The GW approximation: band structures and more

Lucia Reining
Palaiseau Theoretical Spectroscopy Group

The GW approximation: band structures and more

→ Why do we need Green's functions?

→ From Green's functions to observables

→ A new auxiliary world

→ Impact of (dynamical) screening

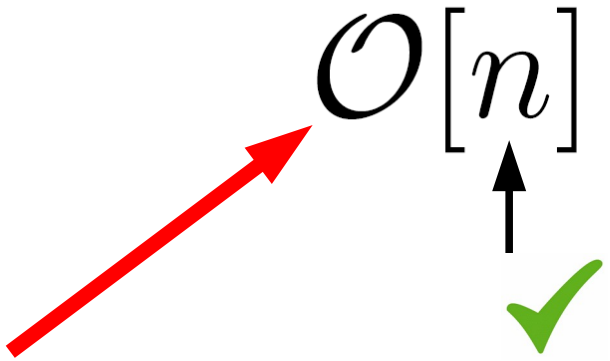
→ Flavours of the GWA

→ What is wrong, and outlook

Density functional theory

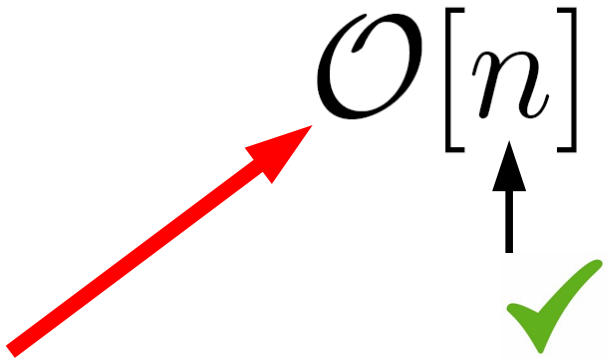
$$\mathcal{O}[n]$$

Density functional theory



And where do we get this functional from ?

Density functional theory



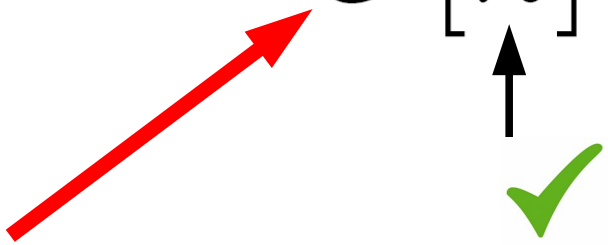
And where do we get this functional from ?

Very often: we do not know

→ we calculate observables in the KS system

Density functional theory

$$\mathcal{O}[n]$$



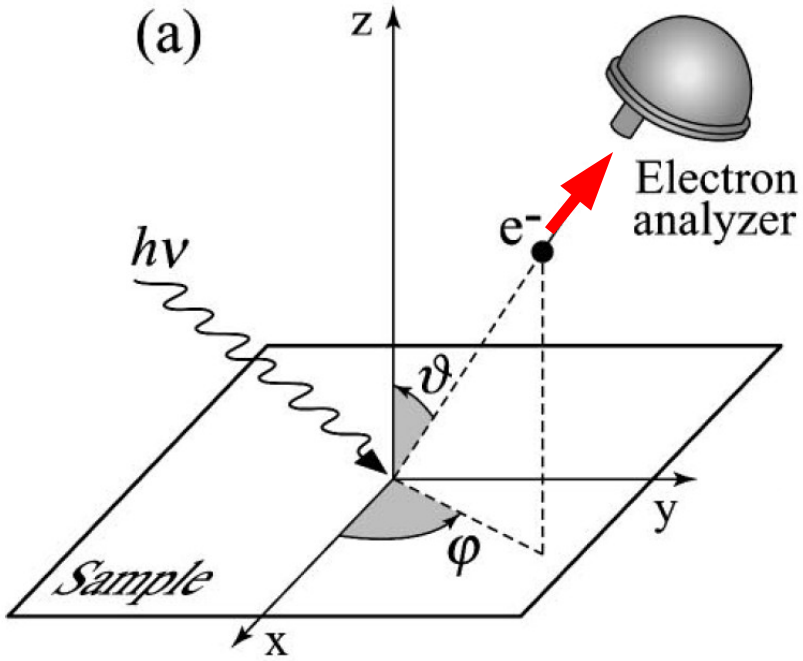
And where do we get this functional from ?

Very often: we do not know

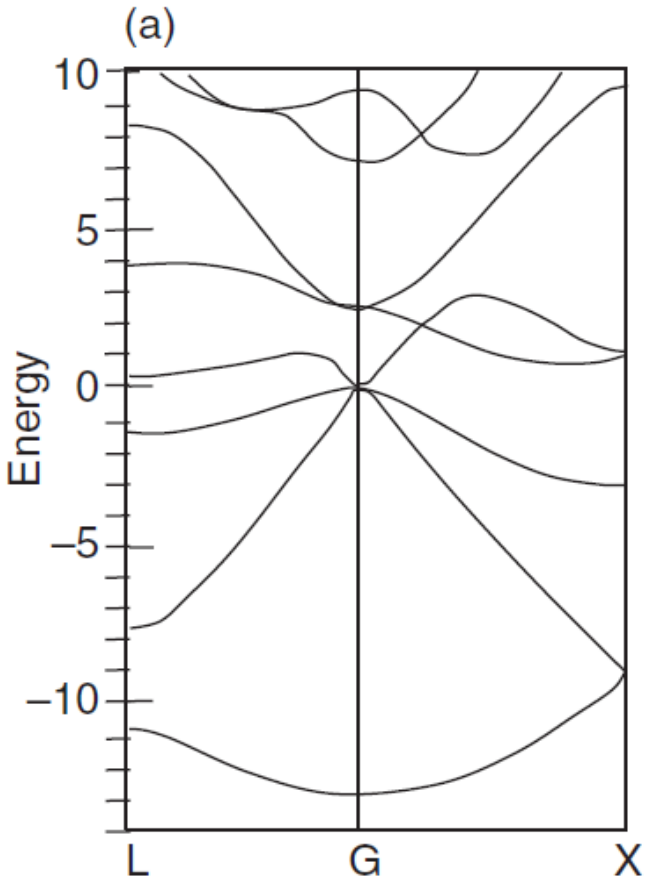
→ we calculate observables in the KS system

(This can be seen as approximate functional)

Can we use this approximation for photoemission spectra?



Photoemission geometry



From Damascelli et al., RMP 75, 473 (2003)

+.....

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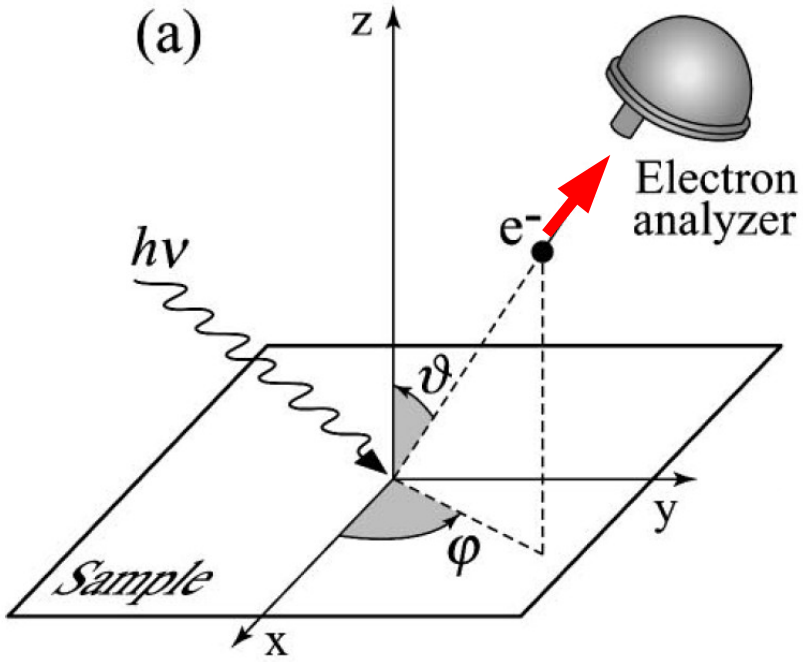

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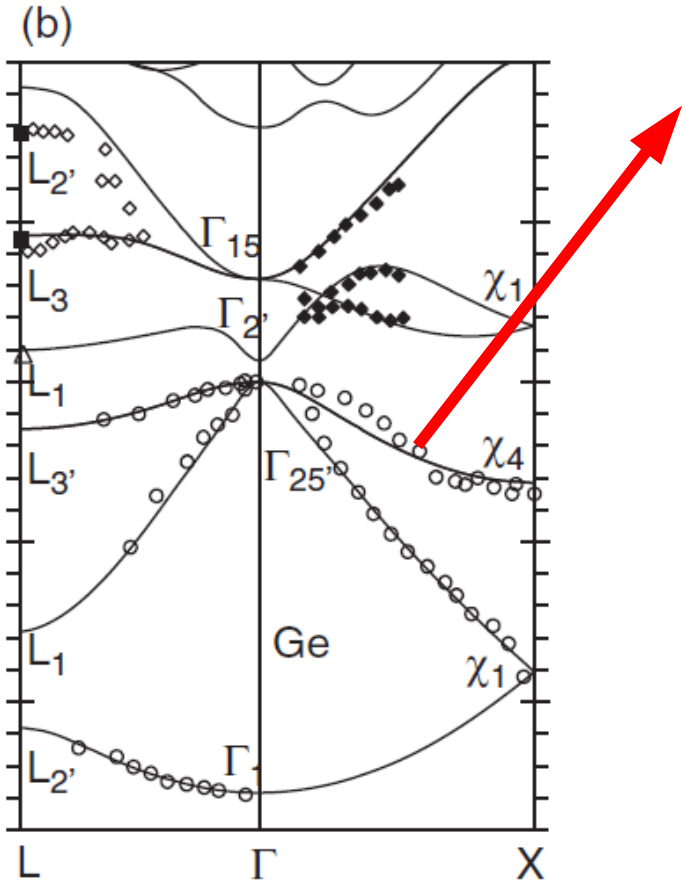

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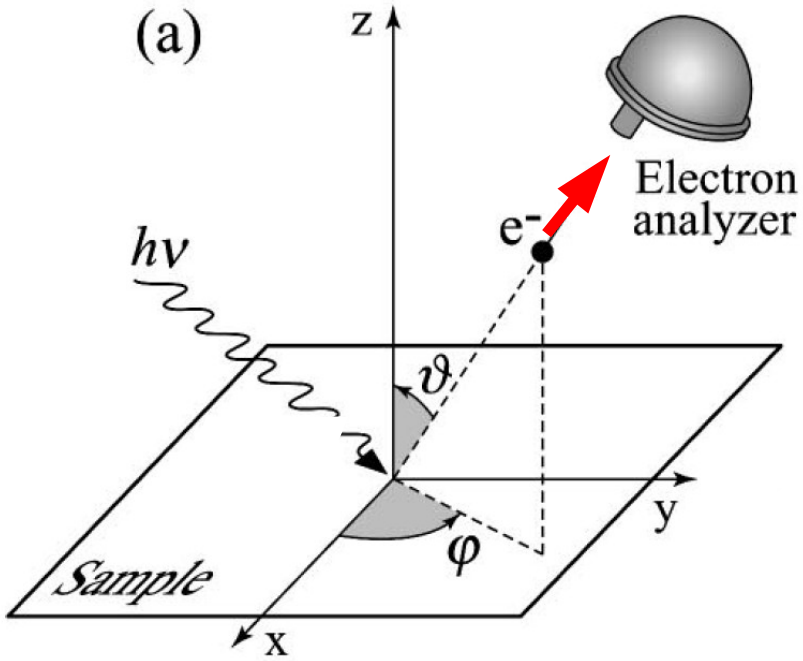

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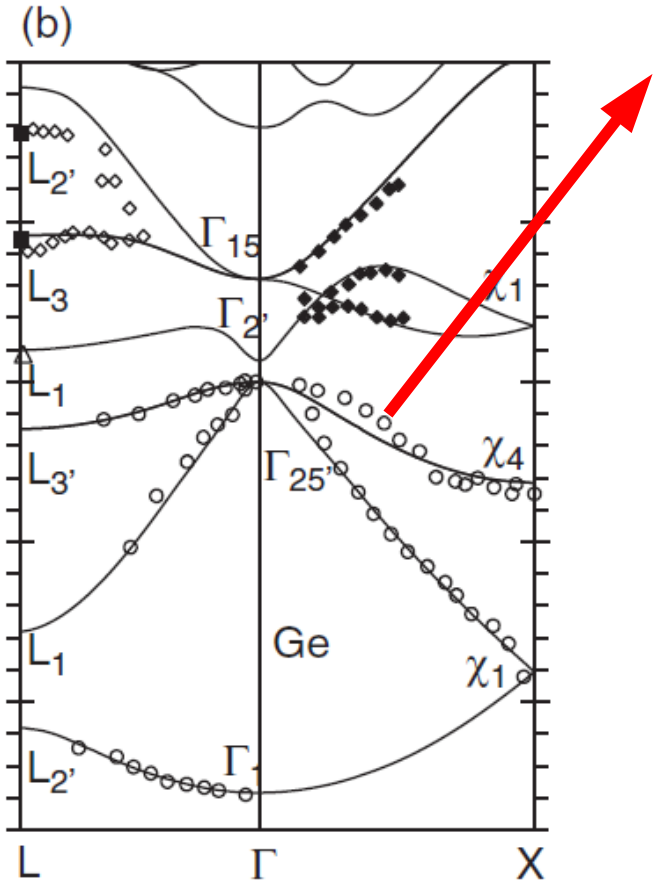

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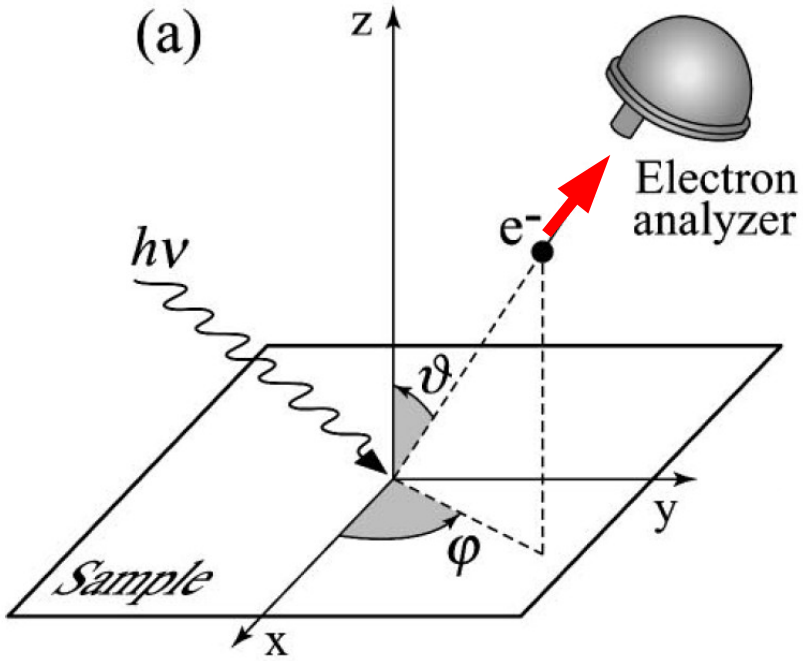

