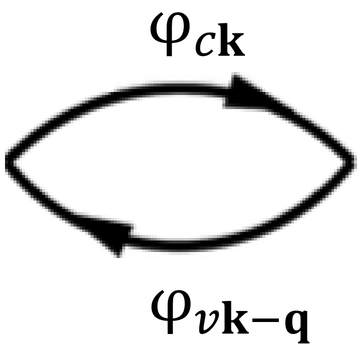
Convergence: N_c E_{cut} N_k

Irreducible polarizability



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$N_{\mathbf{G}} \approx 10^2 - 10^3$

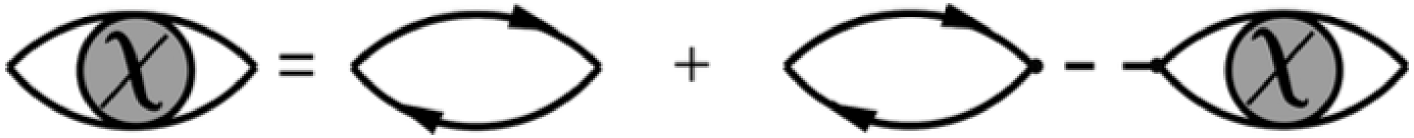
$N_c \approx 10^2$

$N_{\mathbf{k}} \approx 10^2$

Very computational demanding, number of operations scales as: $N_c \times N_{\mathbf{G}}^2 \times N_{\mathbf{k}}^2 \times N_\omega$

Convergence: N_c E_{cut} N_k

Screened interaction W



Reducible polarizability:

$$\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \sum_{\mathbf{G}''} \left[\delta_{\mathbf{G},\mathbf{G}''} - \chi_{0,\mathbf{G},\mathbf{G}''}(\mathbf{q},\omega) v(\mathbf{q}+\mathbf{G}'')\right]^{-1} \chi_{0,\mathbf{G}'',\mathbf{G}'}(\mathbf{q},\omega)$$

Inverse dielectric function:

$$\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \delta_{\mathbf{G},\mathbf{G}'} + v(\mathbf{q}+\mathbf{G})\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$$

Screened interaction:

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

Frequency dependence of W

$$\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \delta_{\mathbf{G},\mathbf{G}'} + v(\mathbf{q}+\mathbf{G})\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$$

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χ_0 and W share the same frequency dependence:
they feature poles at the transition energies: $\Omega_n^{\mathrm{KS}} = \Delta\epsilon_n^{\mathrm{KS}} - i0^+$

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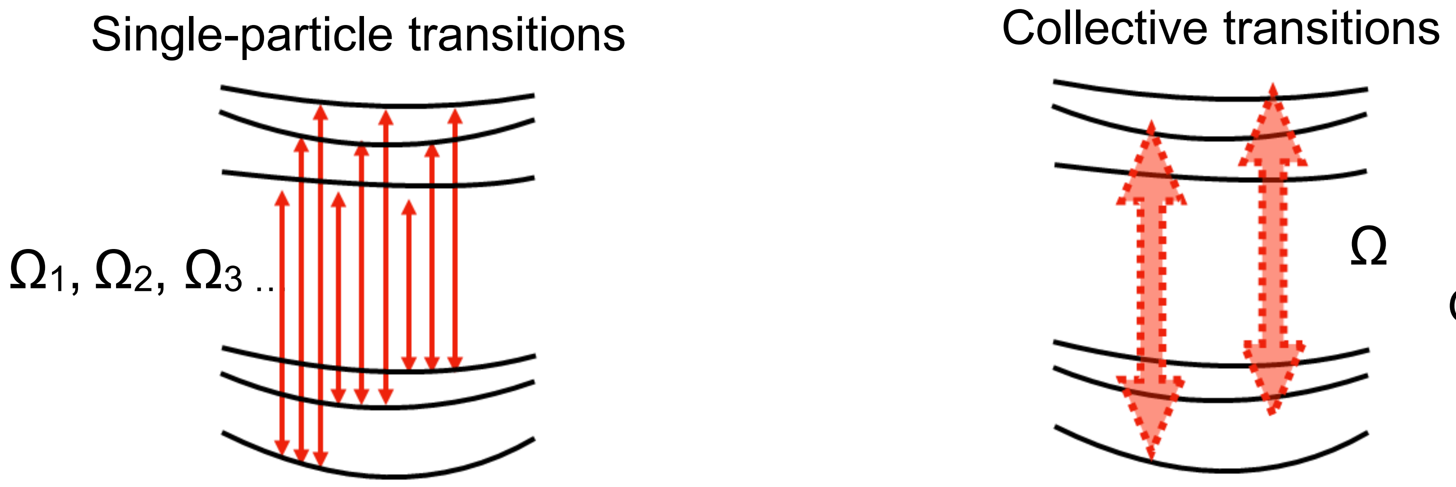
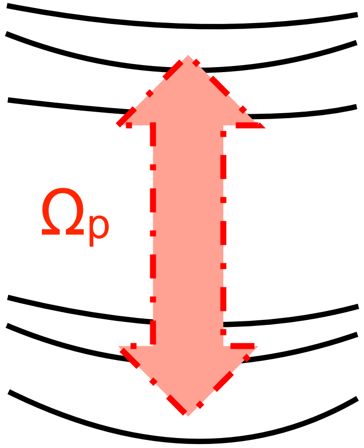


