The Bethe-Salpeter Equation

Lucia Reining & Francesco Sottile
Palaiseau Theoretical Spectroscopy Group

The Bethe-Salpeter Equation

→ A reminder

→ TD-GFT

→ The electron-hole problem

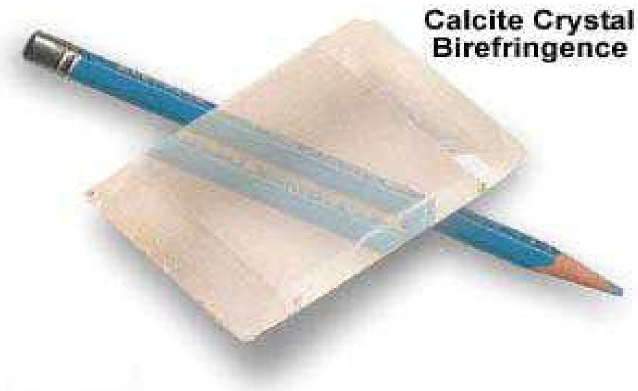
→ Approximations

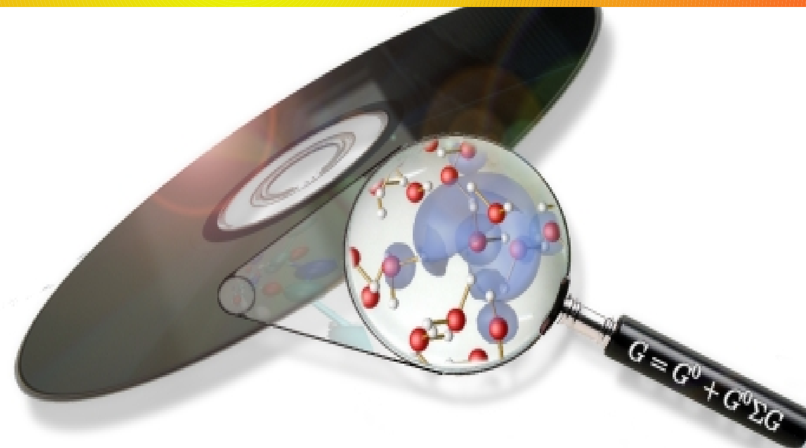
→ Realizations

→ Applications

→ Notes

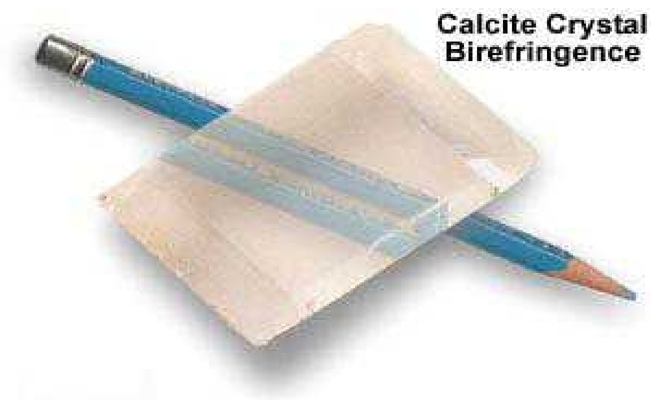
→ Theoretical Spectroscopy: aims and observations

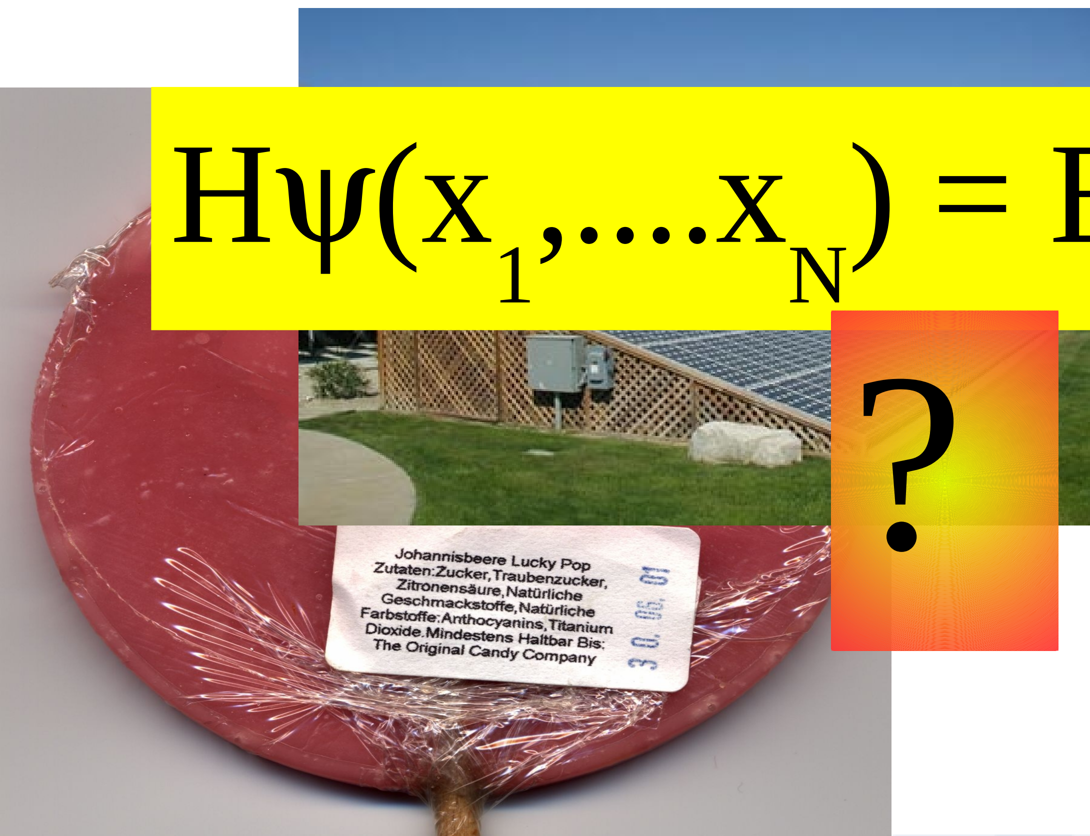




Key quantity $W(\omega) = \varepsilon^{-1}(\omega)\, v$

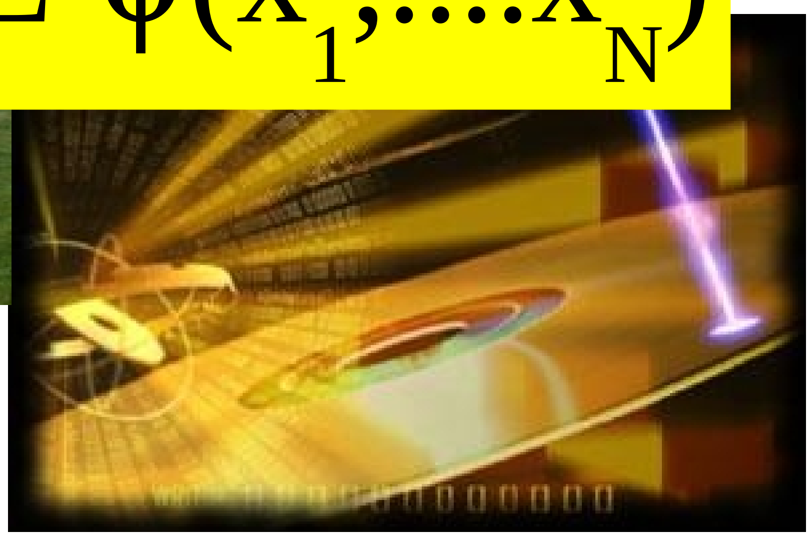
→ Theoretical Spectroscopy: aims and observations





$$H\psi(x_1,\ldots.x_N) = E\,\psi(x_1,\ldots.x_N)$$

?



→ Theoretical Spectroscopy: tools

Effective quantities in an effective world

A practical example, simulate zero gravity

→ Theoretical Spectroscopy: tools

Calculate only what you want,.....so that you can understand!

$$H\psi_n(x_1,....x_N) = E_n\,\psi_n(x_1,....x_N)$$

Want: → total energy E_0

→ expectation values like

* density
* spectral functions
* dielectric function

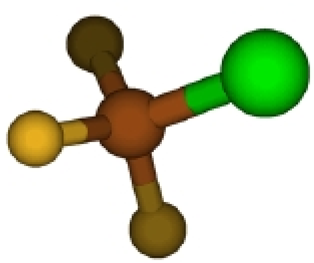
$$V_{tot}(\omega) = \varepsilon^{-1}(\omega) V_{ext}(\omega)$$

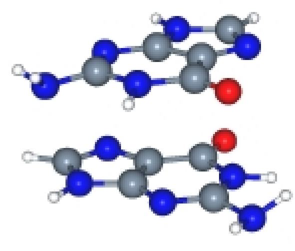
Do not want: → *all many-body* $\psi_n(x_1,....x_N)$

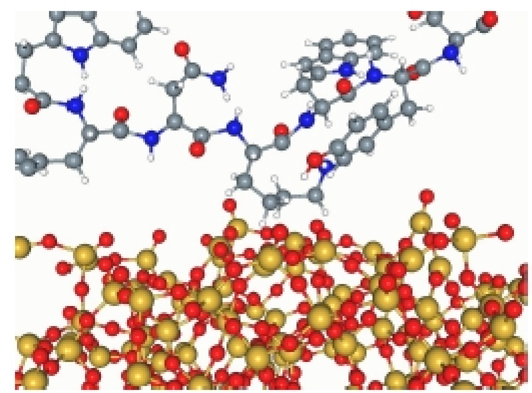
→ The effective quantities:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, .., \mathbf{r}_N, t) \quad \longrightarrow \quad G(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) \quad \longrightarrow \quad \rho(\mathbf{r}, t)$$

CI, QMC | GF methods (GW, BSE) | DF







→ The effective world:

$$\left(-\frac{1}{2}\nabla^2 + v_{\text{eff}}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r})$$

LDA or so

$$v_{\text{eff}}(\mathbf{r}) = \quad v_{\text{ext}}(\mathbf{r}) + v_{\text{H}}([n],\mathbf{r}) + v_{\text{xc}}([n],\mathbf{r})$$

Designed for density and top valence
NOT for bandgaps, for example!!!