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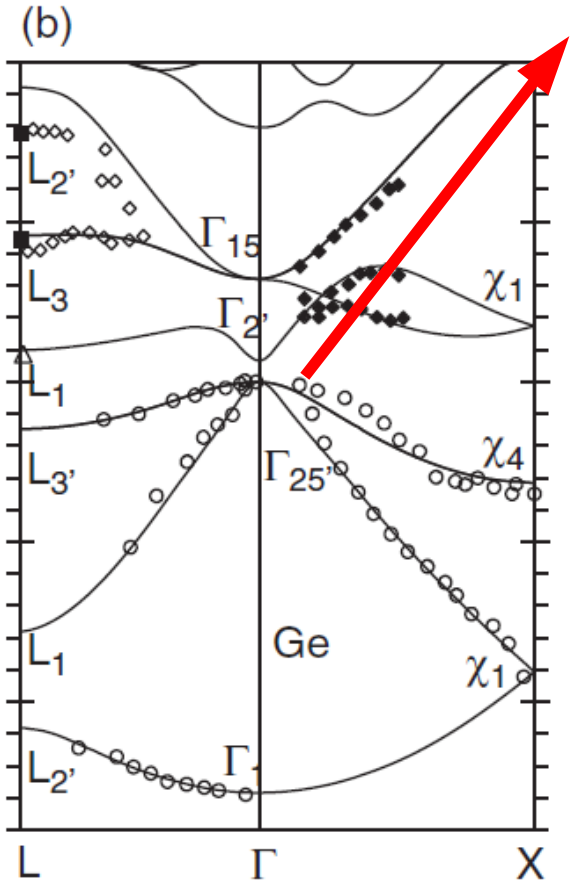

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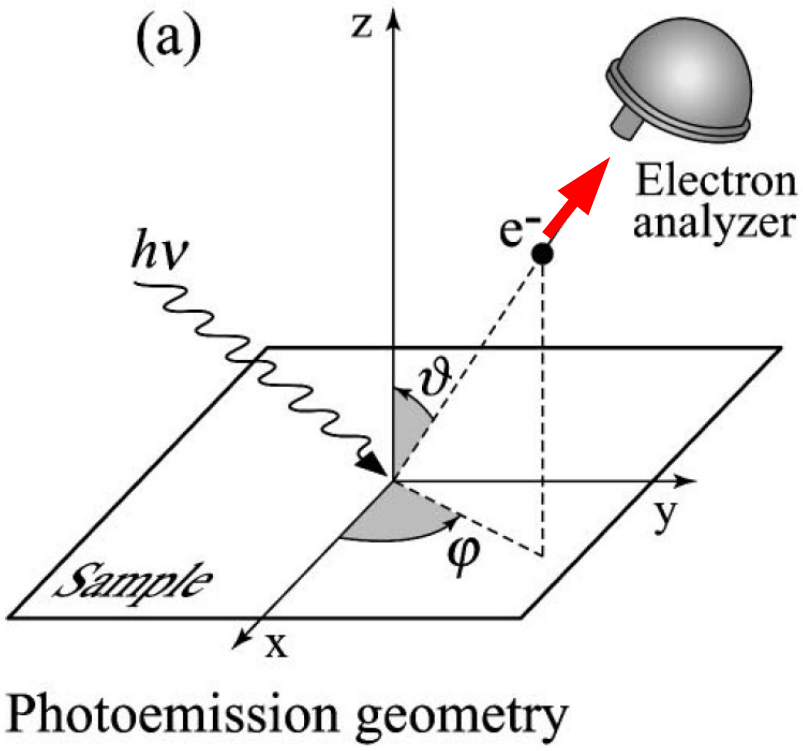

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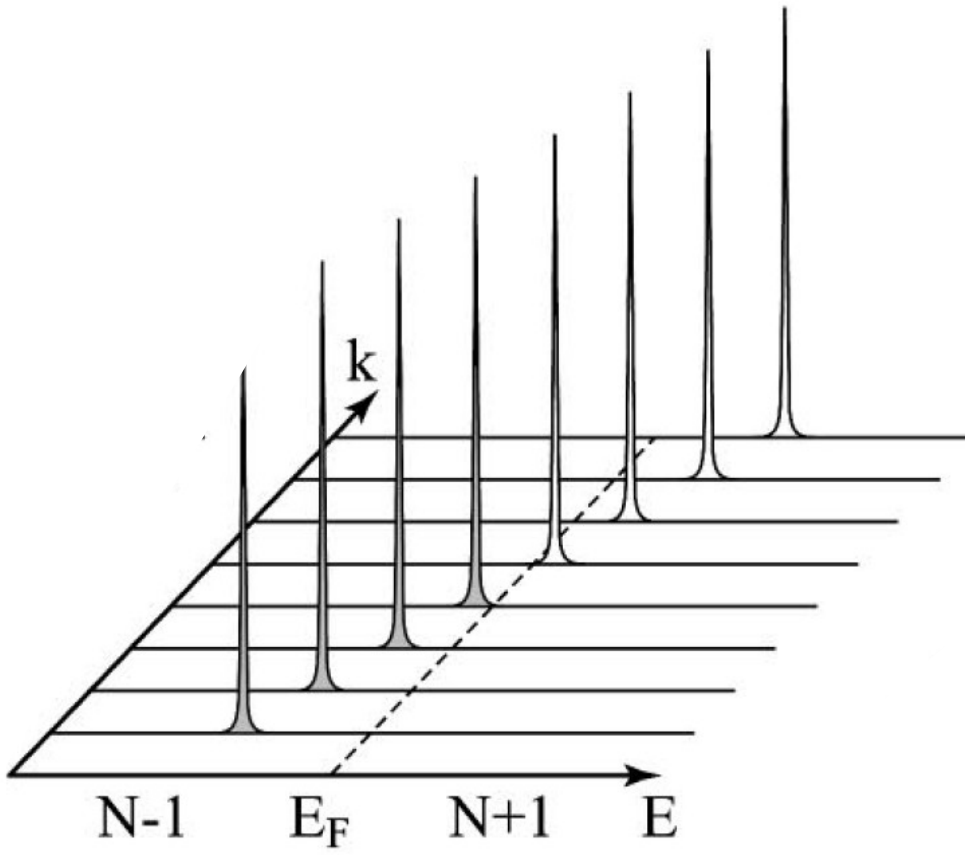

From Damascelli et al., RMP 75, 473 (2003)

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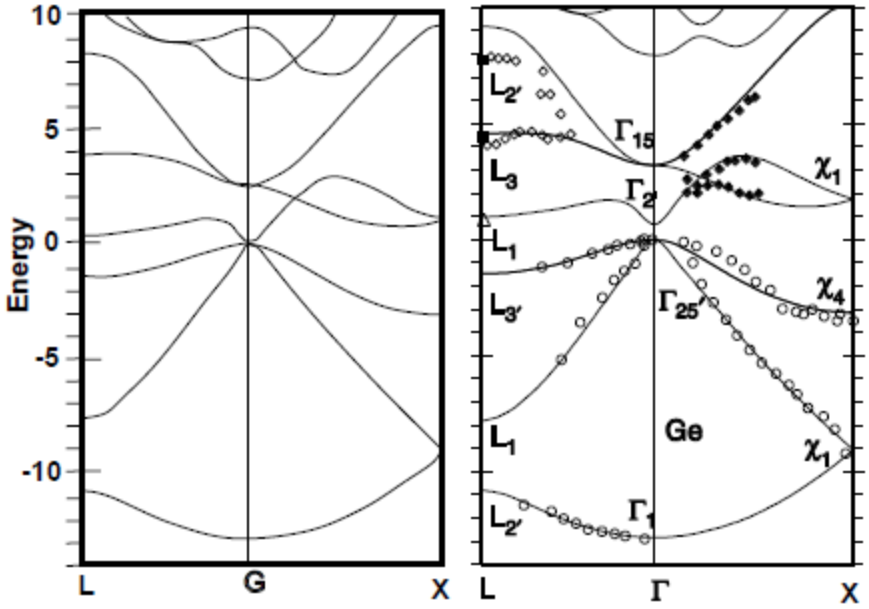
Can we use this approximation for photoemission spectra?

, plus LDA



Band structure of bulk germanium

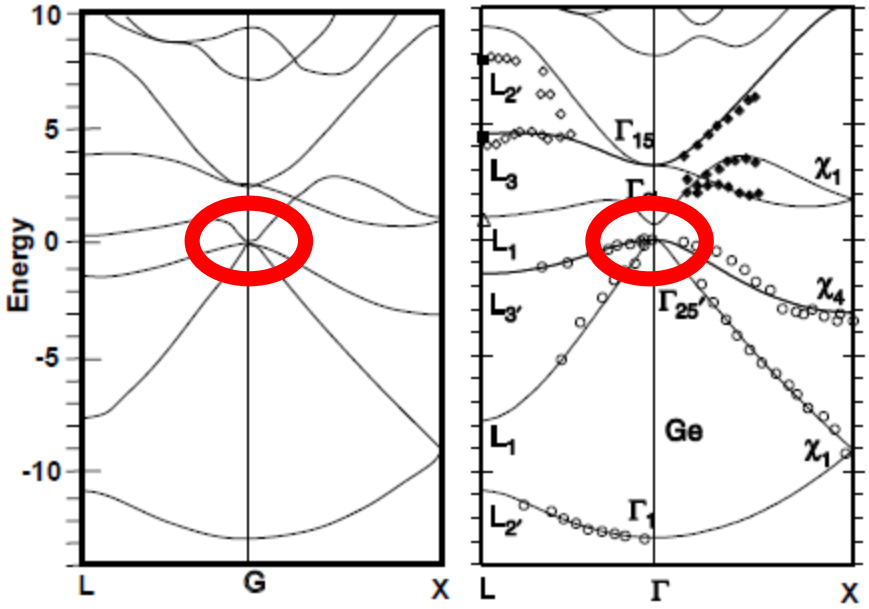
Rohlfing et al., PRB 48, 17791 (1993)

GW calculations, Rohlfing et al., PRB 48, 17791 (1993)

Bandstructure of germanium, theory versus experiment

“The Kohn-Sham band gap problem”

, plus LDA



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Bandstructure of germanium, theory versus experiment

“Exact” KS band gaps (in eV)
using xc potential reconstructed from AFQMC density:

	Si		NaCl
	indirect	direct at Γ	(direct at Γ)
AFQMC	0.69	2.72	5.25
PBE	0.66	2.60	5.08
LDA	0.49	2.55	4.59
Exp:	1.17	>3	8.5

A. Aouina, M. Gatti, S. Chen, S. Zhang, L. Reining Phys. Rev. B 107, 195123

Confirming previous work:

R. W. Godby, M. Schlüter, and L. J. Sham, Phys. Rev. Lett. 56, 2415 (1986); Phys. Rev. B 37, 101 (1988)

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T. Kotani, J. Phys.: Condens. Matter 10, 9241 (1998).

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The exact KS gap is definitely smaller than the photoemission gap

The “band gap problem” comes from the approx. use of the KS system

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BUT: we have no clue about $E_{gap}[n]$!!!!!

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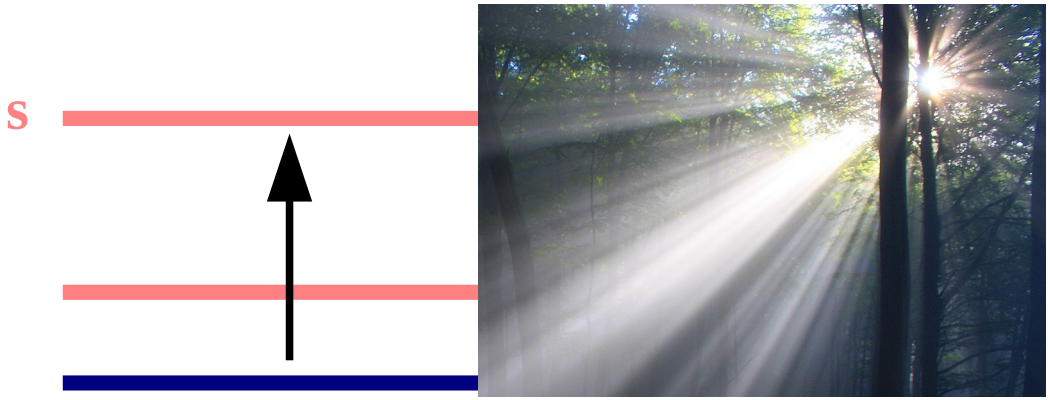
Spectroscopy: have to describe transitions

$$f_{ds}(t) = N \int dx_1 ... dx_N \, \Psi^*(x_1, ...x_N; t) d(x_1) e^{i\omega t} \Psi_s(x_1, ...x_N; t)$$



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$$= e^{i(E_s - E_0 + \omega)t} N \int dx_1 ... dx_N \, \Psi^*(x_1, ...x_N) d(x_1) \Psi_s(x_1, ...x_N)$$

Phase factor: excitation energy

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For the transition amplitude

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Phase factor: excitation energy

For the transition amplitude

Need amplitudes to excited states
and phase factors/energies

For photoemission: we need transition energies and amplitudes N → N-1

$$E_s \equiv E_0 - E_{N-1,s}$$

$$f_s(x_1,t) \equiv e^{iE_s t} N \int dx_2, \ldots\ldots dx_N \, \Psi^*(x_1, \ldots x_N)\Psi_{N-1,s}(x_2, \ldots . x_N)$$

$$f_s(x_1,t) = e^{iE_s t} f_s(x_1)$$

We build an object that contains the desired information (and also N → N+1)

$$G(x_1, x_1', t, t') = -ie^{-iE_s(t-t')}\Big[\Theta(t-t')\Theta(E_s-\mu) - \Theta(t'-t)\Theta(\mu-E_s)\Big] f_s(x_1) f_s^*(x_1')$$

One-body Green's function,

describing propagation of electrons and holes

Written using second quantization:

$$G(x_1, x_1', t, t') = -i\langle N|T[\hat{\Psi}(x_1,t)\hat{\Psi}^\dagger(x_1',t')]|N\rangle$$

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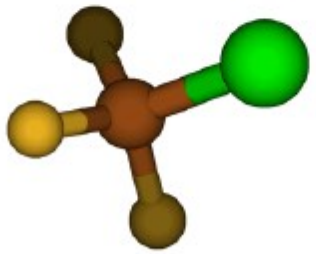
The descriptor:

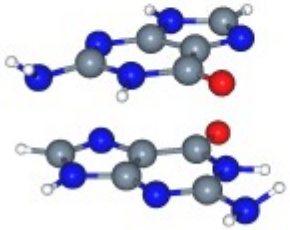
$\Psi(x_1, x_2, ..., x_N; t)$

CI, QMC



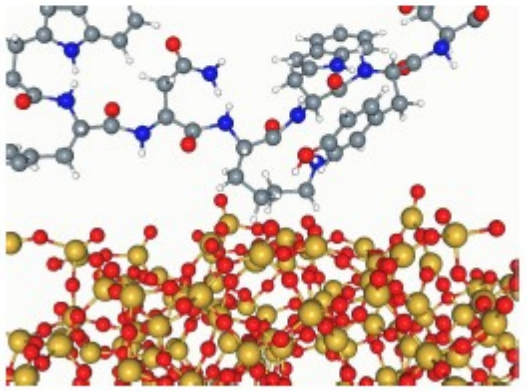
$G(x_1, x_2; t_1, t_2)$

Green's Functions



$n(\mathbf{r}; t)$

Density Functionals



The spectral function is a simple functional of the Green's function

Spectral function: peaks at transition energies, probabilities → intensity

$$\frac{1}{\pi}\left|\mathrm{Im}\, G_{\mathbf{k}}(\omega)\right| = \sum_{\lambda} \left|\mathrm{f}_{\lambda}(\mathbf{k})\right|^2 \delta(\omega - \varepsilon_{\lambda})$$

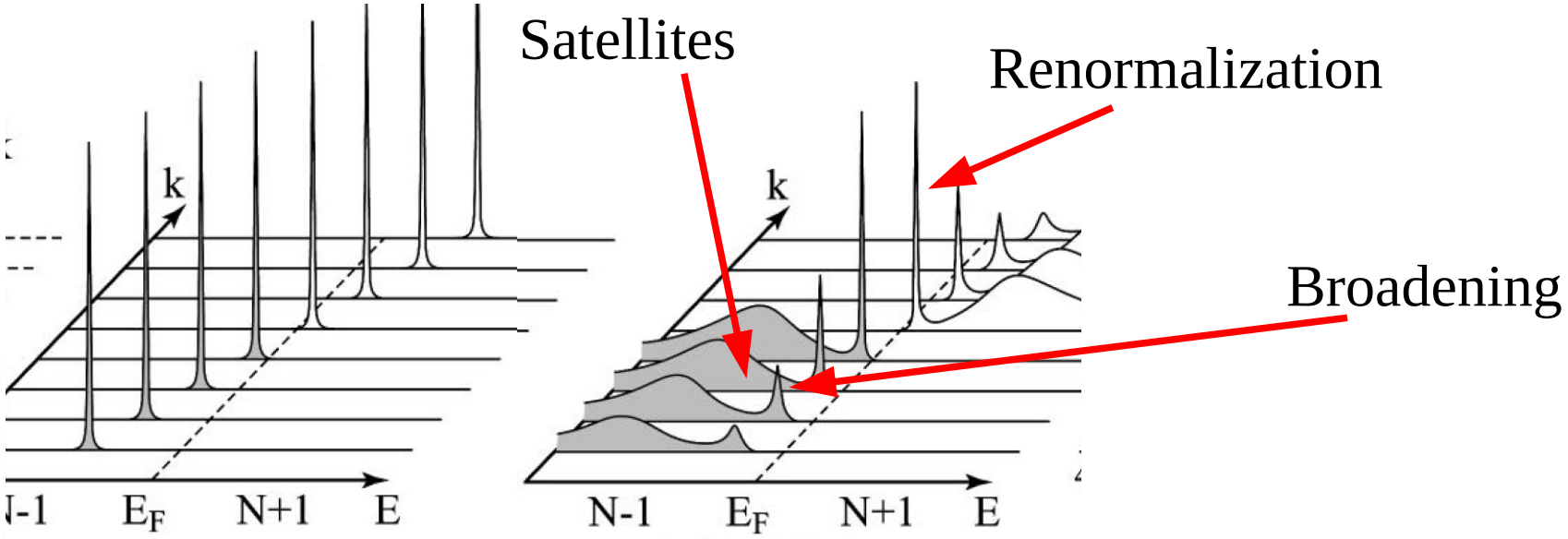
$$G^{T}(x_1, x_2, \omega) = \lim_{\eta \to 0^+} \sum_{\lambda} \frac{\mathrm{f}_{\lambda}(x_1)\mathrm{f}^{*}_{\lambda}(x_2)}{\omega - \varepsilon_{\lambda} + i\eta\, \mathrm{sgn}\,(\varepsilon_{\lambda} - \mu)}$$

$$\varepsilon_{\lambda} = E(N+1, \lambda) - E_0 > \mu \qquad \varepsilon_{\lambda} = E_0 - E(N-1, \lambda) < \mu$$

One-body GF

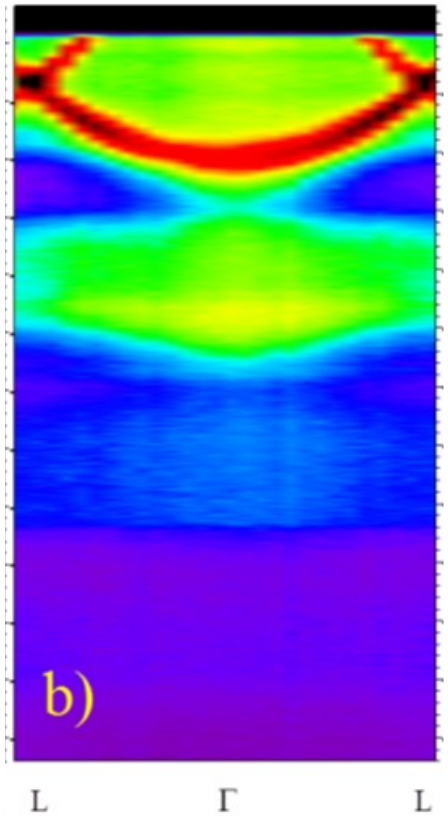
Spectral function: peaks at transition energies, probabilities → intensity

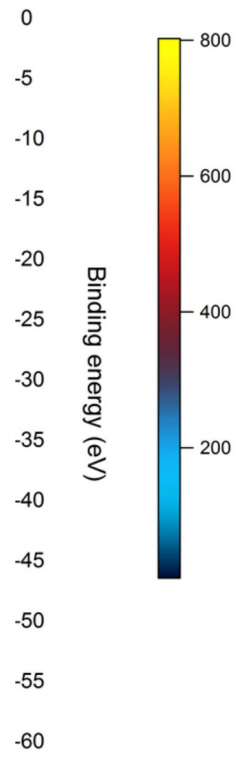
$$A_{\mathbf{k}}(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G_{\mathbf{k}}(\omega)|$$



Photoemission of bulk aluminum

Experiment





Zhou, Reining, Nicolaou, Bendounan, Ruotsalainen, Vanzini, Kas, Rehr, Muntwiler, Strocov, Sirotti, Gatti, PNAS 117 (46), 28596 (2020)

$$\mathcal{O}[n] \rightarrow \mathrm{O}\ ???$$

$$O[G] \rightarrow \mathrm{O}$$ ✓

$$A_{\mathbf{k}}(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G_{\mathbf{k}}(\omega)|$$

$$A(\omega) = \sum_{\mathbf{k}} A_{\mathbf{k}}(\omega)$$

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But where do we get G from?

$$A(\omega) = \sum_{\mathbf{k}} A_{\mathbf{k}}(\omega)$$

$$G(x_1, x_1', t, t') = -i\langle N|T[\hat{\Psi}(x_1, t)\hat{\Psi}^\dagger(x_1', t')]|N\rangle$$

We know how to calculate G in PRINCIPLE……

……but this is exactly what we do NOT want to do in PRACTICE!!!

$$G_u(1,1') = G^0(1,1') + G^0(1,\bar{2})\left\{[u(\bar{2}) + v_H(\bar{2})]G_u(\bar{2},1') + \right.$$
$$\left. + iv_c(\bar{2},\bar{3})\frac{\delta G_u(\bar{2},1')}{\delta u(\bar{3}^+)}\right\}$$

L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics*

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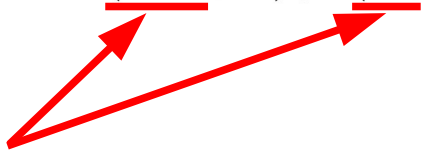
$$\Big(-\frac{\nabla^2}{2} + v_{\mathrm{ext}}(\mathbf{r}) + v_H(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r}) \Big) \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

More advanced simulation chamber

Image from pixabay:
www.noft-traders.com/establish-zero-gravity-zones-with-supply-and-demand/

$$\left(-\frac{\nabla^2}{2} + v_{\rm ext}(\mathbf{r}) + v_H(\mathbf{r}) + v_{\rm xc}(\mathbf{r}) \right) \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

$$\left(-\frac{\nabla^2}{2} + v_{\rm ext}(\mathbf{r}) + v_H(\mathbf{r}) \right) \varphi_i(\mathbf{r};\omega) + \int d\mathbf{r}'\, \Sigma_{\rm xc}(\mathbf{r},\mathbf{r}';\omega) \varphi_i(\mathbf{r}';\omega) = \varepsilon_i(\omega) \varphi_i(\mathbf{r};\omega)$$



New features: → non-locality in space

$$\left(-\frac{\nabla^2}{2} + v_{\rm ext}(\mathbf{r}) + v_H(\mathbf{r}) + v_{\rm xc}(\mathbf{r}) \right) \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

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New features: → non-locality in space

→ non-locality in time, hence, frequency-dependence

Descriptor	Auxiliary "potential"	
$n(\mathbf{r})$	$v_{\mathrm{xc}}(\mathbf{r})$	
$G(\mathbf{r}_1, \mathbf{r}_2, \omega)$	$\Sigma(\mathbf{r}_1, \mathbf{r}_2, \omega)$	
$G(\mathbf{r}, \mathbf{r}, \omega)$	$v_{SF}(\mathbf{r}, \omega)$	

Gatti, Olevano, Reining, Tokatly, PRL 99, 057401 (2007)

$G_{\ell\ell}(\omega)$	$\Sigma_{\ell}^{loc}(\omega)$	DMFT

A. Georges et al., Rev. Mod. Phys. 68, 13 (1996)

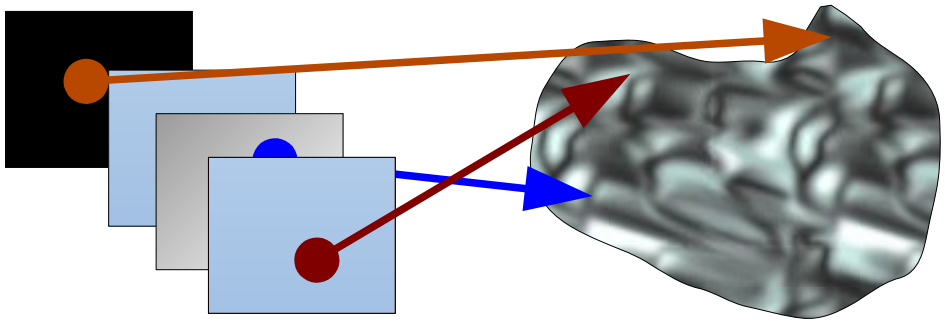
S. Y. Savrasov and G. Kotliar, Phys. Rev. B 69, 245101 (2004)

GFFT approximation strategy **of DMFT**

$\Sigma_\ell^{loc}(\omega)$ $G_{\ell\ell}(\omega)$

$v_{\mathrm{xc}}(\mathbf{r},[n])$ $n_r^h = n(r)$ Local Density Approximation (LDA)

Anderson Impurity Model → Material



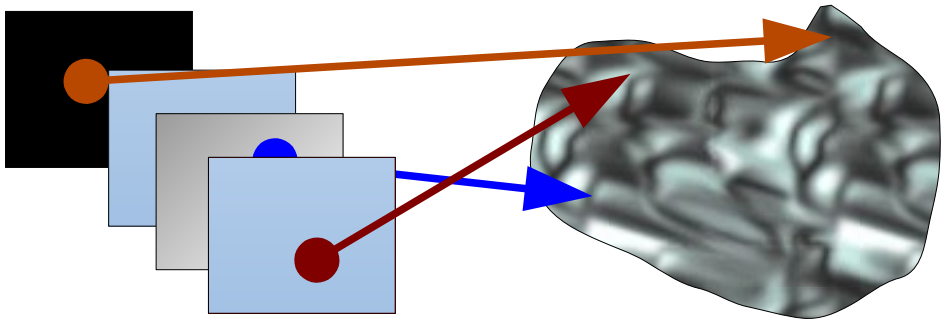
"Same local spectral function" →

GFFT approximation strategy **of DMFT**

$\Sigma_\ell^{loc}(\omega)$ $G_{\ell\ell}(\omega)$ Local GF Approximation**!**

$\Sigma_\ell^{loc}(\omega, [G_{\ell\ell}])$ **Nearsightedness**

Anderson Impurity Model → Material



"Same local spectral function" →

$$\Big(-\frac{\nabla^2}{2} + v_{\rm ext}(\mathbf{r}) + v_H(\mathbf{r}) + v_{\rm xc}(\mathbf{r}) \Big) \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

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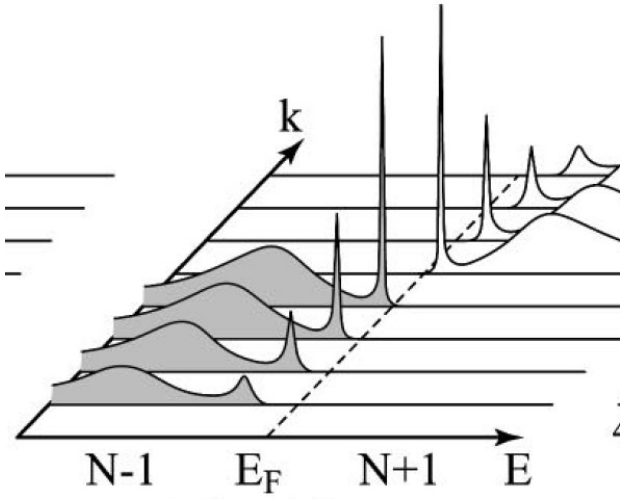
Usually formulated as Dyson equation:

$$G = G_0 + G_0 (v_H + \Sigma_{\rm xc}) G$$

Dyson equation: $G = G_0 + G_0 \Sigma G$

$$A_{\ell\ell}(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G_{\ell\ell}(\omega)|$$