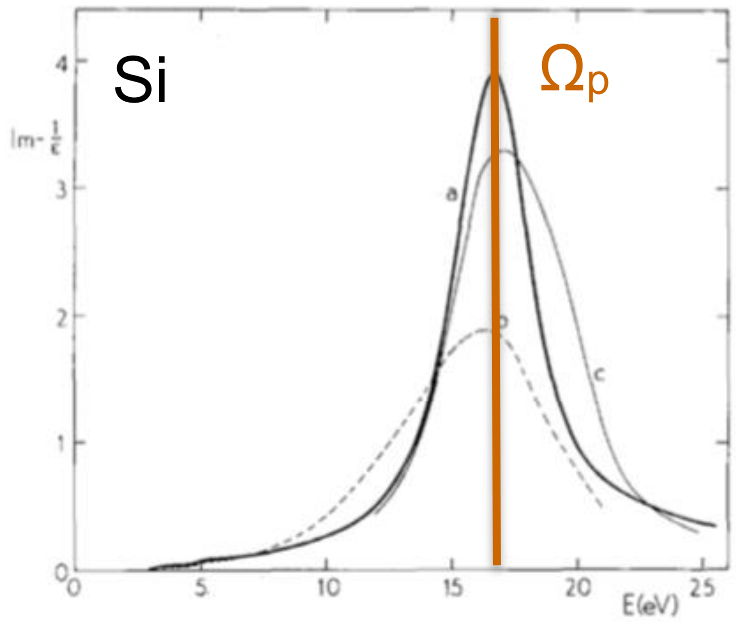
Only most relevant poles included

Frequency dependence of W: the PPA

The plasmon pole approximation (PPA) provides an effective frequency-representation of W



$$EELS(\omega) \propto -\Im \frac{1}{\varepsilon_M(\omega)}$$



J. Stiebling, Z. Physik B 31,355-357 (1978)

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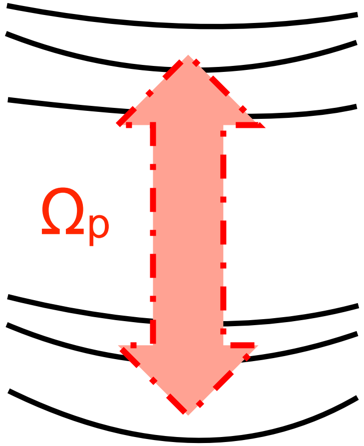

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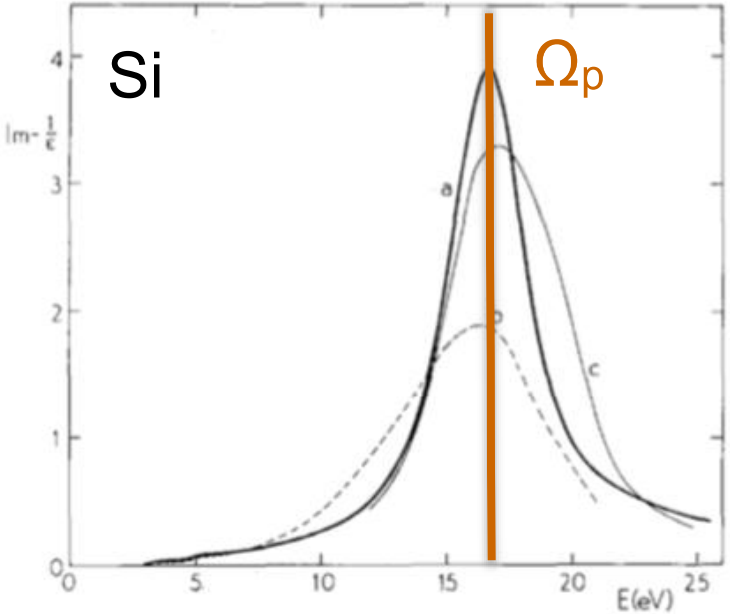