Hohenberg-Kohn-Sham

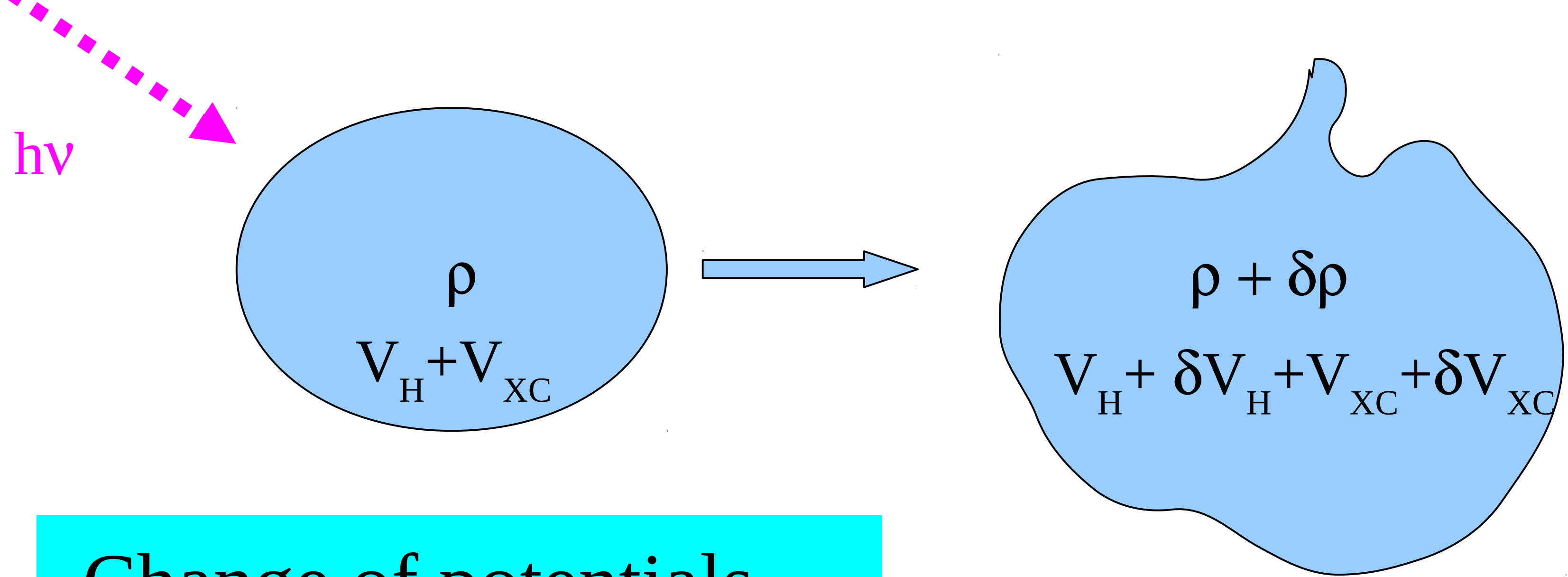
→ Theoretical Spectroscopy: tools

Effective quantities in an effective world

Time-dependent quantities – TD world

TDDFT intuitive :

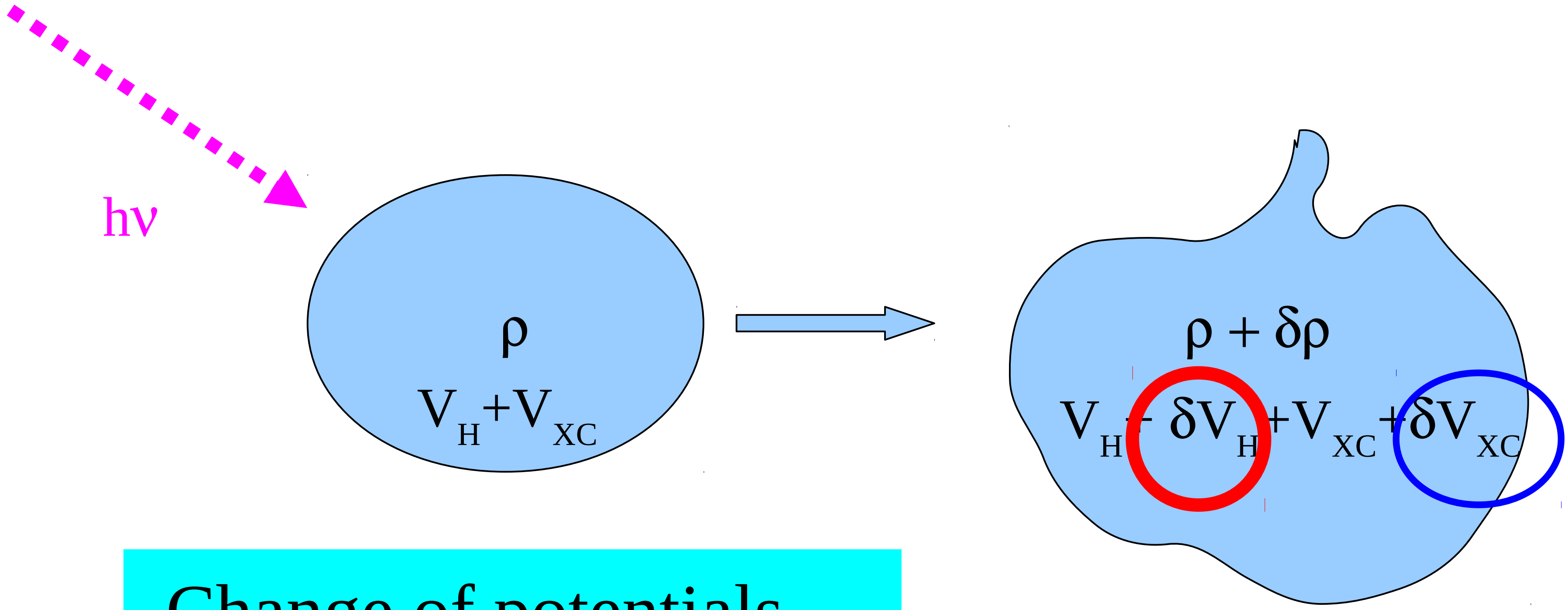
(TD)DFT point of view: moving density



Change of potentials

Excitation ?

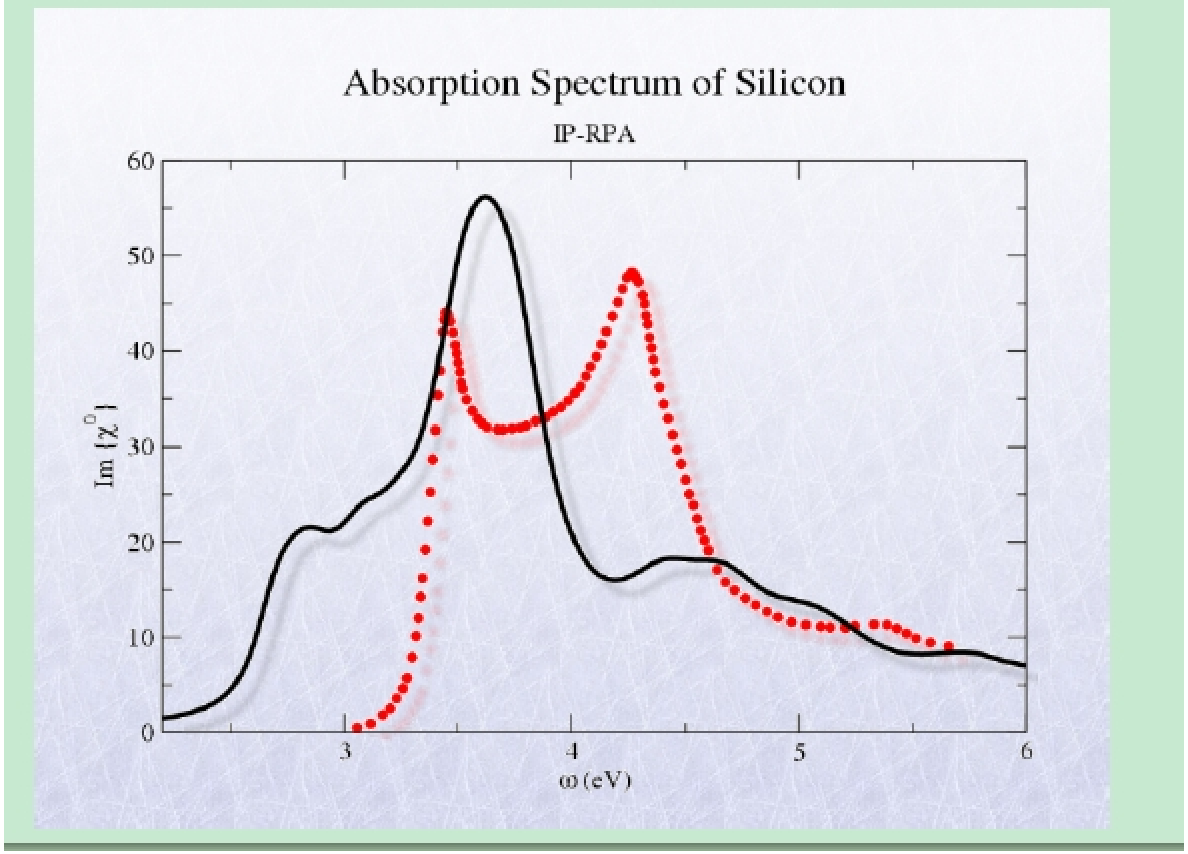
→ Induced potentials



Change of potentials

RPA

TDLDA, ….