Solving the Dyson equation would give a full spectral function

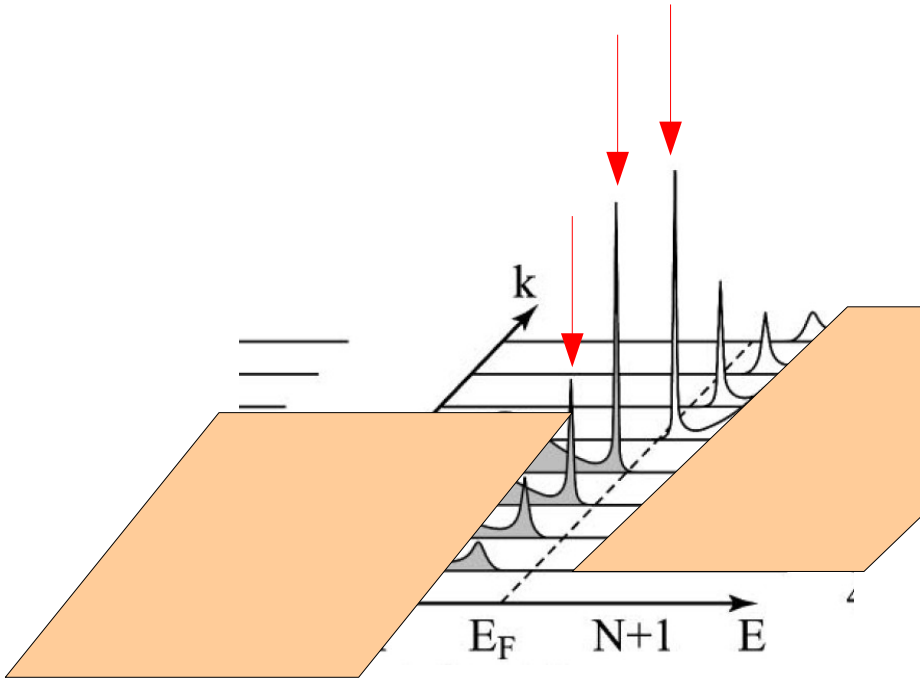


Dyson equation: $G = G_0 + G_0 \Sigma G$

$$A_{\ell\ell}(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G_{\ell\ell}(\omega)|$$

$$G(x_1, x_1', t, t') = -ie^{-iE_s(t-t')} \left[\Theta(t-t')\Theta(E_s-\mu) - \Theta(t'-t)\Theta(\mu-E_s)\right] f_s(x_1) f_s^*(x_1')$$

Quasiparticle approximation:



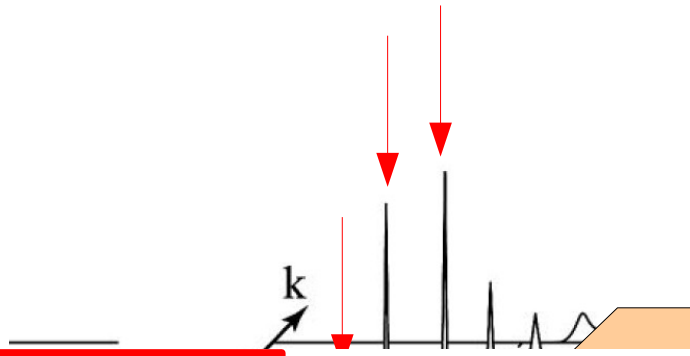
Dyson equation: $G = G_0 + G_0 \Sigma G$

$$A_{\ell\ell}(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G_{\ell\ell}(\omega)|$$

$$G(x_1, x_1', t, t') = -ie^{-iE_s(t-t')} \Big[\Theta(t-t')\Theta(E_s-\mu) - \Theta(t'-t)\Theta(\mu-E_s)\Big] f_s(x_1) f_s^*(x_1')$$

Quasiparticle approximation:

$f_s(x_1)$ like single particle wavefunction.



$$h_0(x_1) f_s(x_1) + \int dx_1' \, \Sigma_{\mathrm{xc}}(x_1, x_1', \varepsilon_s) f_s(x_1') = \varepsilon_s f_s(x_1)$$

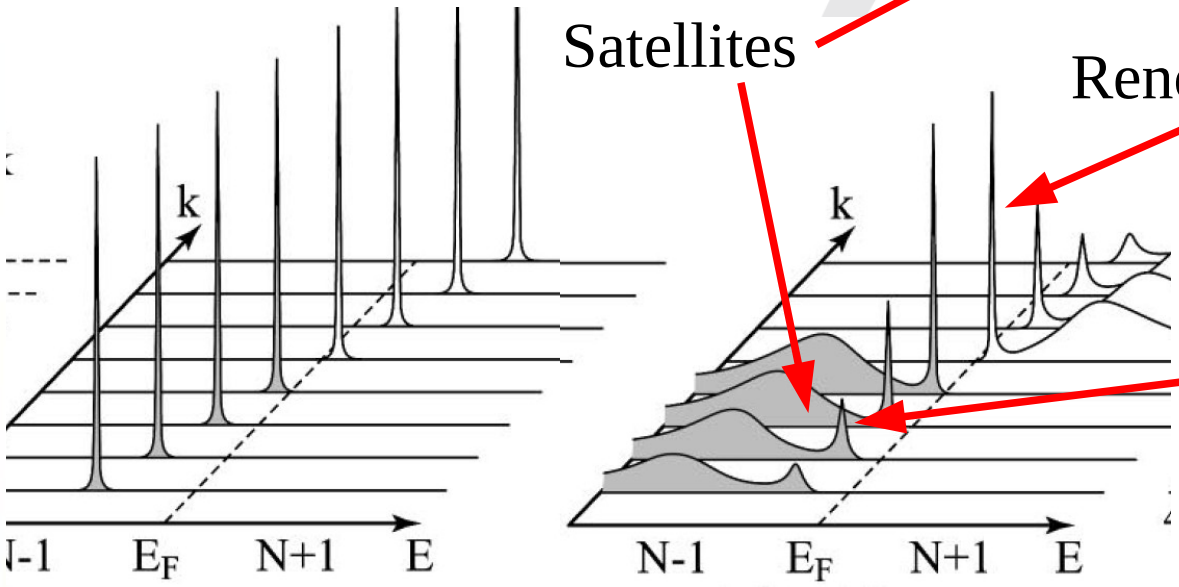
$$h_0(x_1)\phi_s(x_1) + v_{\mathrm{xc}}(x_1)\phi_s(x_1) = \varepsilon_s^0 \phi_s(x_1)$$

Our new fictitious world has a more complicated “potential” w.r.t. KS.
Therefore it can give us more information.

→ The spectral function

beyond the quasi-particle picture.....

$$A_{\mathbf{k}}(\omega) = \frac{1}{\pi}|\mathrm{Im}\, G_{\mathbf{k}}(\omega)| = \frac{1}{\pi}\frac{|\mathrm{Im}\, \Sigma_{\mathbf{k}}(\omega)|}{[\omega - \varepsilon^0_{\mathbf{k}} - \mathrm{Re}\, \Sigma_{\mathbf{k}}(\omega)]^2 + [\mathrm{Im}\, \Sigma_{\mathbf{k}}(\omega)]^2}$$



Satellites

Renormalization

Broadening

The GW approximation: band structures and more

→ Why do we need Green's functions?

→ From Green's functions to observables

→ A new auxiliary world

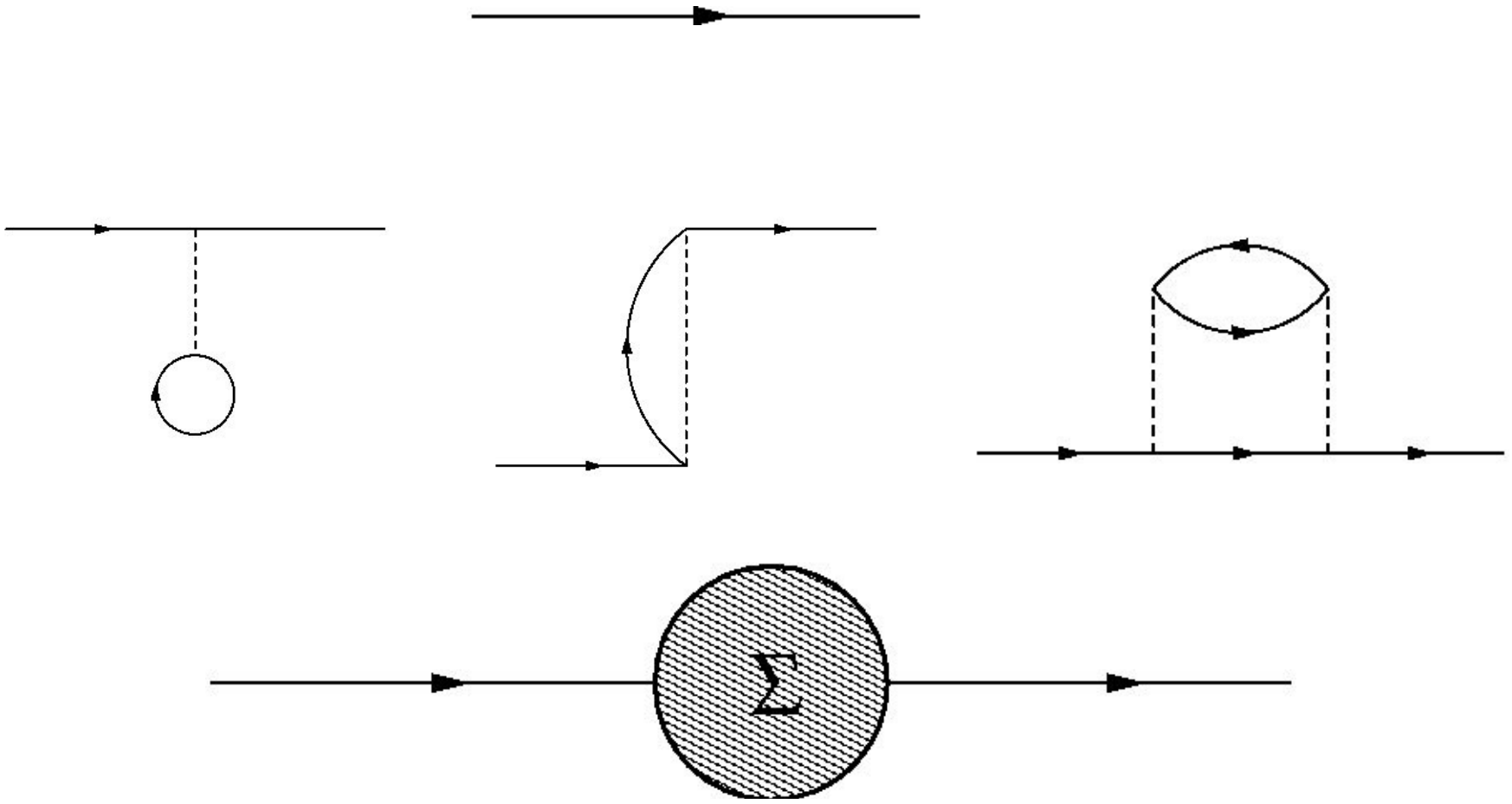
→ Impact of (dynamical) screening

→ Flavours of the GWA

→ What is wrong, and outlook

$$G(x_1, x_1', t, t') = -i\langle N|T[\hat{\Psi}(x_1, t)\hat{\Psi}^\dagger(x_1', t')]|N\rangle$$

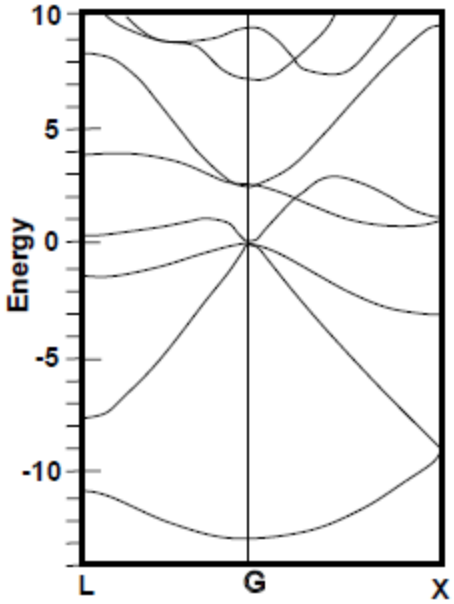
Many things can happen to a particle that propagates in the middle of others.....

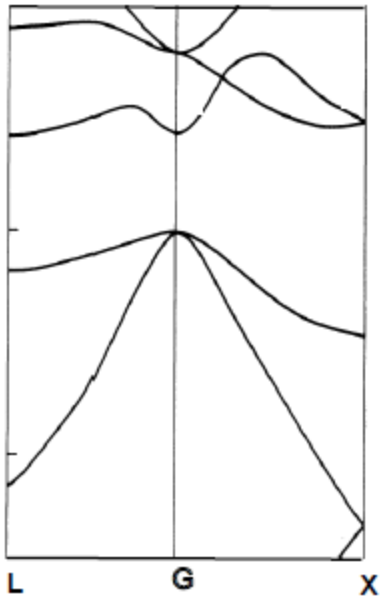


Dyson equation: $G = G_0 + G_0 \Sigma G$

LDA

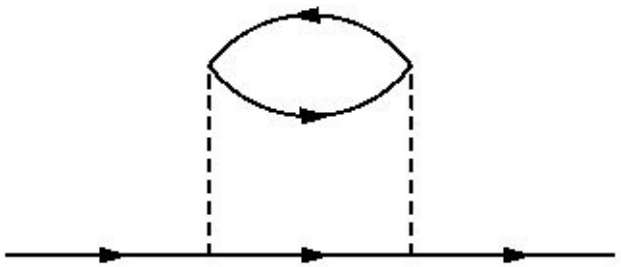
HF





GW calculations, Rohlfing et al., PRB 48, 17791 (1993)

Bandstructure of germanium, theory versus experiment



+ ……..