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Hybertsen and Louie, 1986

PPA applied to **all** $\varepsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega)$

Godby and Needs, 1989

$$(R^{GN}, \Omega^{GN}) : \begin{cases} X^{GN}(0) = X(0) \\ X^{GN}(i\varpi_p) = X(i\varpi_p) \end{cases}$$

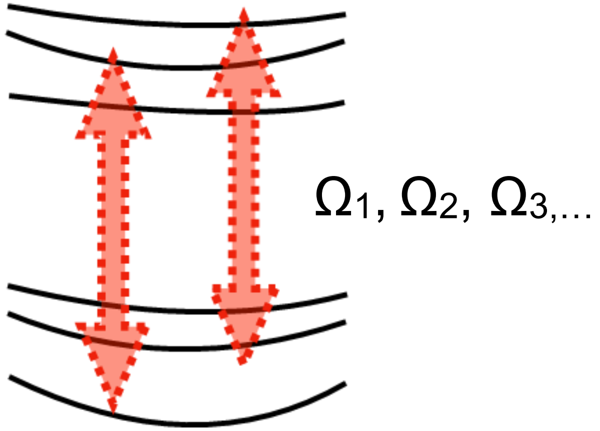
Default: ω_1=0, ω_p=i 1Ha

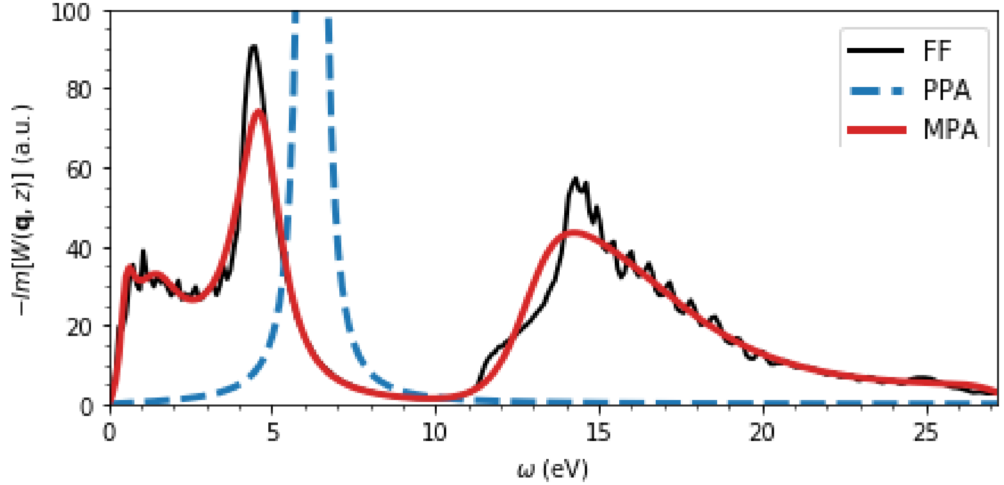
Frequency dependence of W: other methods

Other methods to describe the frequency dependence are available in Yambo:

- **Multipole approximation (MPA)**
  extension of PPA, various collective excitations

- **Real axis integration (FF)**
  describe all single-particle transitions





Guandalini *et al. Phys Rev. B* **109**, 075120 (2024)

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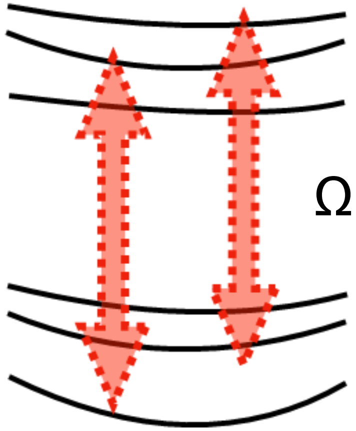