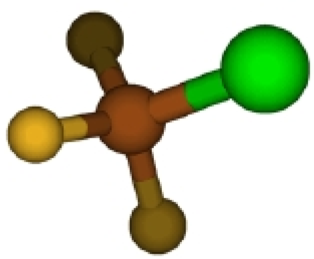


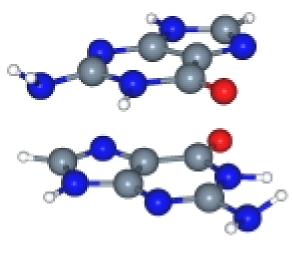
Absorption Spectrum of Silicon
IP-RPA
Im {χ^0}
ω (eV)
0
10
20
30
40
50
60
3
4
5
6

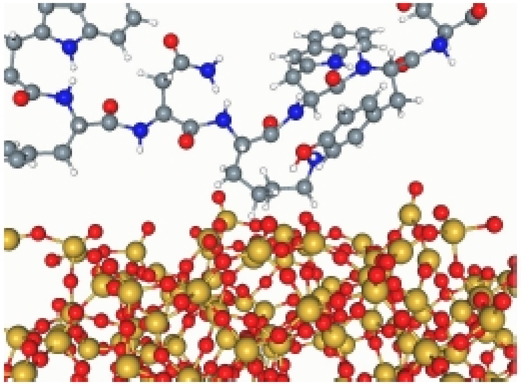
→ The effective quantities:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, .., \mathbf{r}_N, t) \longrightarrow G(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) \longrightarrow \rho(\mathbf{r}, t)$$

CI, QMC | GF methods (GW, BSE) | DF



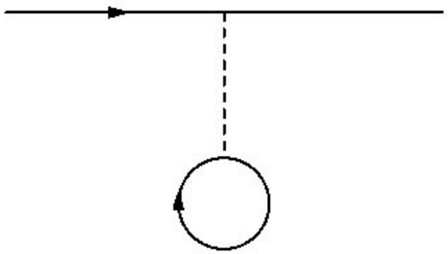


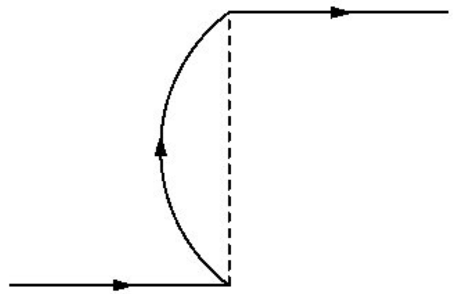


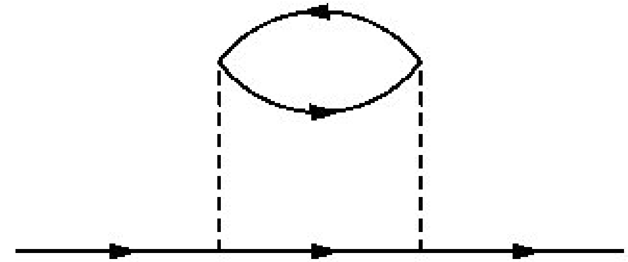
→ Propagators

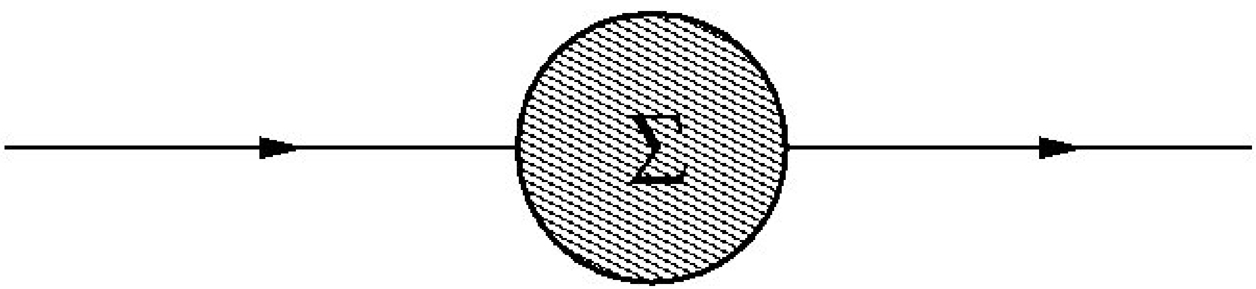
$$\mathcal{G}(1,2) = -i \langle T[\psi(1)\psi^\dagger(2)] \rangle \qquad 1=(r_1,\sigma_1,t_1)$$

$$n(1)=-iG(1,1^+)$$









Dyson equation: $\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \, \Sigma \, \mathcal{G}$

→ The effective world:

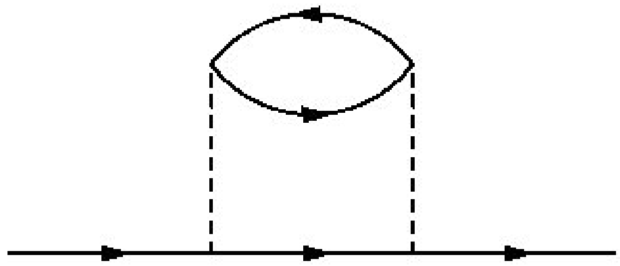
$$\left(-\frac{1}{2}\nabla^2 + v_{\text{eff}}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

$$v_{\text{eff}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + v_{\text{H}}([n],\mathbf{r}) + v_{\text{xc}}([n],\mathbf{r})$$

$$\Sigma(r,r',\varepsilon_i)$$

Designed for electron addition and removal spectra (bandstructure, lifetimes, satellites,....,density,...)

Other: DMFT $\Sigma_{ll}(\omega)$

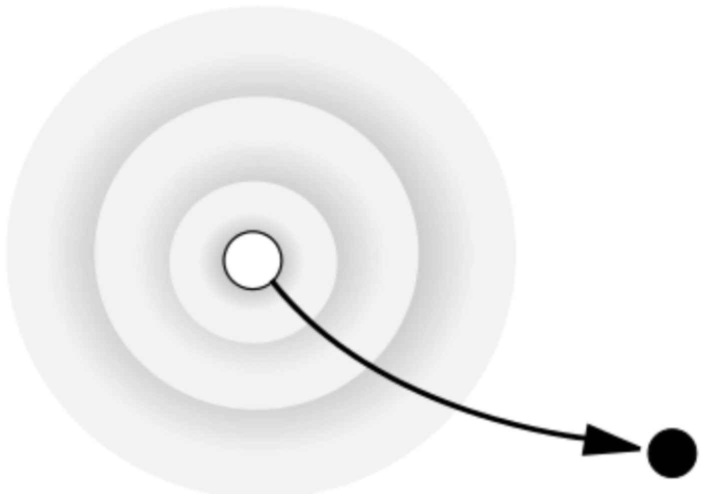


+ ....

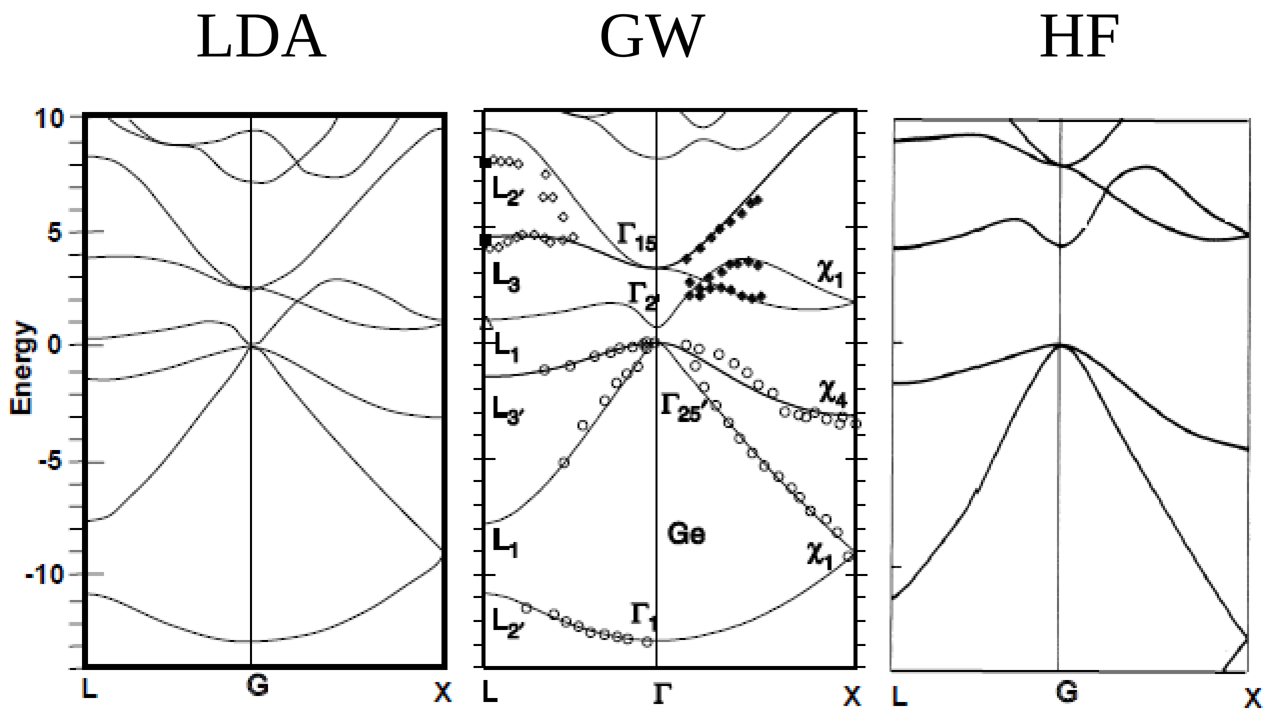
$\rightarrow \Sigma \sim i\,\mathcal{W}\mathcal{G}$ "GW"