→ $\Sigma \sim i\,\mathcal{W}\mathcal{G}$ “GW”

L. Hedin, Phys. Rev. 139:A796–823, 1965

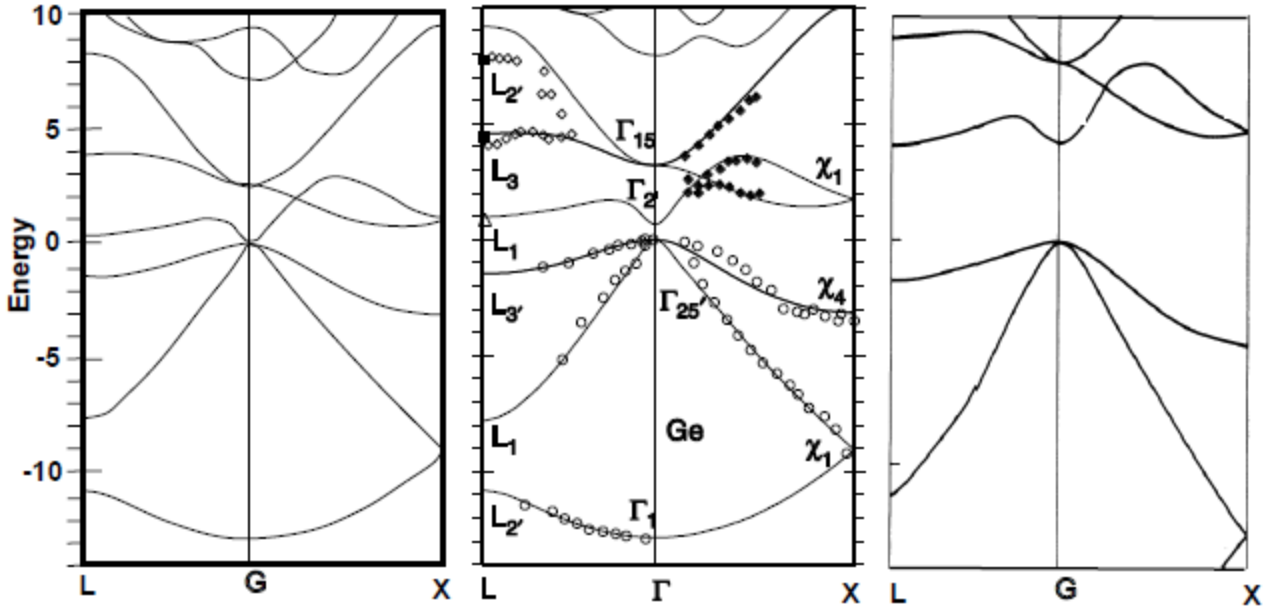
$$W = \varepsilon^{-1}(\omega)\, v$$

GW

Hartree-Fock

Usually good gaps and band structures in GW

LDA GW HF



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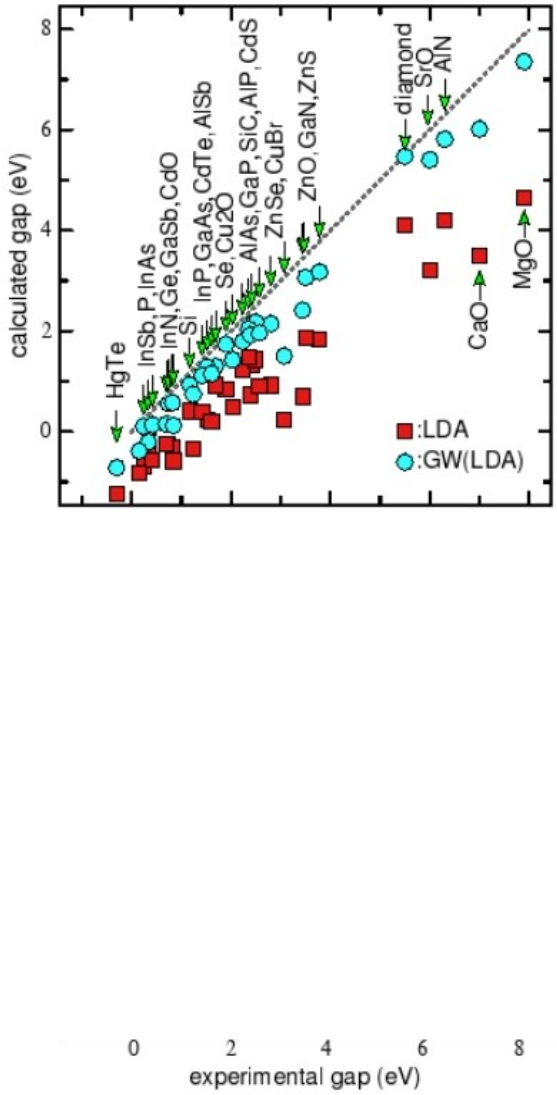
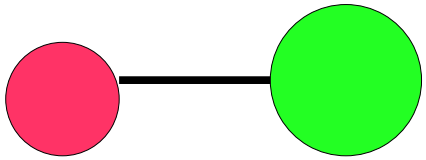
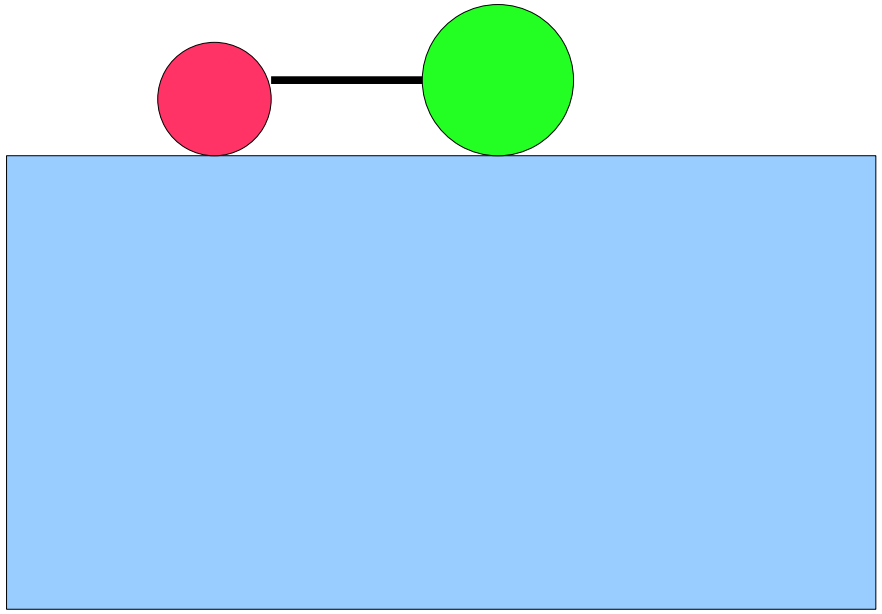


van Schilfgaarde, Kotani, Faleev,
Phys. Rev. Lett. 96, 226402 (2006)

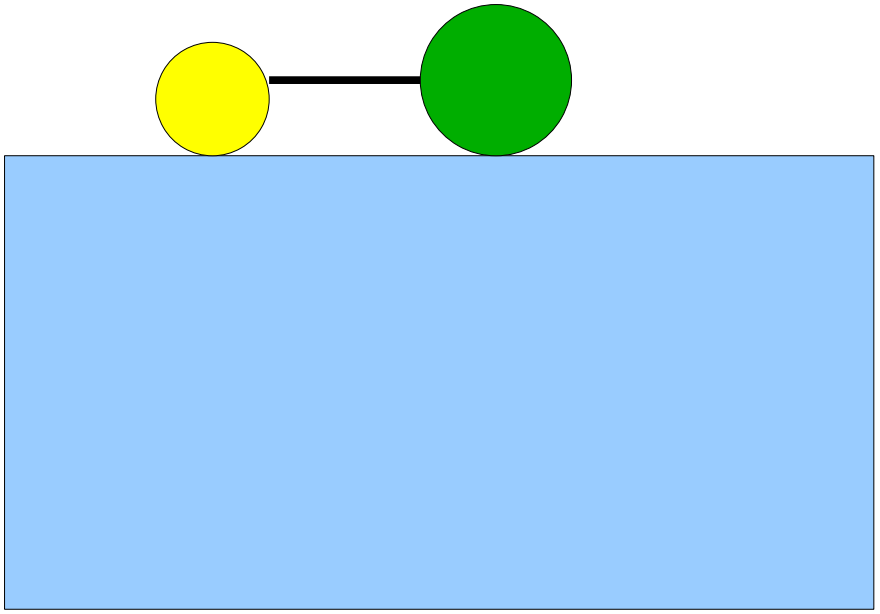
Molecules on surfaces



Molecules on surfaces

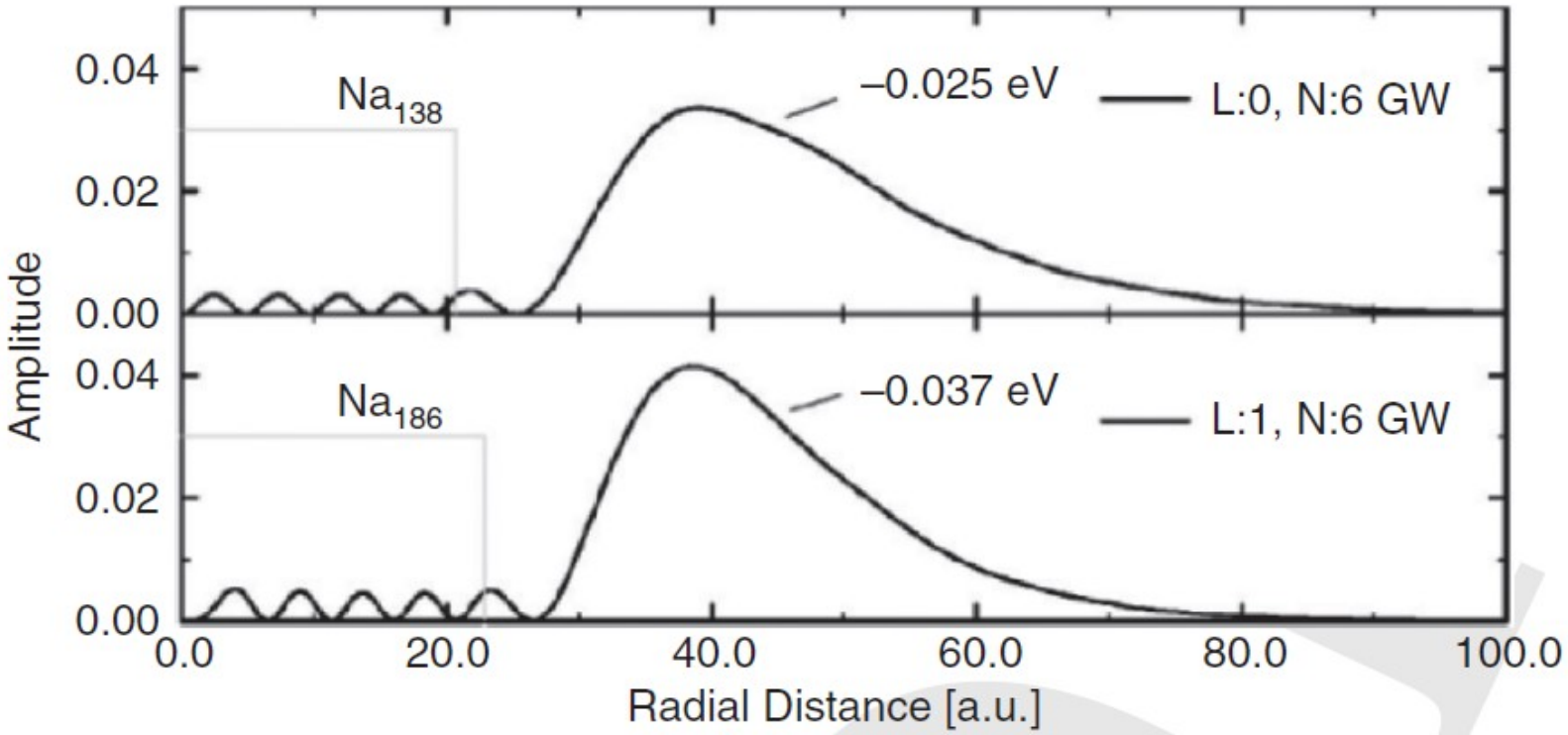


Molecules on surfaces



C. Freysoldt, et al., Phys. Rev. Lett. 103:056803, 2009.
J. M. Garcia-Lastra, et al, Phys. Rev. B 80:245427, 2009.

Image states



P. Rinke, et al., Phys. Rev. A 70:063201, 2004.

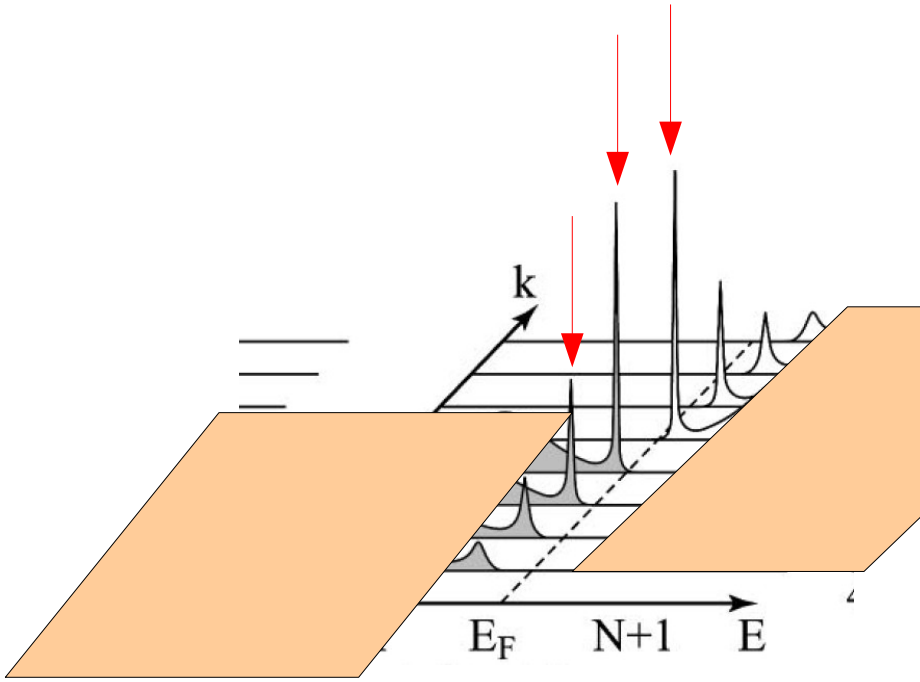
Also: vdW

Dyson equation: $G = G_0 + G_0 \Sigma G$

$$A_{\ell\ell}(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G_{\ell\ell}(\omega)|$$

$$G(x_1, x_1', t, t') = -ie^{-iE_s(t-t')} \left[\Theta(t-t')\Theta(E_s-\mu) - \Theta(t'-t)\Theta(\mu-E_s)\right] f_s(x_1) f_s^*(x_1')$$

Quasiparticle approximation:



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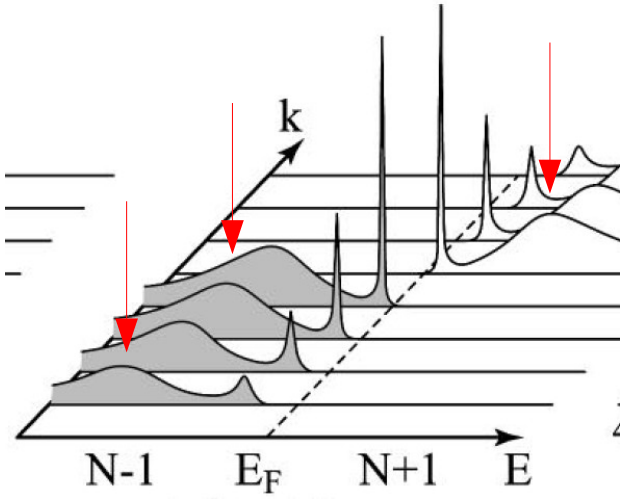
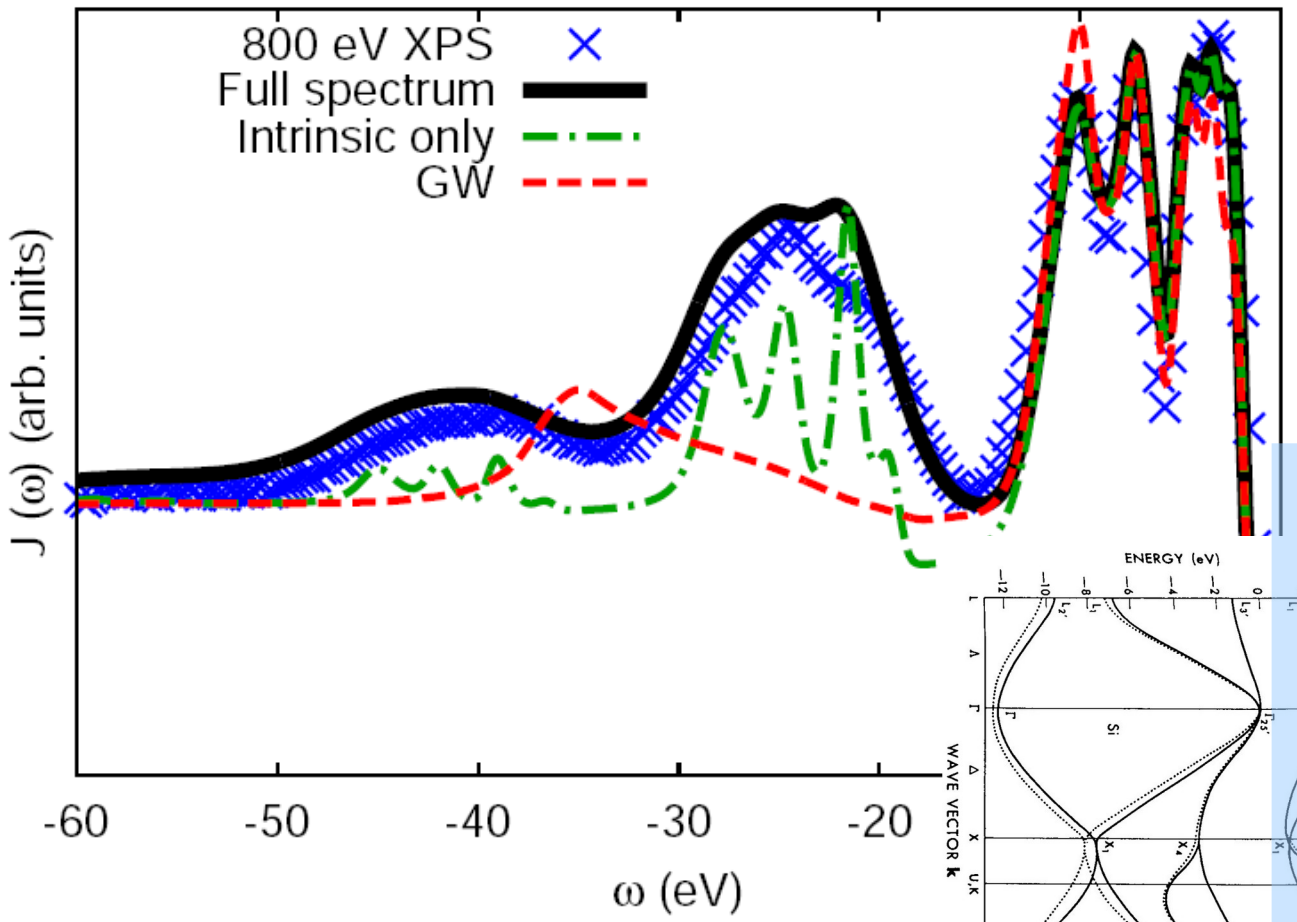
Quasiparticle approximation **and beyond:**

Additional excitations contained in *W(ω)*



→ ARPES of simple bulk silicon:

Obviously far from an i.p. picture!



Cohen and Chelikowsky: "Electronic Structure and Optical Properties of Semiconductors" Solid-State Sciences 75, Springer-Verlag 1988)

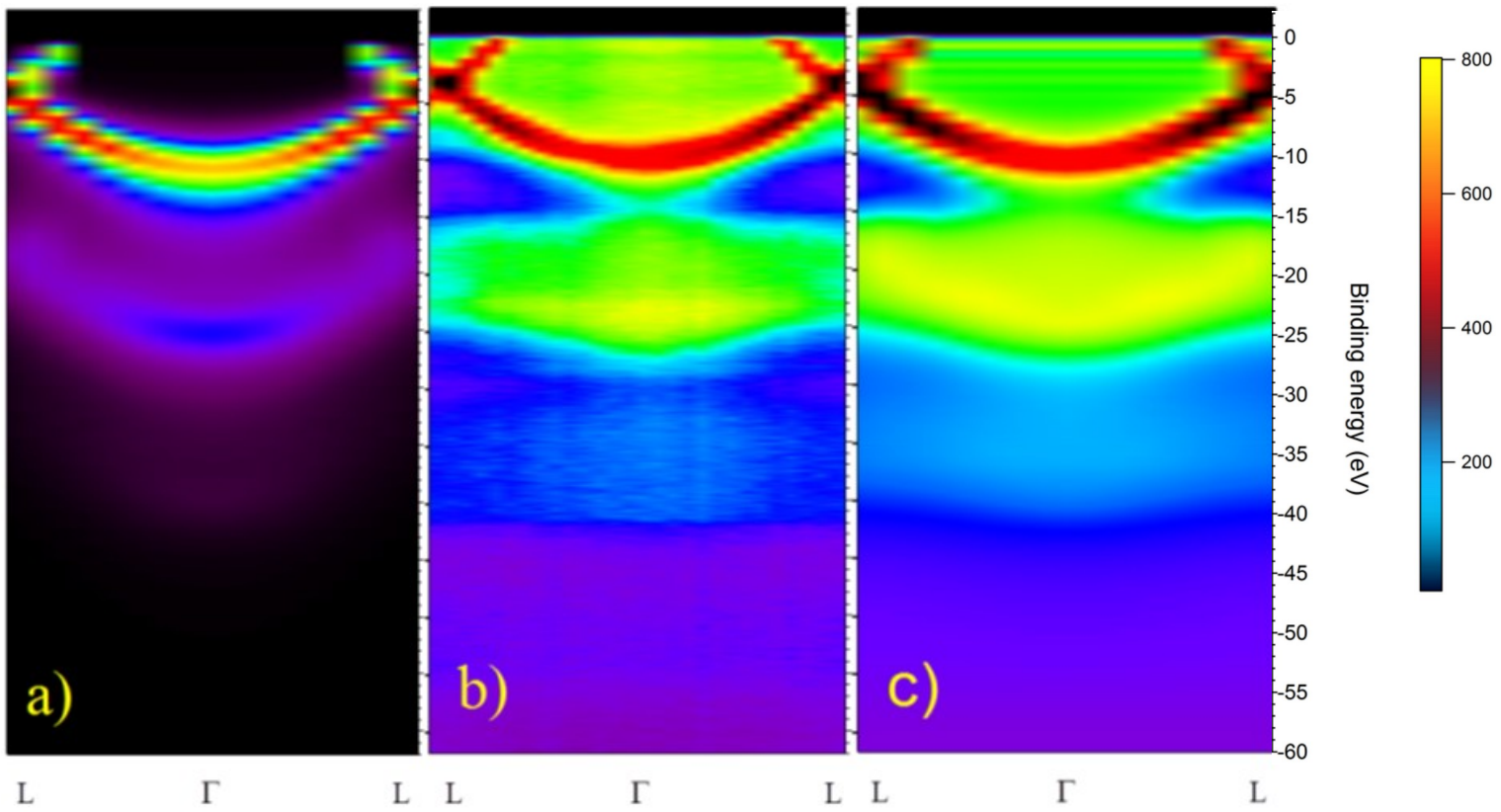
Exp.: F. Sirotti et al., TEMPO beamline SOLEIL

Photoemission of bulk aluminum

GW+C spectrum

Experiment

GW+C++



Zhou, Reining, Nicolaou, Bendounan, Ruotsalainen,Vanzini, Kas, Rehr, Muntwiler, Strocov, Sirotti, Gatti, PNAS 117 (46), 28596 (2020)

The GW approximation: band structures and more

→ Why do we need Green's functions?

→ From Green's functions to observables

→ A new auxiliary world

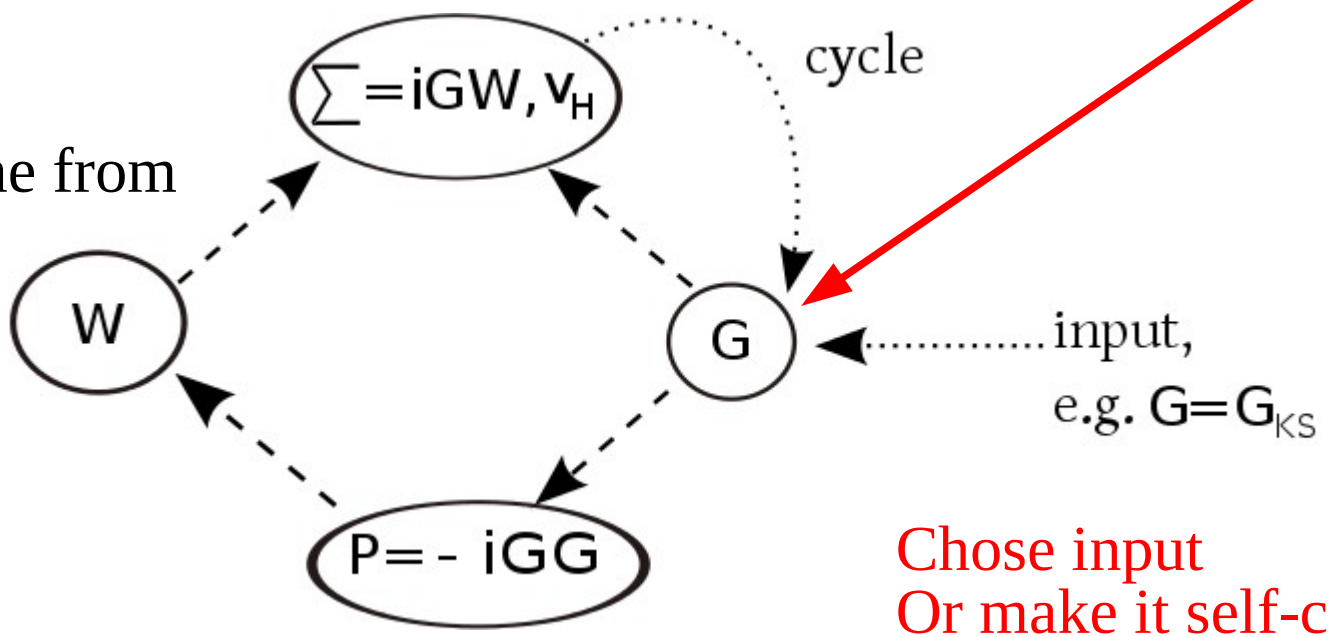
→ Impact of (dynamical) screening

→ Flavours of the GWA

→ What is wrong, and outlook

Output G or QP energies

G in input and output...



Can come from TDDFT

Chose input
Or make it self-consistent

RPA
Or beyond

Dyson equation: $G = G_0 + G_0 \Sigma G$

$$A_{\ell\ell}(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G_{\ell\ell}(\omega)|$$

$$G(x_1, x_1', t, t') = -ie^{-iE_s(t-t')} \left[\Theta(t-t')\Theta(E_s-\mu) - \Theta(t'-t)\Theta(\mu-E_s)\right] f_s(x_1) f_s^*(x_1')$$

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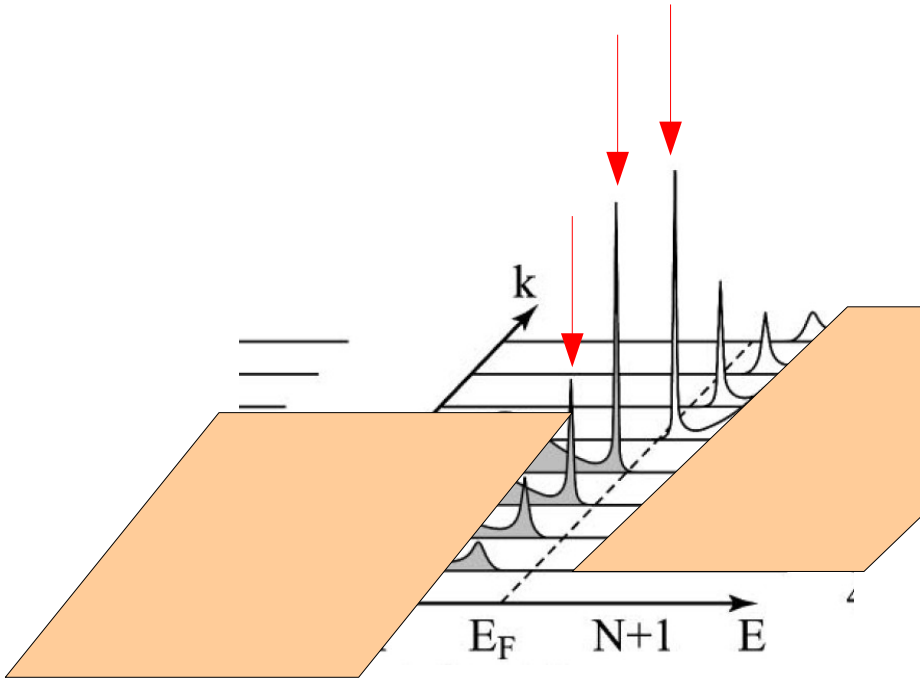
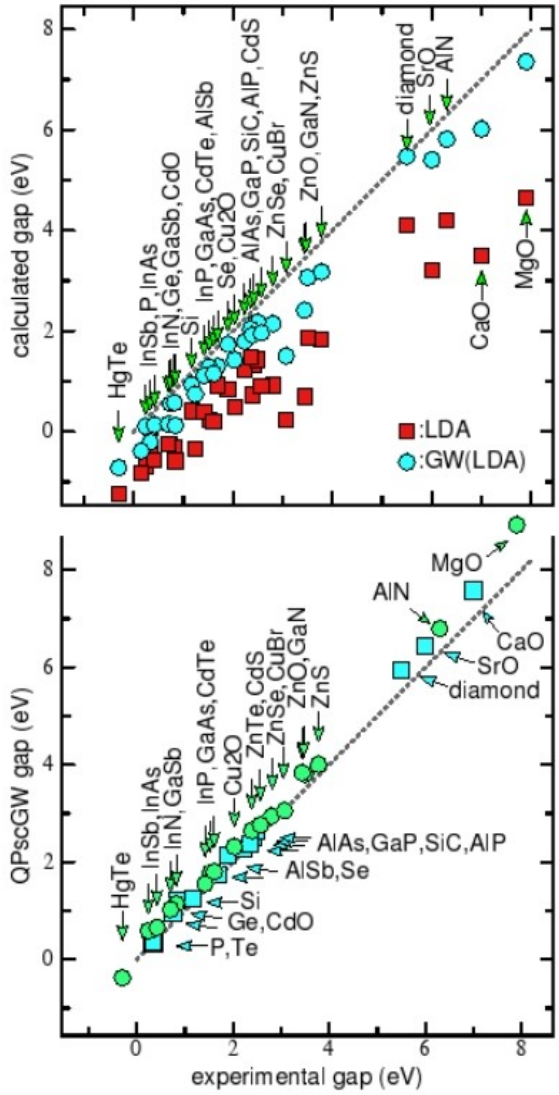