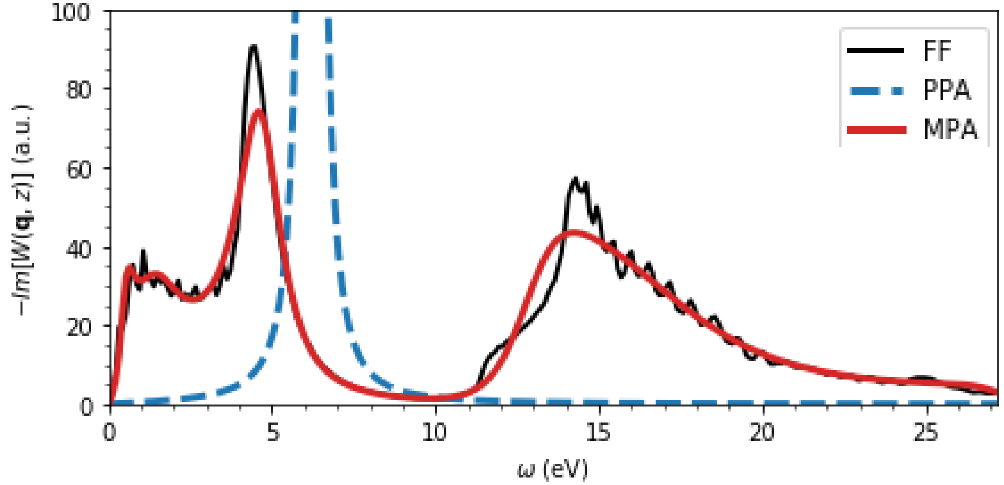

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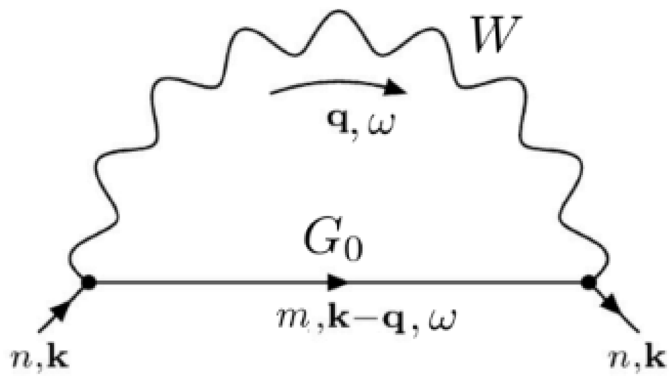
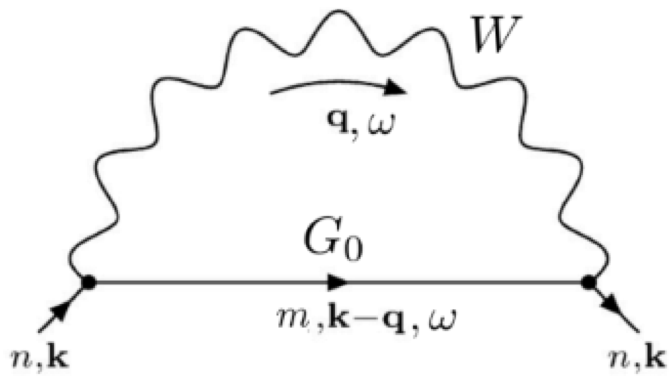
Keep in mind
Computational cost ∝ N(ω)!

The G_0W_0 self-energy



$$\Sigma_{n\mathbf{k}}(\omega) = -\int \frac{d\omega'}{2\pi i} \int \frac{d\mathbf{q}}{(2\pi)^3} \sum_m G_{0,m\mathbf{k}-\mathbf{q}}(\omega+\omega') W^{nn\mathbf{k}}_{mm\mathbf{k}-\mathbf{q}}(\omega')$$