L. Hedin (1965)

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



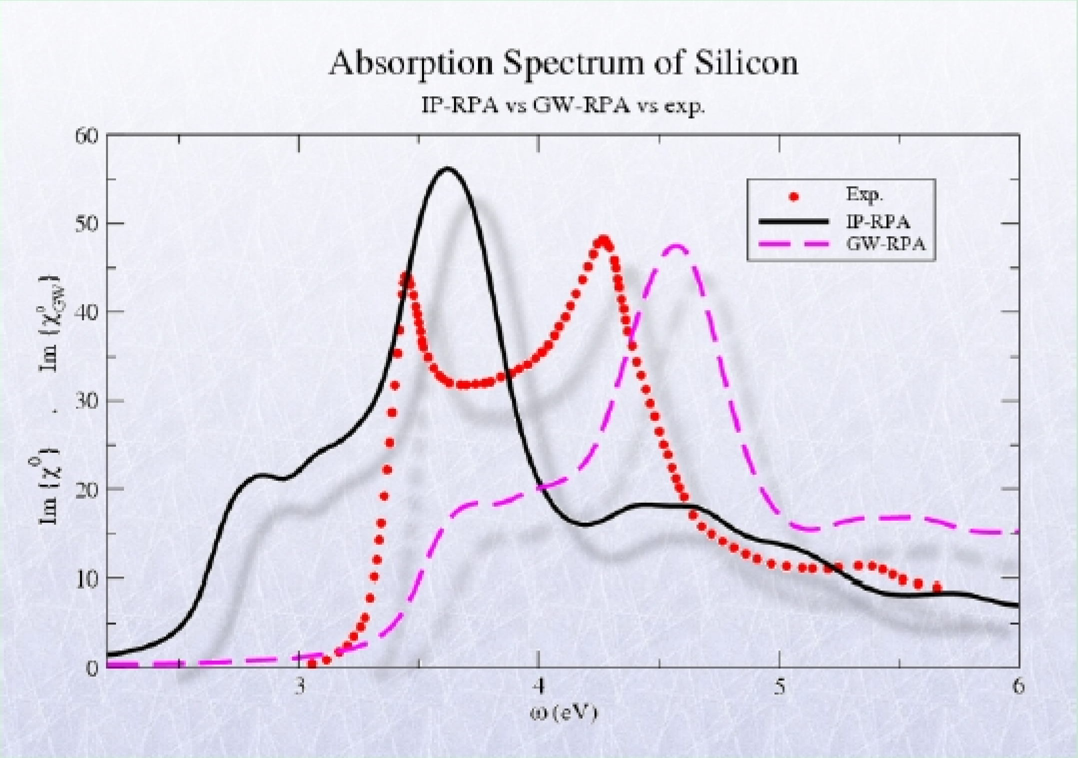
GW today: standard for bandstructures



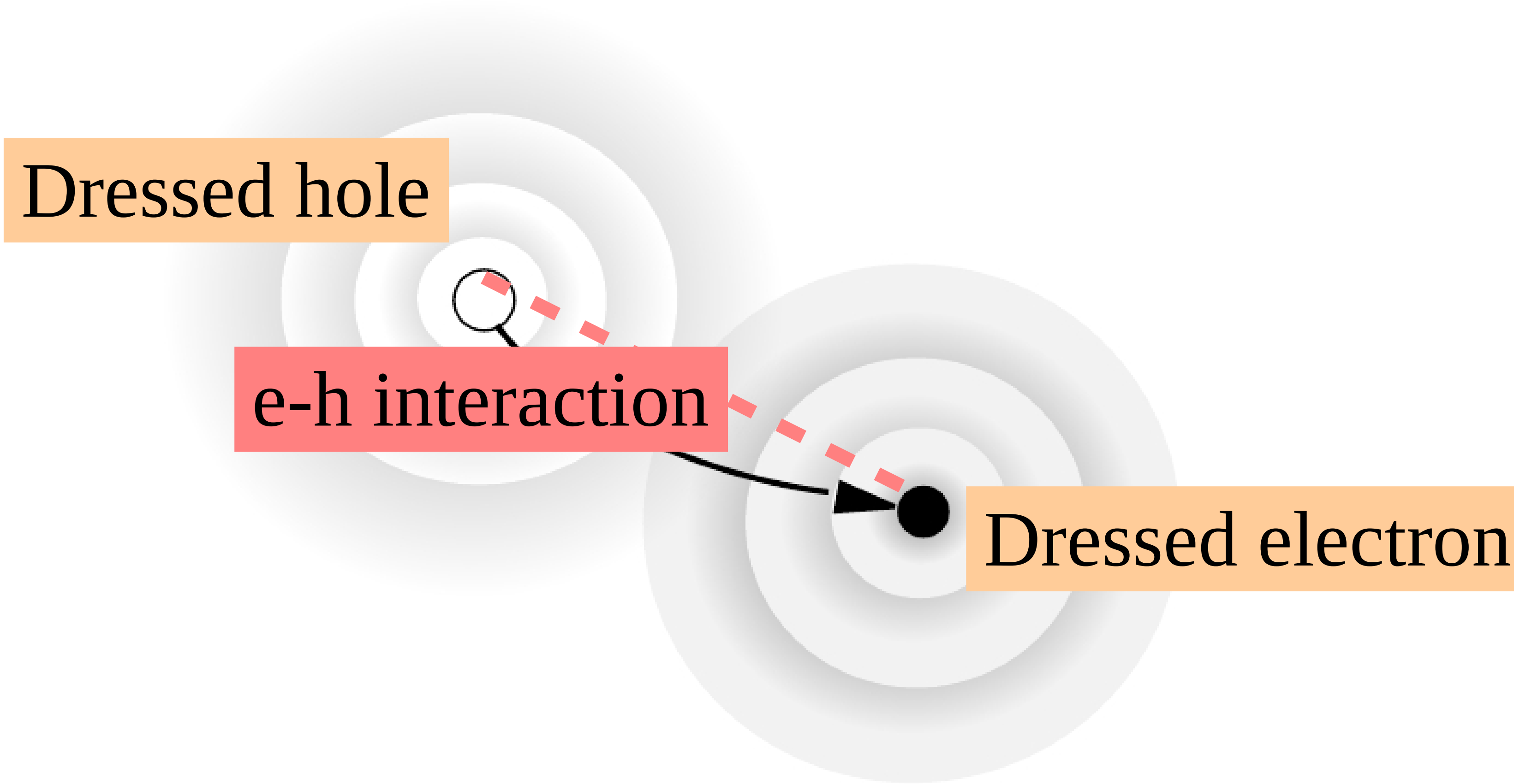
Bandstructure of germanium, theory versus experiment

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

Spectra in GW-RPA



→ What is missing?



e-h problem: Bethe-Salpeter equation

TD-.... ?

TD-GFT

Time evolution of the MBPT equations?

$(\partial/\partial t)G$..... Kwong and Bonitz, Phys. Rev. Lett. **84**, 1768 (2000)

van Leeuwen work

TD-GFT

Time evolution of the MBPT equations?

$(\partial/\partial t)G$..... Kwong and Bonitz, Phys. Rev. Lett. **84**, 1768 (2000)

van Leeuwen work

Tough!!!!!!!

The electron-hole problem : LR

Hedin's equations

$$\Sigma(1,2) = i \int d(34) G(1,3) \tilde{\Gamma}(3,2,4) W(4,1^+)$$

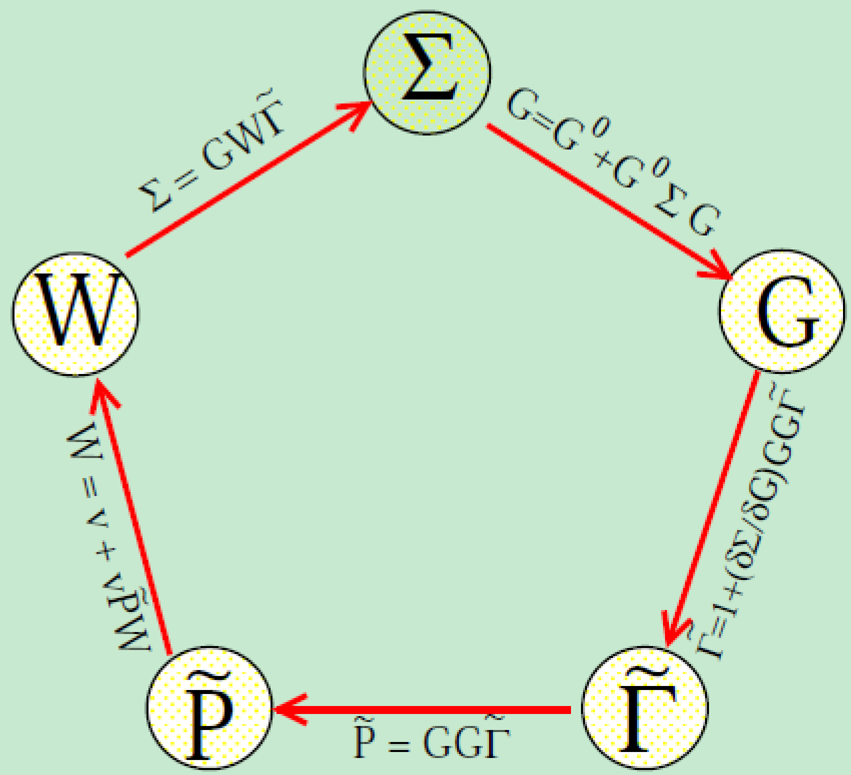
$$G(1,2) = G^0(1,2) + \int d(34) G^0(1,3) \Sigma(3,4) G(4,2)$$

$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \int d(4567) \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6) G(7,5) \tilde{\Gamma}(6,7,3)$$

$$\tilde{P}(1,2) = -i \int d(34) G(1,3) G(4,1^+) \tilde{\Gamma}(3,4,2)$$

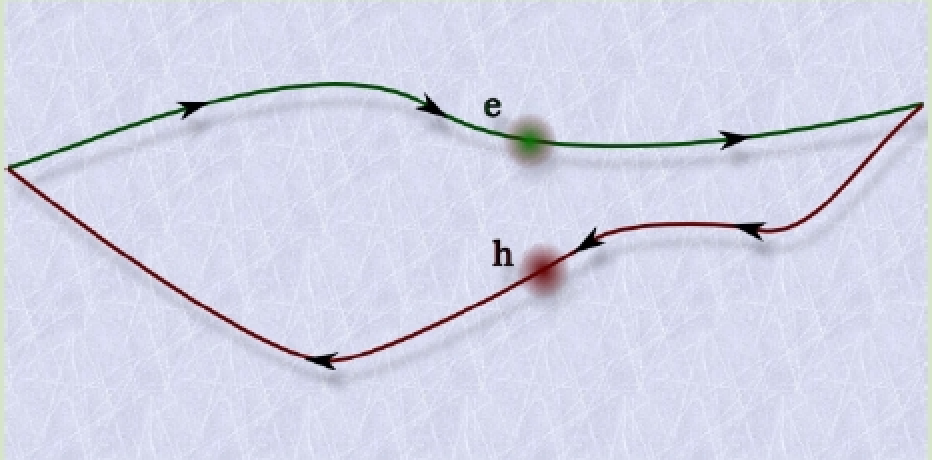
$$W(1,2) = v(1,2) + \int d(34) v(1,3) \tilde{P}(3,4) W(4,2)$$