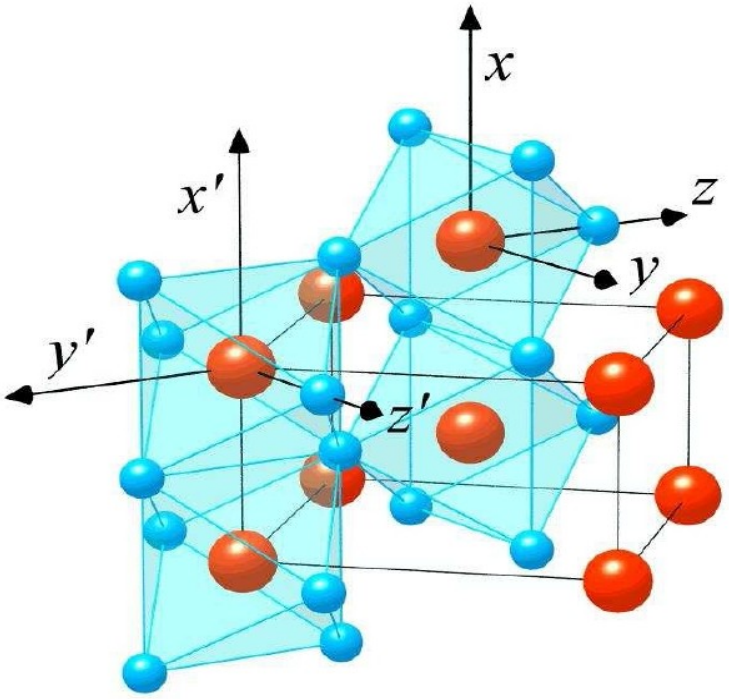
Usually good gaps and band structures in GW



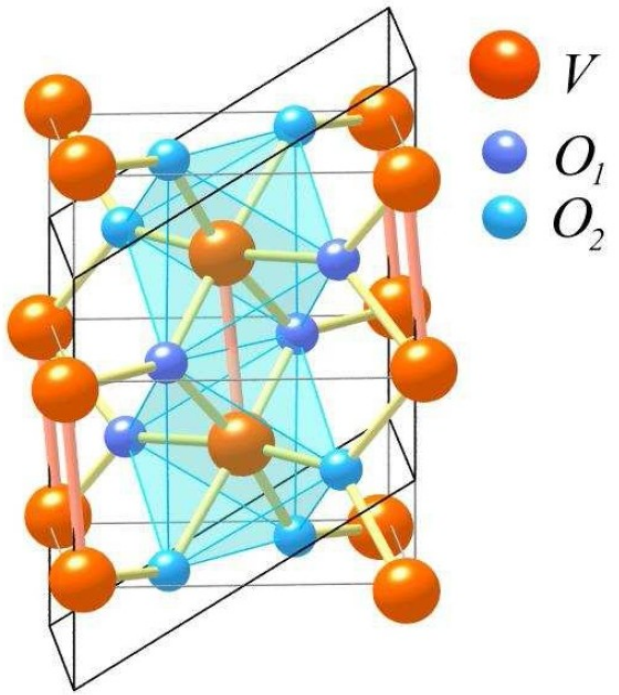
van Schilfgaarde, Kotani, Faleev, Phys. Rev. Lett. 96, 226402 (2006)

Gaps...even for TMO's

VO_2

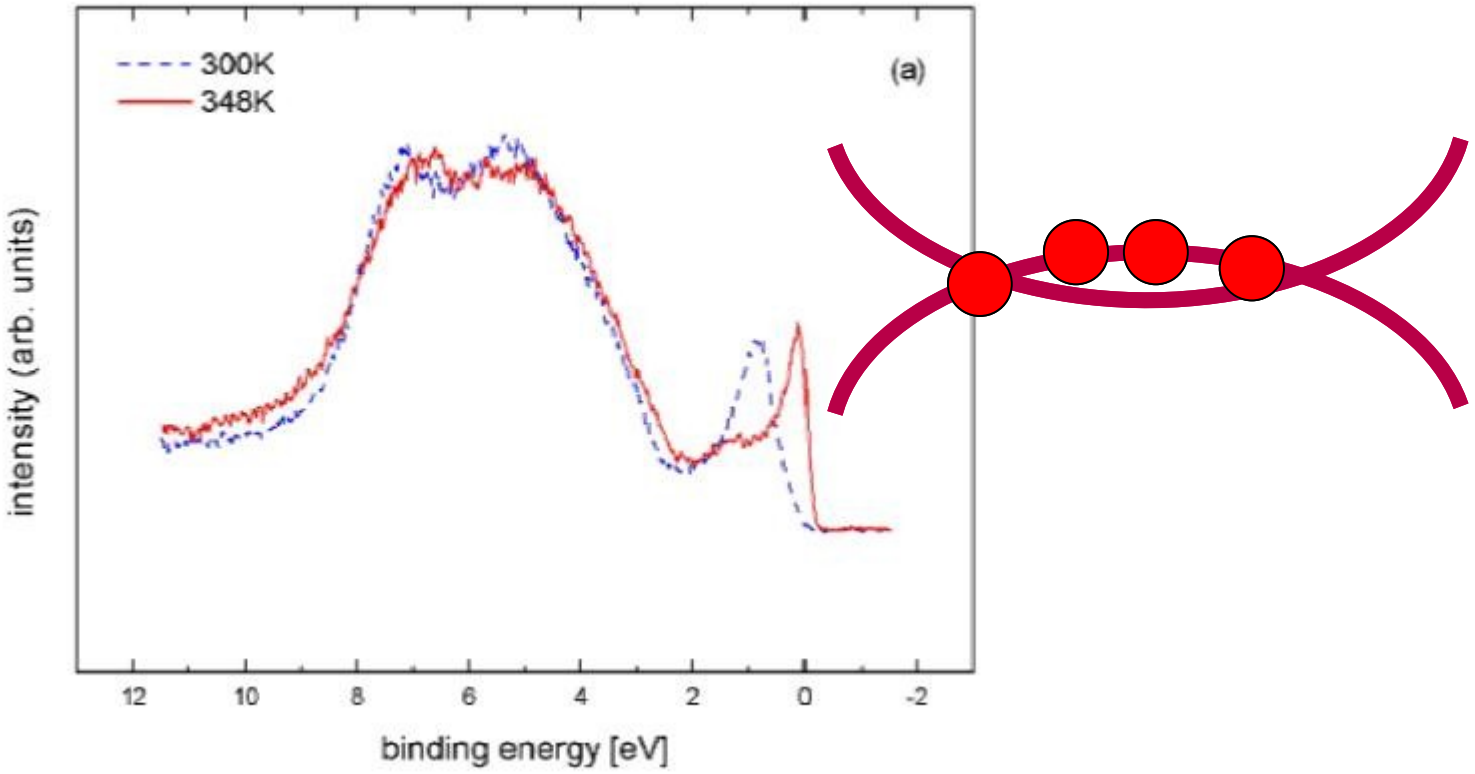


rutile



monoclinic

Matteo Gatti et al.



T. C. Koethe et al., Phys. Rev. Lett. 97, 116402 (2006).

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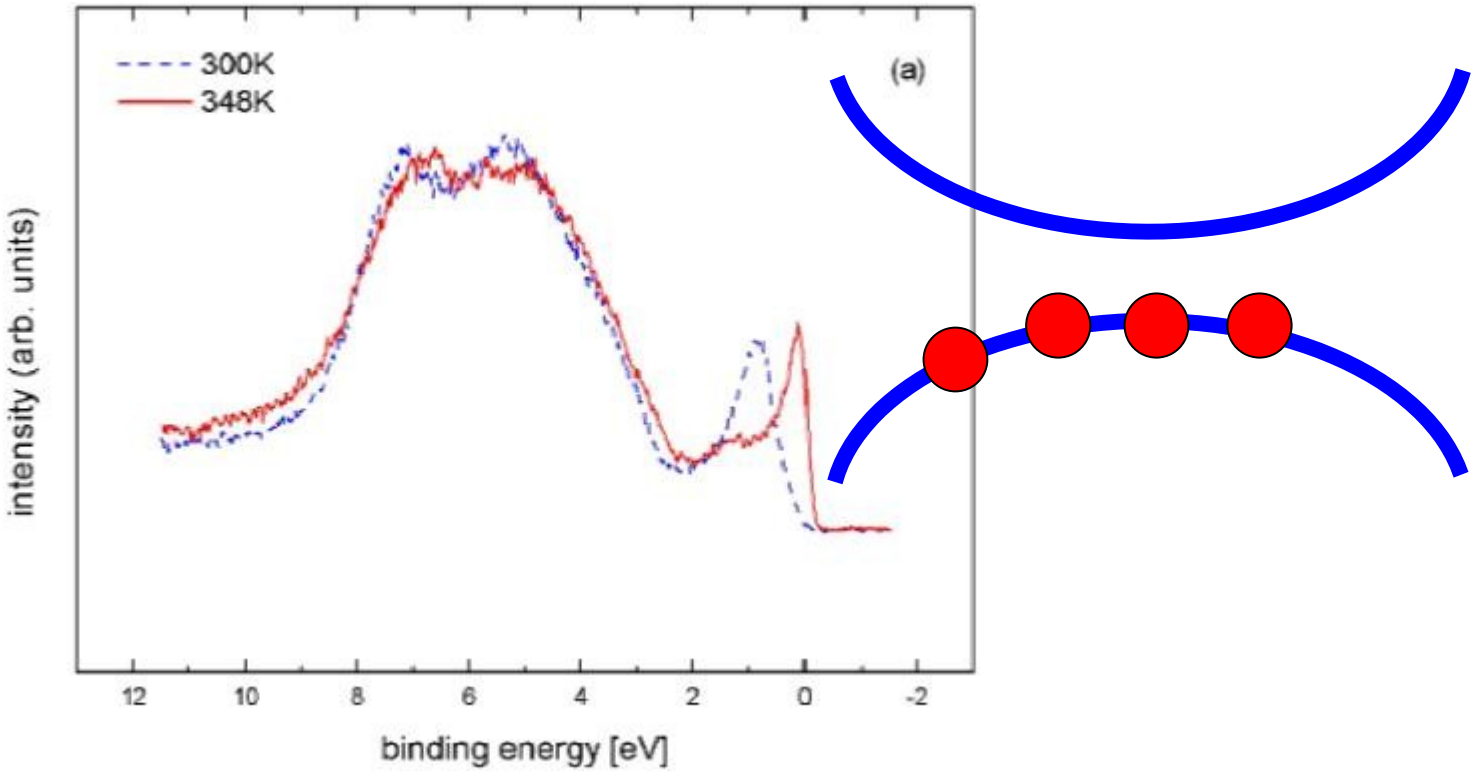

In GW: M. Gatti, F. Bruneval, V. Olevano and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007)