The G_0W_0 self-energy



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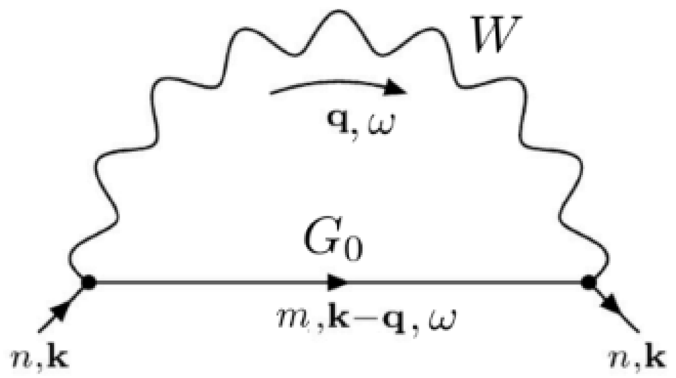
$$G_{0,m\mathbf{k}}(\omega) = \frac{f_{m\mathbf{k}}}{\omega - \varepsilon_{m\mathbf{k}} - i\eta} + \frac{1-f_{m\mathbf{k}}}{\omega + \varepsilon_{m\mathbf{k}} + i\eta}$$

Double integral in momentum and frequency

$$W^{nn\mathbf{k}}_{mm\mathbf{k}-\mathbf{q}}(\mathbf{q},\omega) = \sum_{\mathbf{G}\mathbf{G}'} \rho^*_{nm\mathbf{k}}(\mathbf{q}+\mathbf{G}) W_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) \rho_{nm\mathbf{k}}(\mathbf{q}+\mathbf{G}')$$

The G_0W_0 self-energy



$$\Sigma_{n\mathbf{k}}(\omega) = \Sigma^x_{n\mathbf{k}} + \Sigma^c_{n\mathbf{k}}$$

$$W = v + W^c$$

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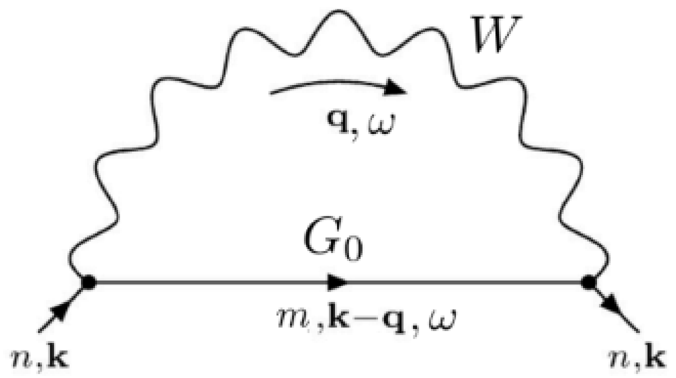
The G_0W_0 self-energy



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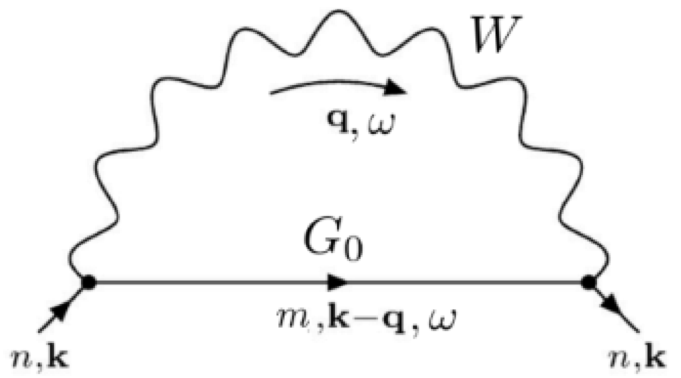
$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_m \sum_{\mathbf{G}\mathbf{G}'} \int \frac{d\mathbf{q}}{(2\pi)^3} \rho^*_{nm\mathbf{k}}(\mathbf{q}+\mathbf{G}) W^c_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) \rho_{nm\mathbf{k}}(\mathbf{q}+\mathbf{G}')$$

Analytical espression provided by the method used (PPA for instance)

The G_0W_0 self-energy: PPA



$$\Sigma_{n\mathbf{k}}(\omega) = \Sigma^x_{n\mathbf{k}} + \Sigma^c_{n\mathbf{k}}$$