Hedin's pentagon



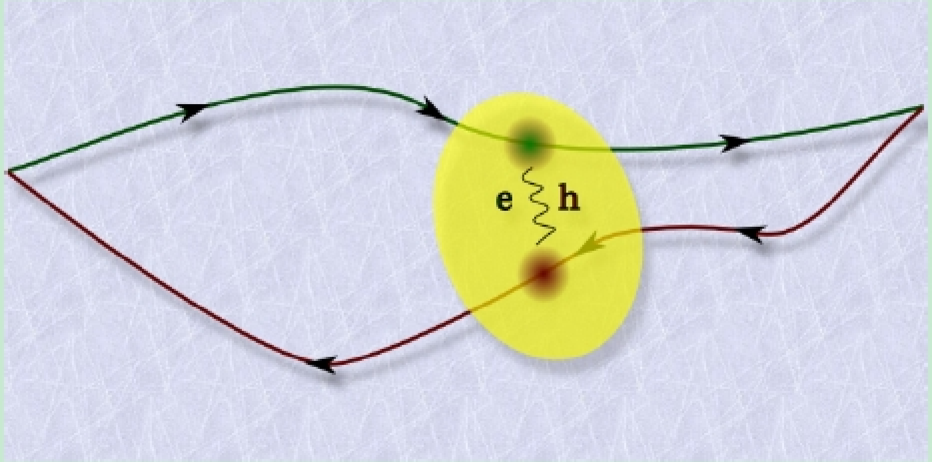
GG Polarizability

$$\tilde{P}(1,2) = -i \quad G(1,2)G(2,1^+)$$



GGΓ Polarizability

$$\tilde{P}(1,2) = -i \int d(34) G(1,3) G(4,1^{+}) \tilde{\Gamma}(3,4,2)$$



$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \\ + \int d(4567)\frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6) G(7,5) \tilde{\Gamma}(6,7,3)$$

Towards the Bethe-Salpeter

$$\tilde{\Gamma} = 1 + \frac{\delta\Sigma}{\delta G} GG\tilde{\Gamma}$$

$$GG\tilde{\Gamma} = GG + GG\frac{\delta\Sigma}{\delta G} GG\tilde{\Gamma}$$

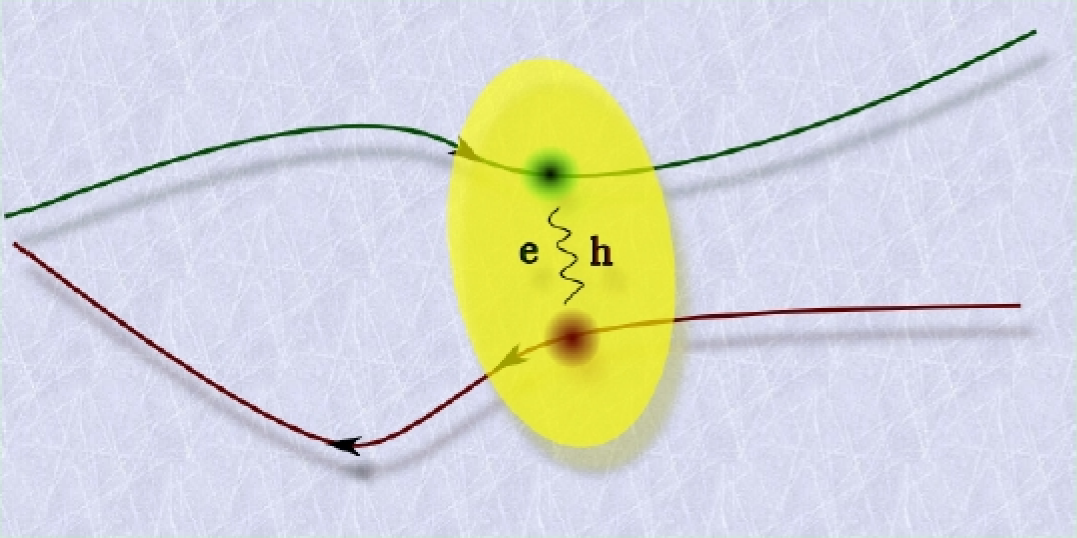
$$\tilde{L} = L^0 + L^0\frac{\delta\Sigma}{\delta G}\tilde{L}$$

$$\tilde{L}(1234) = L^0(1234) + L^0(1256)\frac{\delta\Sigma(56)}{\delta G(78)}\tilde{L}(7834)$$

Towards the Bethe-Salpeter Equation

From electron and hole propagation to **the electron-hole interaction**

$$\tilde{L}(1234) = L^0(1234) + L^0(1256)\frac{\delta\Sigma(56)}{\delta G(78)}\tilde{L}(7834)$$



Irreducible form of the Bethe-Salpeter equation

$$\tilde{L}(1234) = L^0(1234) + L^0(1256)\frac{\delta\Sigma(56)}{\delta G(78)}\tilde{L}(7834)$$

Reducible quantity

$$L = \tilde{L} + \tilde{L}vL$$

Bethe-Salpeter Equation

$$L(1234) = L^0(1234) + L^0(1256)\left[v(57)\delta(56)\delta(78) + \frac{\delta\Sigma(56)}{\delta G(78)}\right]L(7834)$$

$$\frac{\delta V_H}{\delta V_{ext}} = \frac{\delta V_H}{\delta n}\frac{\delta n}{\delta V_{ext}} = v\chi$$

$$\frac{\delta V_{xc}}{\delta V_{ext}} = \frac{\delta V_{xc}}{\delta n}\frac{\delta n}{\delta V_{ext}} = f_{xc}\chi$$

$$\chi = \chi^0 + \chi^0\left(v + f_{xc}\right)\chi$$

with $\mathbf{f_{xc}}$ = **exchange-correlation kernel**

Comparison with Linear Response quantities

$$\chi(12) = \frac{\delta n(1)}{\delta V_{ext}(2)}$$

$$L(1234) = \frac{\delta G(12)}{\delta \tilde{V}_{ext}(34)}$$

Comparison with Linear Response quantities

$$\chi(12) = \frac{\delta n(1)}{\delta V_{ext}(2)}$$

$$L(1133) = \frac{\delta G(11)}{\delta \tilde{V}_{ext}(33)}$$

Comparison with Linear Response quantities

$$\chi(12) = \frac{\delta n(1)}{\delta V_{ext}(2)}$$

$$L(1133) = \frac{\delta n(1)}{\delta V_{ext}(3)}$$

Comparison with Linear Response quantities

$$\chi(12) = \frac{\delta n(1)}{\delta V_{ext}(2)}$$

$$L(1133) = \frac{\delta n(1)}{\delta V_{ext}(3)}$$

Bethe-Salpeter Equation

$$L(1234) = L^0(1234) + L^0(1256)\left[v(57)\delta(56)\delta(78) + \frac{\delta\Sigma(56)}{\delta G(78)}\right] L(7834)$$

Comparison with Linear Response quantities

$$\chi(12) = \frac{\delta n(1)}{\delta V_{ext}(2)}$$

$$L(1133) = \frac{\delta n(1)}{\delta V_{ext}(3)}$$

Bethe-Salpeter Equation

$$L(1234) = L^0(1234) + L^0(1256)\left[v(57)\delta(56)\delta(78) + \frac{\delta\Sigma(56)}{\delta G(78)}\right]L(7834)$$

Have to solve 4 point equation, then take a part!

We have the (4-point)
Bethe-Salpeter equation.
And now ?

Approximations

First point: Choosing Σ

$$L(1234) = L^0(1234) + L^0(1256)\left[v(57)\delta(56)\delta(78) + \frac{\delta\Sigma(56)}{\delta G(78)}\right]L(7834)$$

Screened Coulomb term

$$\Sigma^{GW}(1,2) = iG(12)W(21)$$

⇒ **Standard Bethe-Salpeter equation (Time-Dependent Screened Hartree-Fock)**

Choice of $\Sigma = GW$

Everything should be coherently chosen

$\Rightarrow$ ground state calculation $\longrightarrow \quad \phi_i, \epsilon_i$

$\Rightarrow$ $G^0_{\mathrm{KS}} \quad ; \quad \varepsilon^{-1}_{\mathrm{RPA}}(\mathbf{r}, \mathbf{r}', \omega) \quad ; \quad W(\mathbf{r}, \mathbf{r}', \omega) = \varepsilon^{-1}_{\mathrm{RPA}} v$

$\Rightarrow$ $\Sigma(\mathbf{r}, \mathbf{r}', \omega) = \int d\omega' \, G^0_{\mathrm{KS}}(\mathbf{r}, \mathbf{r}', \omega') W(\mathbf{r}, \mathbf{r}', \omega + \omega')$

$\Rightarrow$ $E_i = \epsilon_i + \Delta_i^{\mathrm{GW}} \quad ; \quad \psi_i \simeq \phi_i$

$\Rightarrow$ $G^{\mathrm{GW}}(\mathbf{r}, \mathbf{r}', \omega)$

$$L = GG + GG\left[v - W\right]L$$

$\Rightarrow$ Approx. $\dfrac{\delta W}{\delta G} = 0$

W static

Realizations

$$L(1234,\omega) = L^0(1234,\omega) + L^0(1256,\omega)K(5678)L(7834,\omega)$$

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = L^{0\,(n_3 n_4)}_{(n_1 n_2)}(\omega) + L^{0\,(n_5 n_6)}_{(n_1 n_2)}(\omega)K^{(n_7 n_8)}_{(n_5 n_6)}L^{(n_3 n_4)}_{(n_7 n_8)}(\omega)$$

We work in transition space...

$$L(1234,\omega) \Rightarrow L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) =$$

$$= \int d(1234)L(1234,\omega)\phi_{n_1}(1)\phi^*_{n_2}(2)\phi_{n_3}(3)\phi^*_{n_4}(4) = \ll L \gg$$

Clever choice of the basis ϕ_n

$$L_{(n_1 n_2)}^{(n_3 n_4)}(\omega) = L_{(n_1 n_2)}^{0\,(n_3 n_4)}(\omega) + L_{(n_1 n_2)}^{0\,(n_5 n_6)}(\omega) K_{(n_5 n_6)}^{(n_7 n_8)} L_{(n_7 n_8)}^{(n_3 n_4)}(\omega)$$

... some “trivial” mathematical arzigogoli ...

$$L_{(n_1 n_2)}^{(n_3 n_4)}(\omega) = \left[(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + K_{(n_1 n_2)}^{(n_3 n_4)} \right]^{-1}$$

$$L_{(n_1 n_2)}^{(n_3 n_4)}(\omega) = [(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg]^{-1}$$

The Excitonic Hamiltonian

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = [(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg]^{-1}$$

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = \frac{1}{H^{exc} - \omega}$$

$$H^{exc} = (E_{n_2} - E_{n_1})\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg$$

Resonant vs Coupling

$n_1, n_2, n_3, n_4 = v, c \quad (\mathbf{k})$

$$H^{reso} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + \ll v \gg - \ll W \gg$$

(Where are we going....???)