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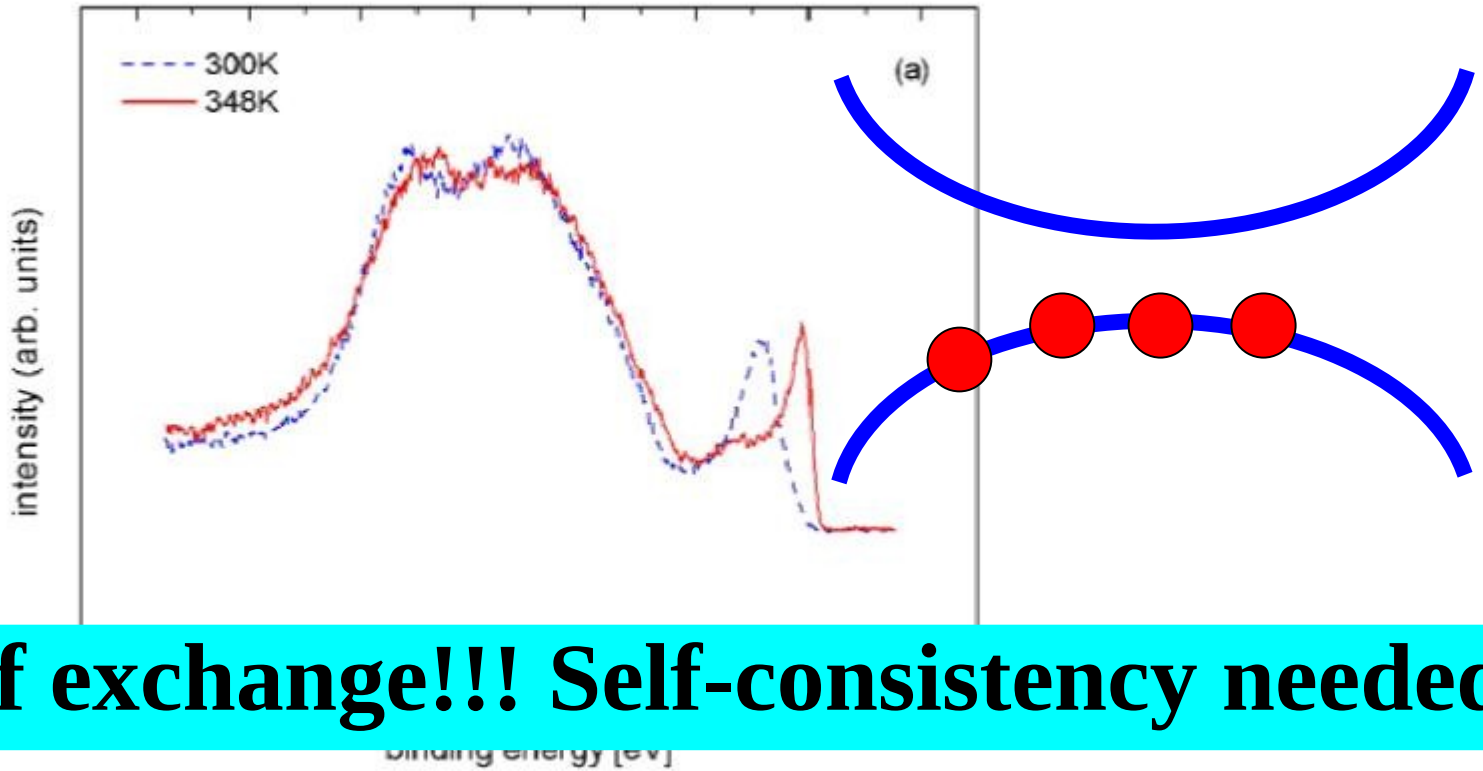
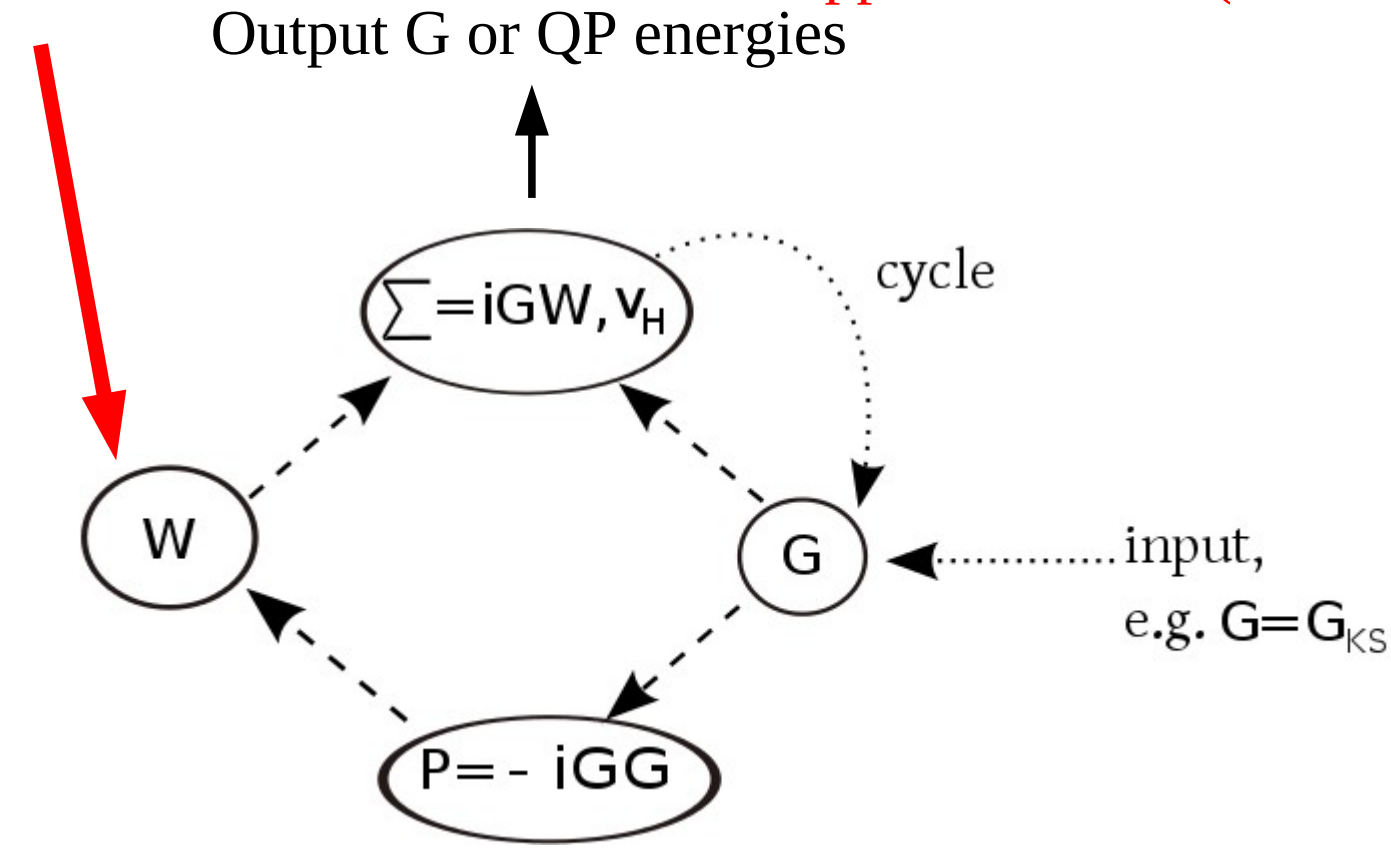


Effect of exchange!!! Self-consistency needed

In GW: M. Gatti, F. Bruneval, V. Olevano and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007)

Can be calculated with different approximations (see TDDFT)



The GW approximation: band structures and more

→ Brief reminder Lecture I

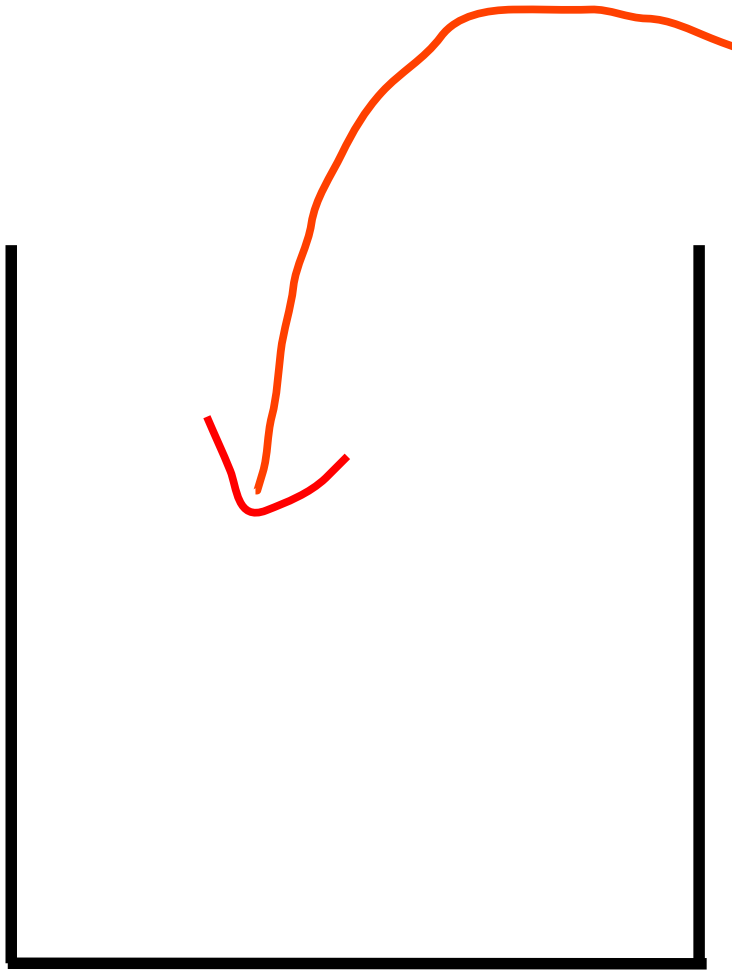
→ Diagrams

→ Importance of screening

→ Impact of dynamical screening

→ Flavours of the GWA

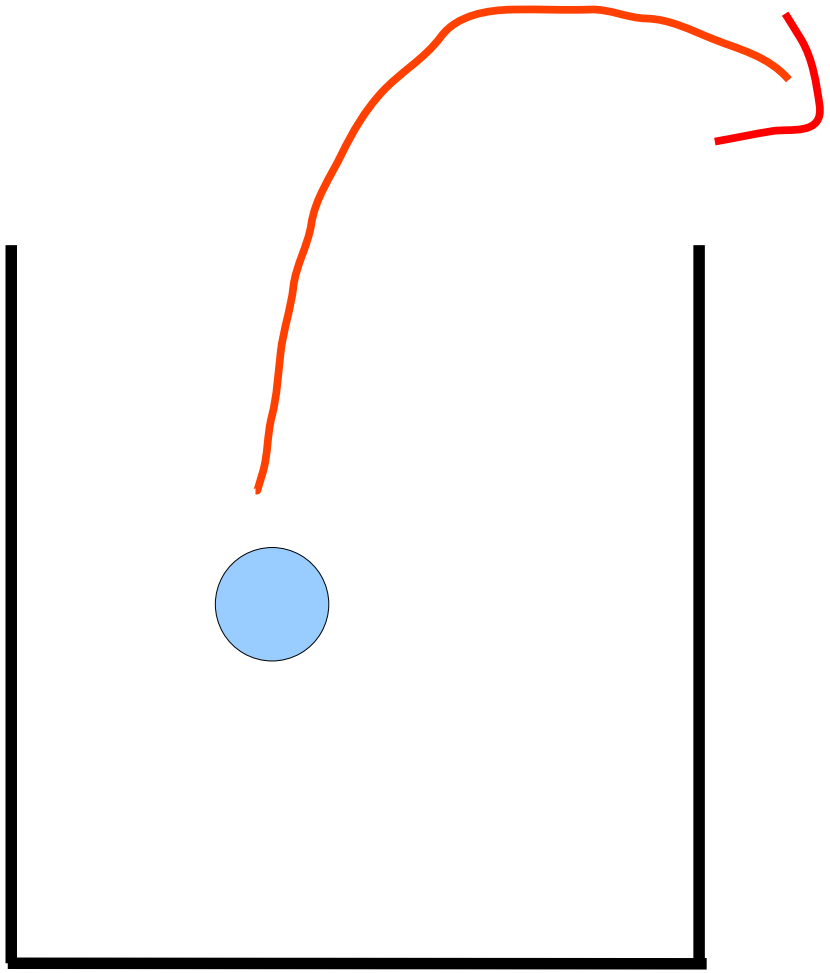
→ What is wrong, and outlook



$$W = v_c$$

HF = exact

Romaniello P., Guyot S., and Reining L., J. Chem. Phys. 131, 154111 (2009)

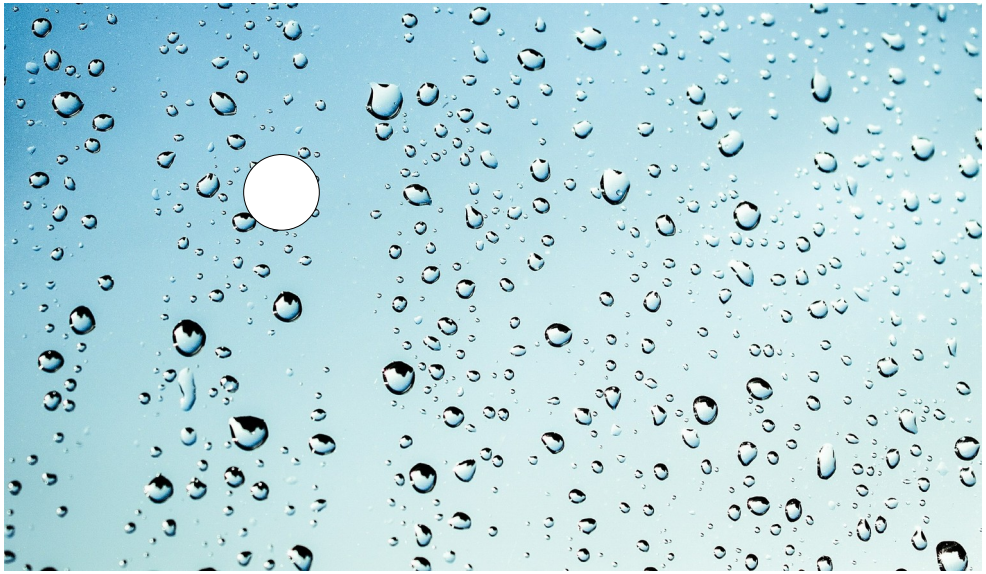


$$W \neq v_c$$

self-screening

Romaniello P., Guyot S., and Reining L., J. Chem. Phys. 131, 154111 (2009)

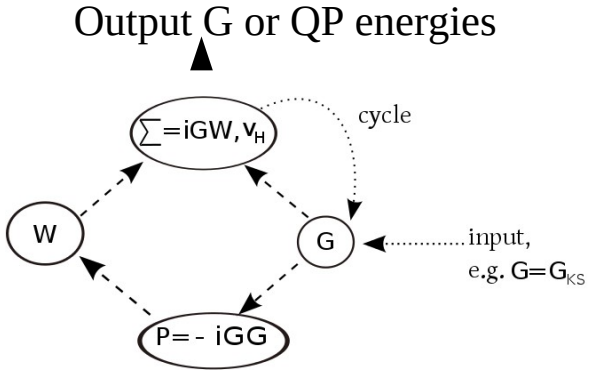
GW is good for QP energies of electrons in “normal” densities



GW fails when explicit correlation with individual electrons is neded

So, how should one do a GW calculation?

Don't forget, GW is itself an approximation!



My personal advice/current knowledge:

→ Make sure your density is good:

* by using a good local KS potential (e.g. no LDA for localized states) → $\Sigma(E_{KS})$

* or by using some sort of QP-self-consistency for G (can be hybrids!) → $\Sigma(E_{QP})$

→ Make sure your W (screening) is "good":

* it can be useful to compare it to experiment
* self-consistent RPA is usually underscreening
* **but:** hints that KS-RPA convenient, and that vertex beyond GW would weaken screening (Note: self-screening problem)

Suggested Reading

L. Hedin, “On correlation effects in electron spectroscopies and the GW approximation,” J. Phys. C 11:R489–528, 1999. *Short review, very good for photoemission!*

F. Aryasetiawan and O. Gunnarsson, “The GW method,” Rep. Prog. Phys. 61:237–312, 1998; and:

W. G. Aulbur, L. Jonsson, and J. W. Wilkins, “Quasiparticle calculations in solids,” Solid State Phys. 54:1–218, 2000;
Two nice and quite complete reviews on GW

Strinati, G., “Application of the Green’s function method to the study of the optical-properties of semiconductors,” Rivista del Nuovo Cimento 11, 1, 1988. *Pedagogical review of the theoretical framework underlying today’s Bethe–Salpeter calculations. Derivation of the main equations and link to spectroscopy.*

Onida, G., Reining, L., and Rubio, A., “Electronic excitations: density-functional versus many-body Greens-function approaches,” Rev. Mod. Phys. 74, 601, 2002.
Review of ab initio calculations of electronic excitations with accent on optical properties and a comparison between Bethe–Salpeter and TDDFT

R.M. Martin, L. Reining, D.M. Ceperley, “Interacting Electrons: Theory and Computational Approaches, Cambridge May 2016
Recent book containing many-body perturbation theory, DMFT and QMC