$$W = v + W^c$$

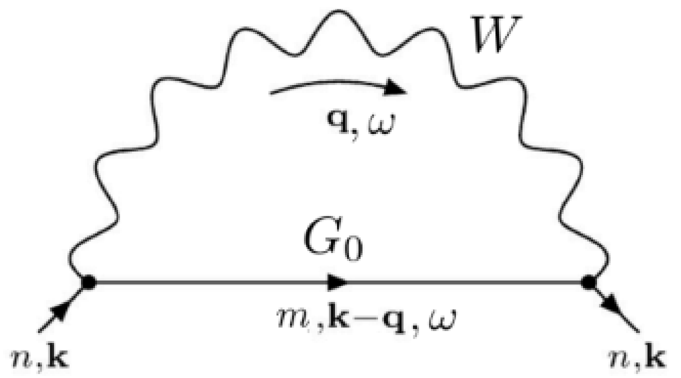
$$\Sigma^x_{n\mathbf{k}} = -\sum_v \sum_{\mathbf{G}} \int \frac{d\mathbf{q}}{(2\pi)^3} v(\mathbf{q}+\mathbf{G}) |\rho_{nv\mathbf{k}}(\mathbf{q}+\mathbf{G})|^2$$

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_m \sum_{\mathbf{G}\mathbf{G}'} \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{\rho^*_{nm\mathbf{k}}(\mathbf{q}+\mathbf{G}) R_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) \rho_{nm\mathbf{k}}(\mathbf{q}+\mathbf{G}')}{\omega + [\Omega_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) + i\eta]\,\mathrm{sgn}(\mu - \varepsilon_{m\mathbf{k}-\mathbf{q}}) - \varepsilon_{m\mathbf{k}-\mathbf{q}}}$$

plasmon residue

plasmon energy

The G_0W_0 self-energy: PPA



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Convergence:

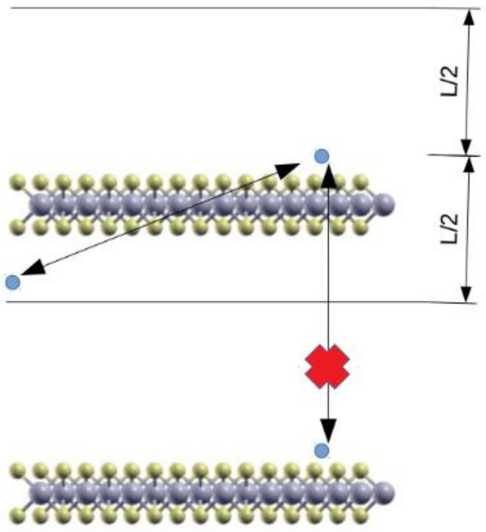
- N_c
- E_{cut}
- N_k

The k-point convergence

The k-point requirements in GW usually traces to the long-range interaction:

$$v(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

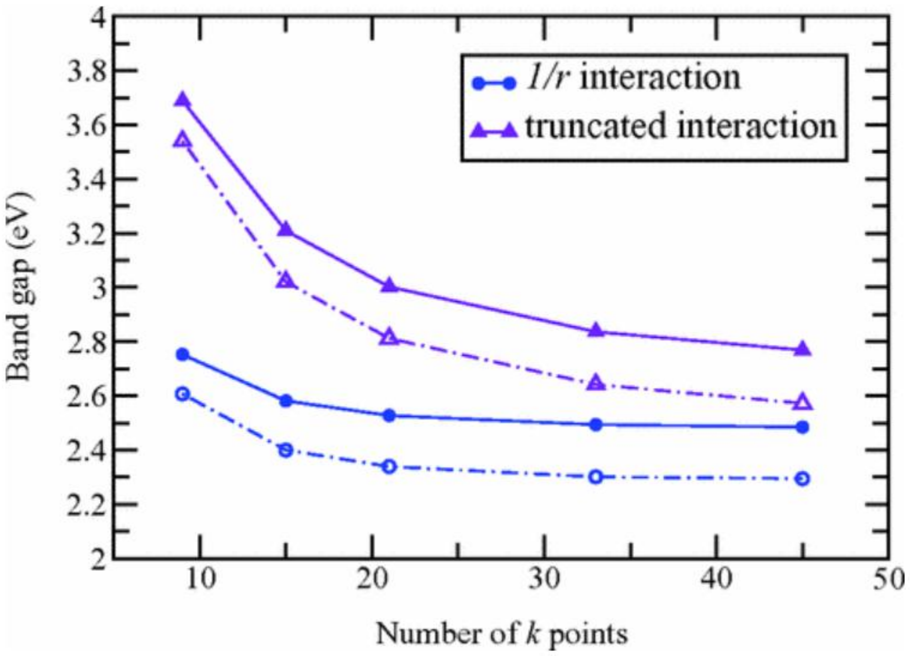
2D systems are particularly critical



Truncated Coulomb potential:

$$v^{\mathrm{slab}}(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{\Theta(L/2 - |z_1 - z_2|)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