$n_1, n_2, n_3, n_4 = v, c \quad (\mathbf{k})$

$$H^{reso} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + \ll v \gg - \ll W \gg$$

(Where are we going....???)

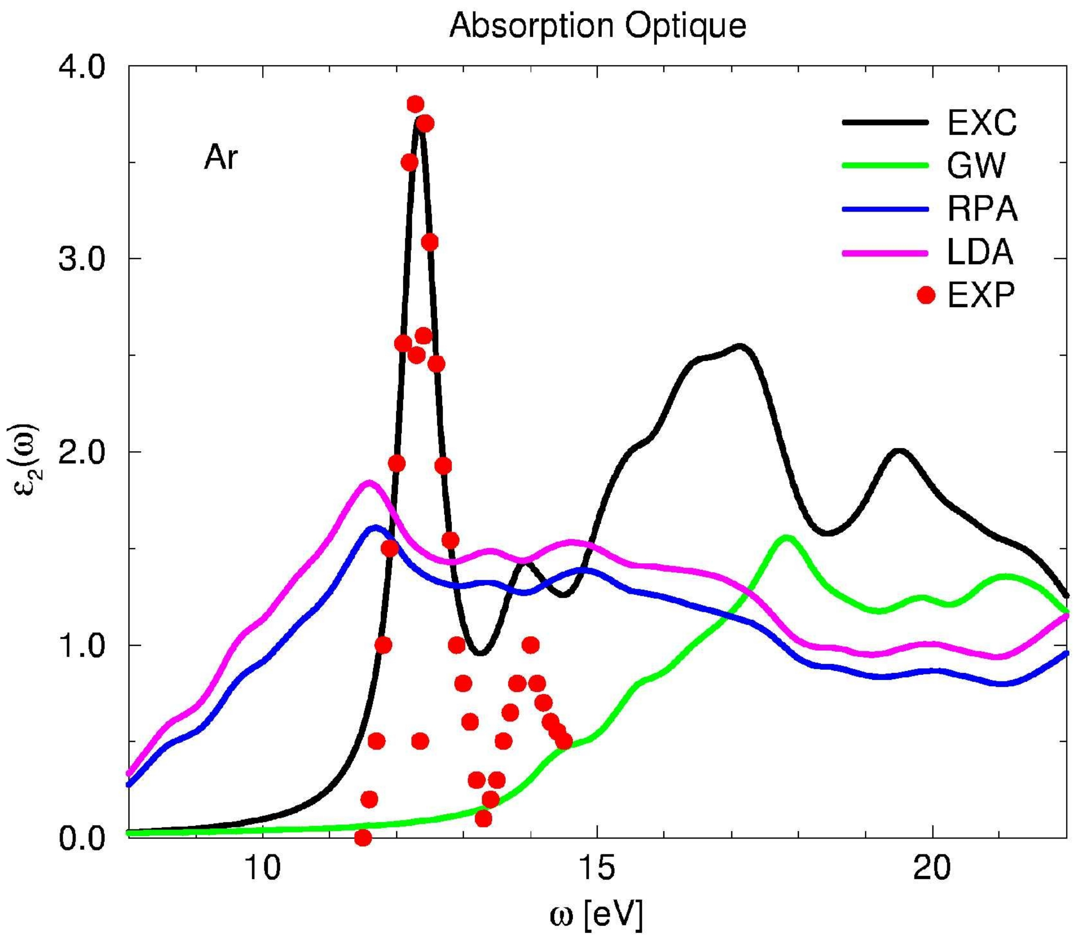
$n_1, n_2, n_3, n_4 = v, c \quad (\mathbf{k})$

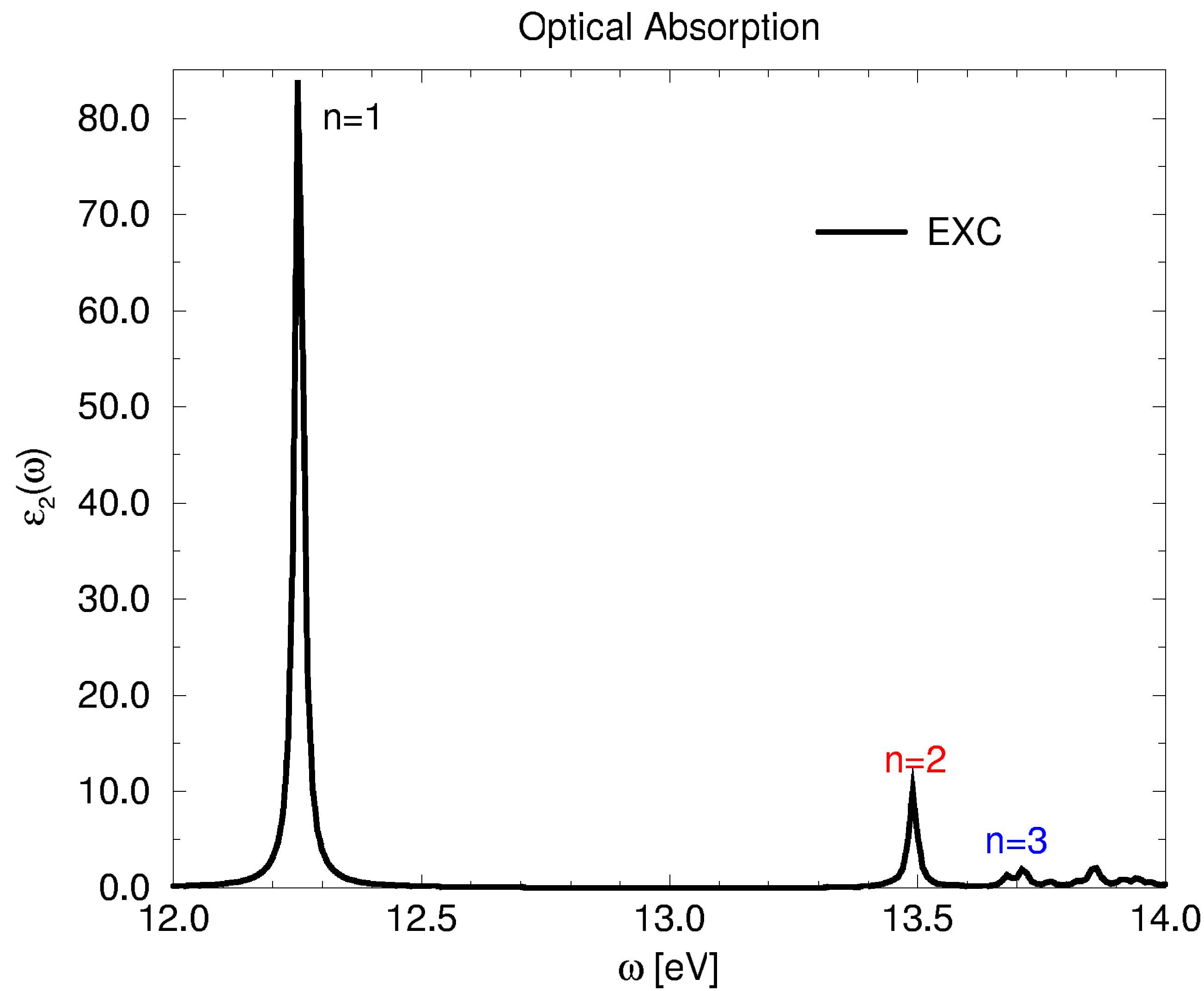
$$H^{reso} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + \cancel{\ll V \gg} - \ll W \gg$$

$k^2/2m^*$ → $-\dfrac{\nabla^2}{2m^*}$

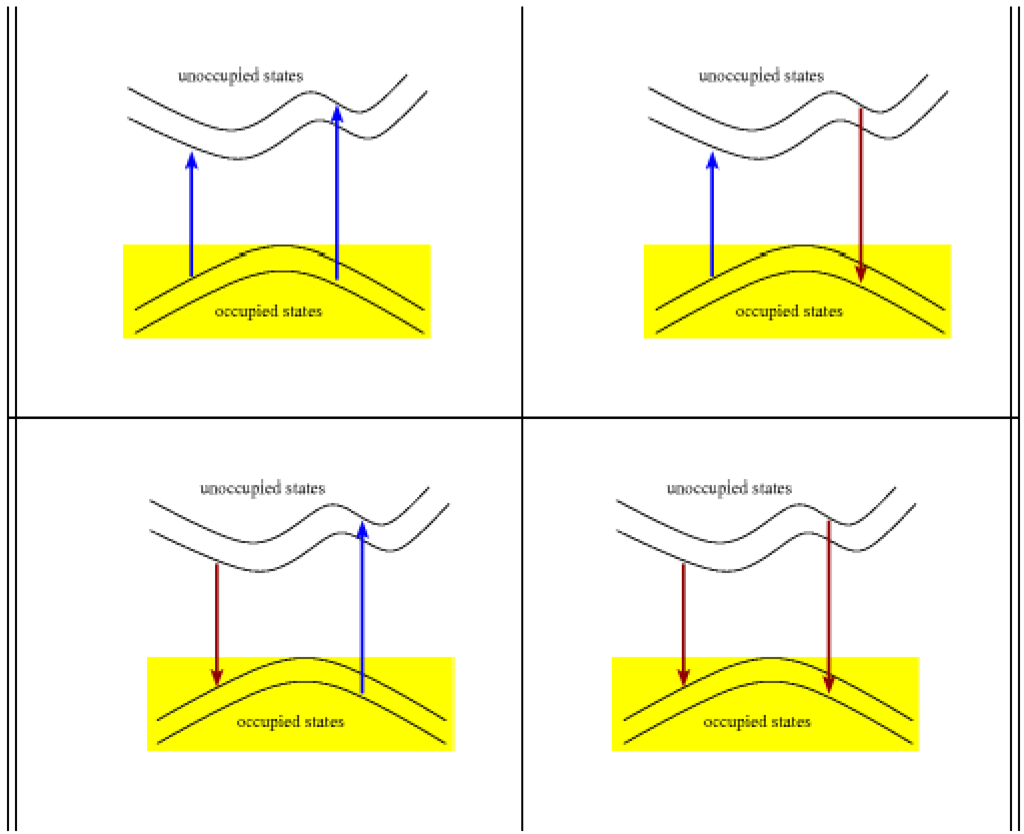
$-1/\varepsilon k^2$ → $-1/\varepsilon r$

Wannier exciton – "hydrogen atom"


Absorption Optique
Ar
EXC
GW
RPA
LDA
EXP
4.0
3.0
2.0
1.0
0.0
10
15
20
$\varepsilon_2(\omega)$
ω [eV]



Optical Absorption
n=1
EXC
n=2
n=3
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
ε2(ω)
12.0
12.5
13.0
13.5
14.0
ω [eV]


unoccupied states
occupied states
unoccupied states
occupied states
unoccupied states
occupied states
unoccupied states
occupied states

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = [(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg]^{-1}$$

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = [H^{exc} - \omega]^{-1}$$

$$H^{exc} = [(E_{n_2} - E_{n_1})\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg]$$

Diagonalization

Iterative inversion

Diagonalization case (only resonant approx)

$$L_{vc}^{v'c'} = [(E_c - E_v)\,\delta_{vv'}\delta_{cc'} - \omega + \ll v \gg - \ll W \gg]^{-1}$$

$$\frac{1}{H - \omega I} = \sum_{\lambda} \frac{|A_\lambda >< A_\lambda|}{E_\lambda - \omega}$$

Spectrum within BSE

$$L(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\lambda} \frac{\sum_{vc} A_\lambda^{(vc)} \phi_v(\mathbf{r}) \phi_c^*(\mathbf{r}) \phi_v^*(\mathbf{r}') \phi_c(\mathbf{r}') A_\lambda^{*(vc)}}{\omega - E_\lambda^{exc} + i\eta}$$

Spectrum in BSE (only resonant)

$$\mathrm{Abs}^{\mathrm{BSE}}(\omega) = Im\,\langle L(\omega)\rangle = \sum_{\lambda} \left| \sum_{vc} A_{\lambda}^{(vc)} \langle c|D|v\rangle \right|^2 \delta\left(\omega - E_{\lambda}^{exc}\right)$$

$$\mathrm{Abs}^{\mathrm{IP\text{-}RPA}}(\omega) = Im\,\langle \chi^0(\omega)\rangle = \sum_{vc} \left|\langle c|D|v\rangle\right|^2 \delta\left(\omega - (\epsilon_c - \epsilon_v)\right)$$

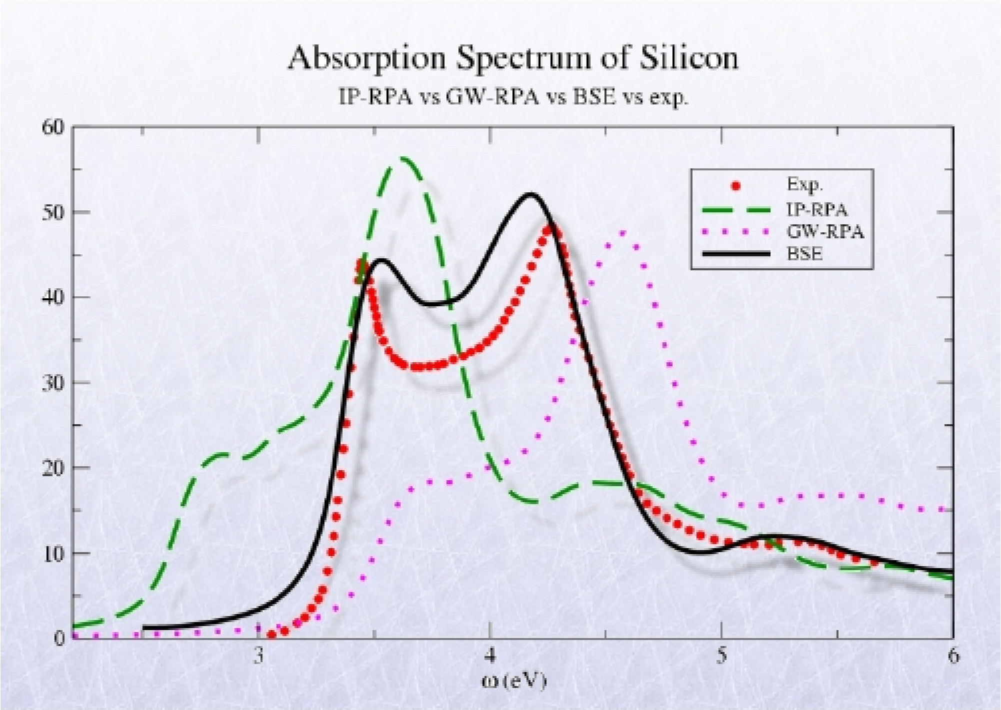
BSE - creating and diagonalizing a (big) matrix

$$\Rightarrow H^{exc}_{(vc)(v'c')} A^{(v'c')}_{\lambda} = E^{exc}_{\lambda} A^{(vc)}_{\lambda}$$

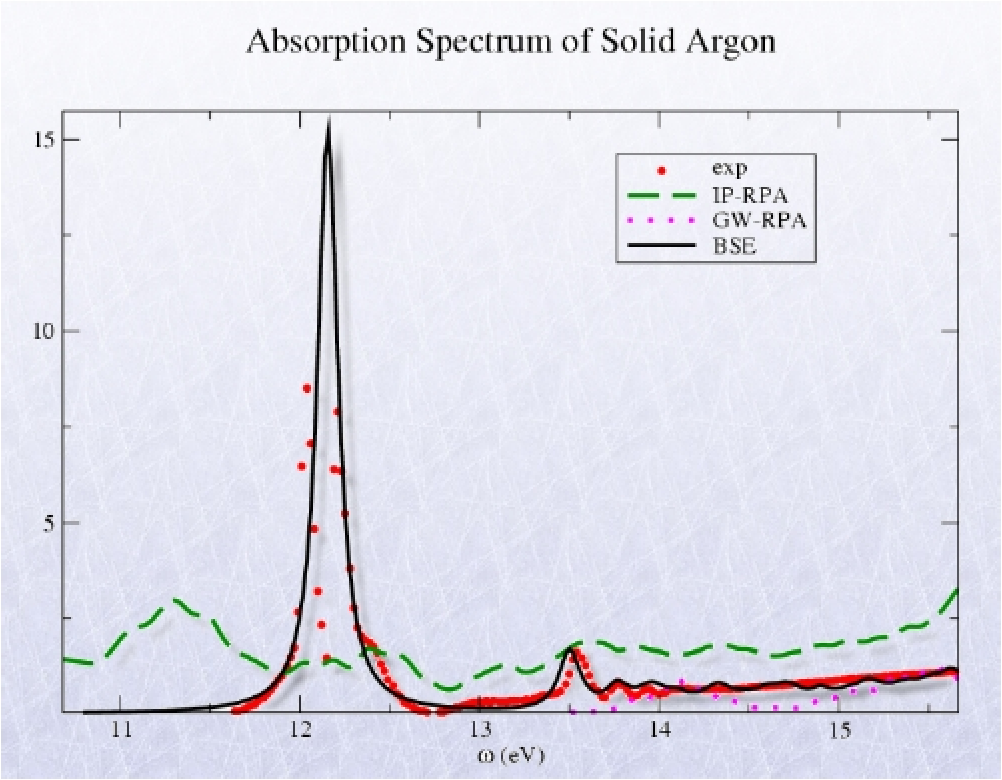
$$\Rightarrow L^{(v'c')}_{(vc)}(\omega) = \sum_{\lambda} \frac{A^{(vc)}_{\lambda} A^{*(v'c')}_{\lambda}}{\omega - E^{exc}_{\lambda} + i\eta}$$

Standard Approximations for BSE

- Ground-state
  - pseudopotential
  - V_{xc} local density approximation
- Quasi-particle Many-Body Theory
  - GW approximation for Σ
  - W rpa, plasmon-pole model
  - $\psi_{\mathrm{GW}} = \phi_{\mathrm{KS}}$
- Bethe-Salpeter equation
  - $\frac{\delta W}{\delta G} = 0$
  - W rpa, static
  - only resonant term