MoS_2 (G_0W_0)



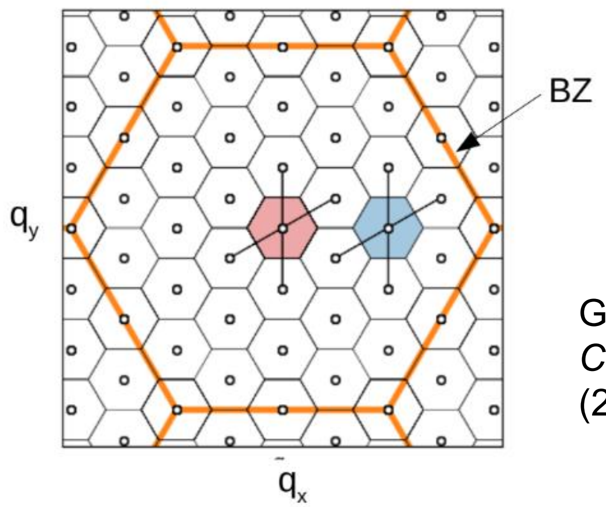
Hüser F. et al. *Phys. Rev. B* **88**, 245309 (2013)

The k-point convergence

Improved treatments of the Coulomb potential are available in Yambo:

V-average method:

- Regularises the q→0 limit of the Coulomb potential
- It acts on the whole of $\Sigma_{n\mathbf{k}}$



Guandalini et al. *npj Comput. Mat.* **9,** 44 (2023)

The k-point convergence

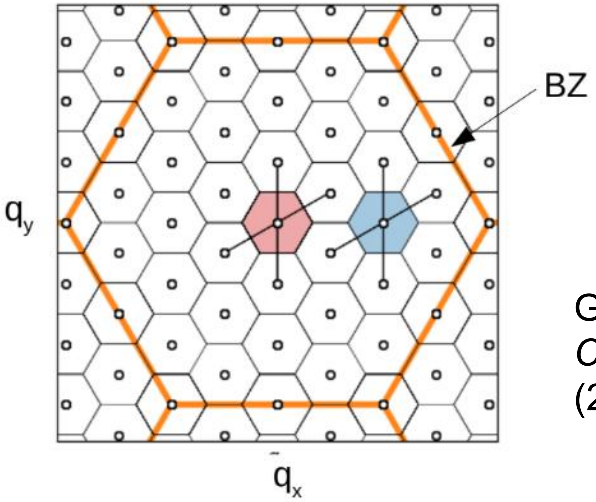
Improved treatments of the Coulomb potential are available in Yambo:

V-average method:

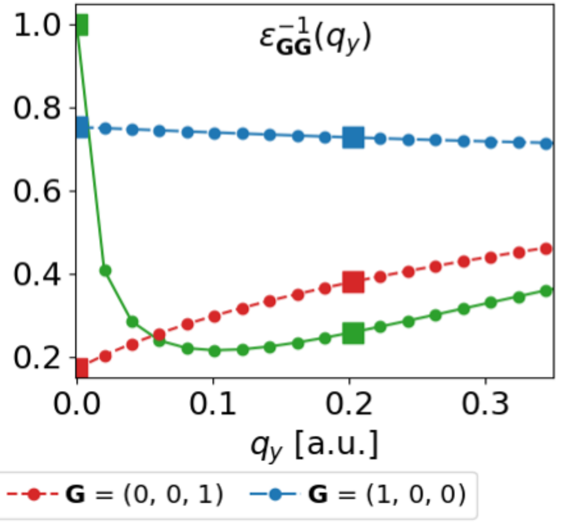
- Regularises the q→0 limit of the Coulomb potential
- It acts on the whole of $\Sigma_{n\mathbf{k}}$

W-average method:

- Regularises the q→0 limit of the screened Coulomb potential
- It acts just inside $\Sigma^{c}_{n\mathbf{k}}$, suggested for the cases where ε^{-1} is not piecewise linear in **q**



Guandalini et al. *npj Comput. Mat*. **9,** 44 (2023)



How to calculate QPs

$$G = G_0 + G_0 \Sigma G$$

Quasi-particles' energies determined self-consistently:

$$E_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}} + \langle \varphi_{n\mathbf{k}} | \Sigma(E_{n\mathbf{k}}) - v_{xc} | \varphi_{n\mathbf{k}} \rangle$$

Linearization enforced (Newton's method):

$$E_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}} + Z_{n\mathbf{k}} \langle \varphi_{n\mathbf{k}} | \mathrm{Re}\Sigma(\varepsilon_{n\mathbf{k}}) - v_{xc} | \varphi_{n\mathbf{k}} \rangle$$

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Renormalization factors

$$Z_{n\mathbf{k}} = \left[1 - \left. \frac{d\ \mathrm{Re}\Sigma_{n\mathbf{k}}}{d\omega} \right|_{\omega = \varepsilon_{n\mathbf{k}}} \right]^{-1}$$

by finite differences with $\Delta\omega = 0.1$ eV
(Σ evaluated at 2 frequencies)

The G$_0$W$_0$ method in one slide

DFT: $\{\varepsilon_{n\mathbf{k}}\}$, $\{\psi_{n\mathbf{k}}\}$

$$G_{0,n\mathbf{k}}(\omega) = \frac{f_{n\mathbf{k}}}{\omega - \varepsilon_{n\mathbf{k}} - i\eta} + \frac{1 - f_{n\mathbf{k}}}{\omega + \varepsilon_{n\mathbf{k}} + i\eta}$$

$$\chi_{0,\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = 2\sum_{v,c}\int_{BZ}\frac{d\mathbf{k}}{(2\pi)^3}\rho_{cv\mathbf{k}}(\mathbf{q},\mathbf{G})\rho^*_{cv\mathbf{k}}(\mathbf{q},\mathbf{G}')\left[\frac{1}{\omega + \varepsilon_{v\mathbf{k}-\mathbf{q}} - \varepsilon_{c\mathbf{k}} + i\eta} - \frac{1}{\omega + \varepsilon_{c\mathbf{k}} - \varepsilon_{v\mathbf{k}+\mathbf{q}} - i\eta}\right]$$

$$\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \sum_{\mathbf{G}''}\left[\delta_{\mathbf{G},\mathbf{G}''} - \chi_{0,\mathbf{G},\mathbf{G}''}(\mathbf{q},\omega)v(\mathbf{q}+\mathbf{G}'')\right]^{-1}\chi_{0,\mathbf{G}'',\mathbf{G}'}(\mathbf{q},\omega)$$

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

$$\Sigma^x_{n\mathbf{k}} = -\sum_{v}\sum_{\mathbf{G}}\int\frac{d\mathbf{q}}{(2\pi)^3}v(\mathbf{q}+\mathbf{G})|\rho_{nv\mathbf{k}}(\mathbf{q}+\mathbf{G})|^2$$

$$E_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}} + Z_{n\mathbf{k}}\langle\varphi_{n\mathbf{k}}|\mathrm{Re}\Sigma(\varepsilon_{n\mathbf{k}}) - v_{xc}|\varphi_{n\mathbf{k}}\rangle$$

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{m}\sum_{\mathbf{G}\mathbf{G}'}\int\frac{d\mathbf{q}}{(2\pi)^3}\rho^*_{nm\mathbf{k}}(\mathbf{q}+\mathbf{G})W^c_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega)\rho_{nm\mathbf{k}}(\mathbf{q}+\mathbf{G}')$$

The G_0W_0 method in one slide

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$$G_{0,n\mathbf{k}}(\omega) = \frac{f_{n\mathbf{k}}}{\omega - \varepsilon_{n\mathbf{k}} - i\eta} + \frac{1 - f_{n\mathbf{k}}}{\omega + \varepsilon_{n\mathbf{k}} + i\eta}$$

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$$\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \sum_{\mathbf{G}''}\left[\delta_{\mathbf{G},\mathbf{G}''} - \chi_{0,\mathbf{G},\mathbf{G}''}(\mathbf{q},\omega)v(\mathbf{q}+\mathbf{G}'')\right]^{-1}\chi_{0,\mathbf{G}'',\mathbf{G}'}(\mathbf{q},\omega)$$

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Conclusions

Approximations used:

GW+RPA screening

G_0W_0
(No self-consistency)

Plasmon pole approximation (PPA)

Newton's solution for the QPs