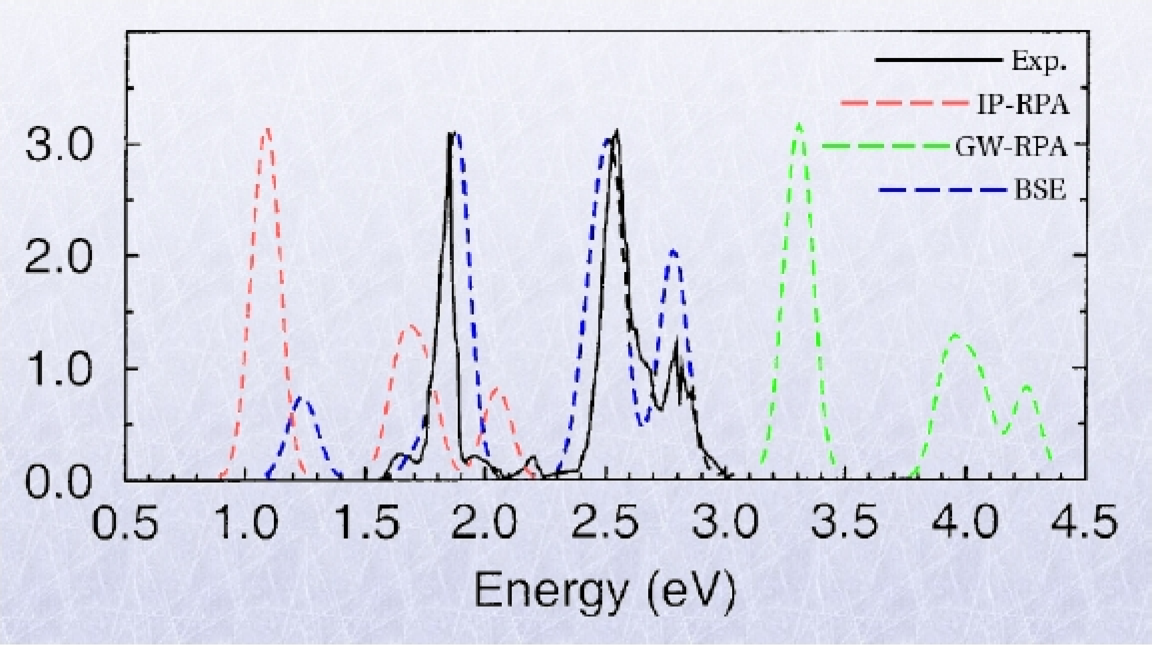


Albrecht *et al.*, PRL **80**, 4510 (1998)

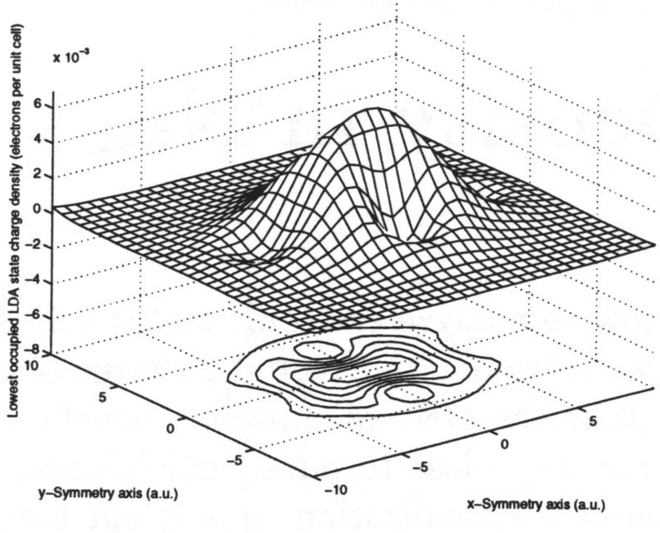


Sottile, Marsili, *et al.*, PRB (2007).

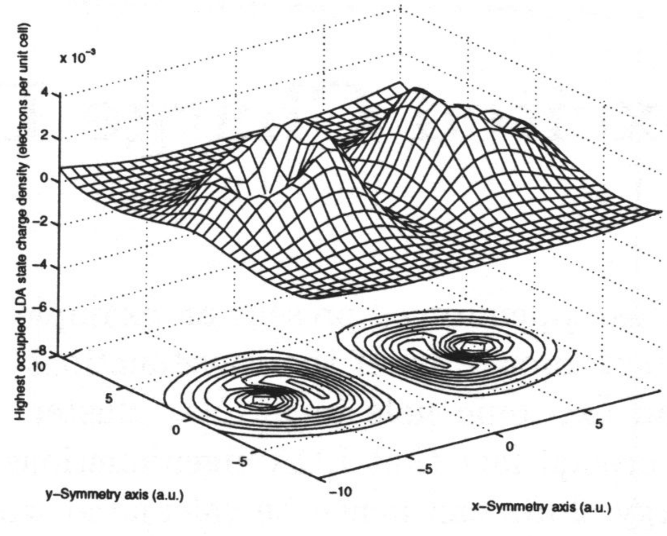
Bethe-Salpeter equation results: Molecule (Na_4)



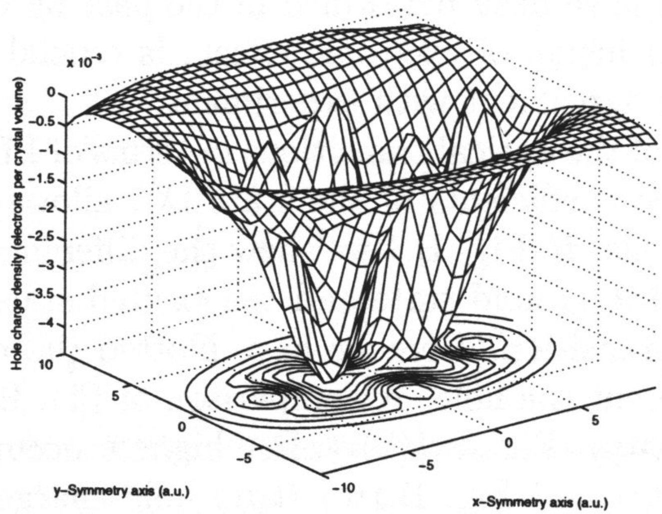
Onida *et al.*, PRL **75**, 818 (1995)



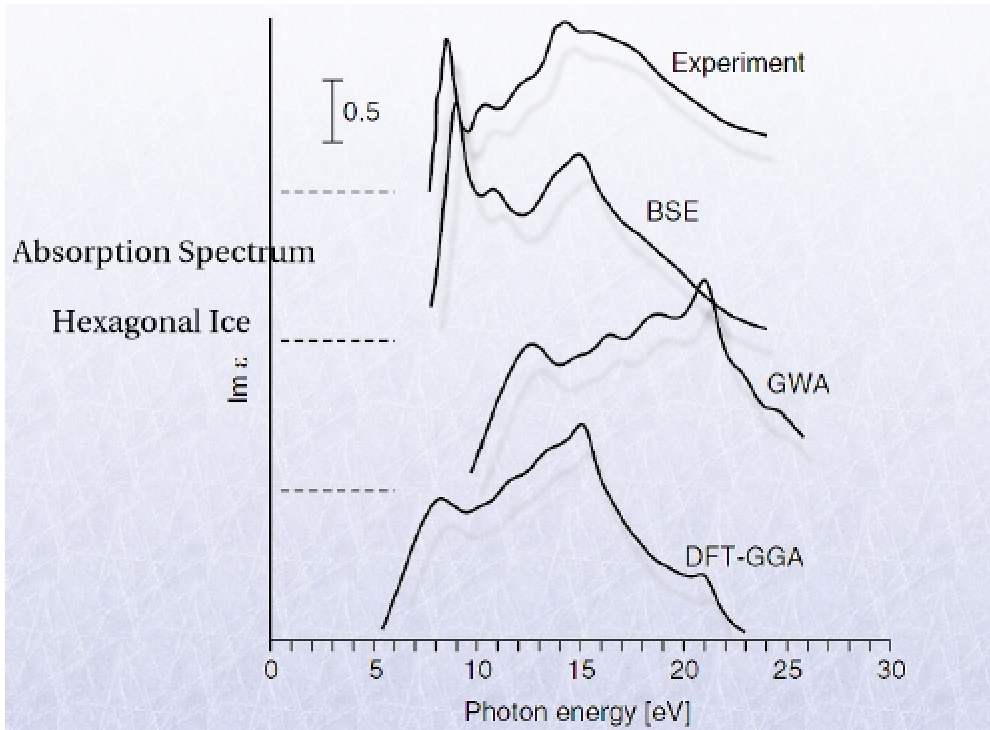
(a) Charge density of the lowest occupied LDA state.



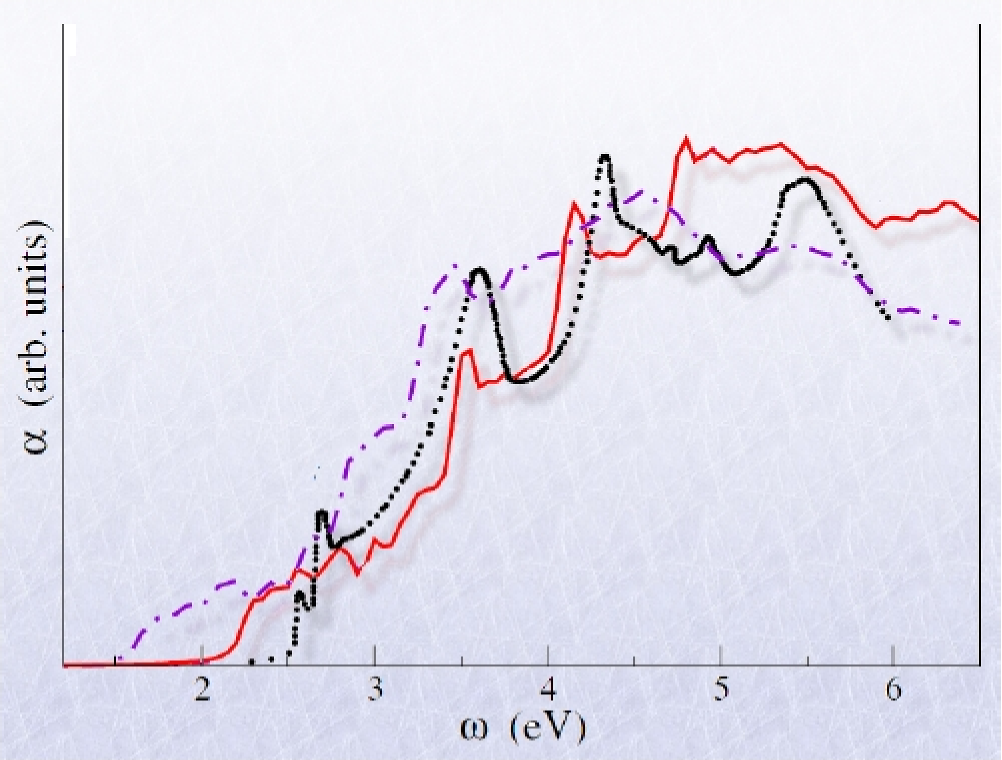
(b) Charge density of the highest occupied LDA state.



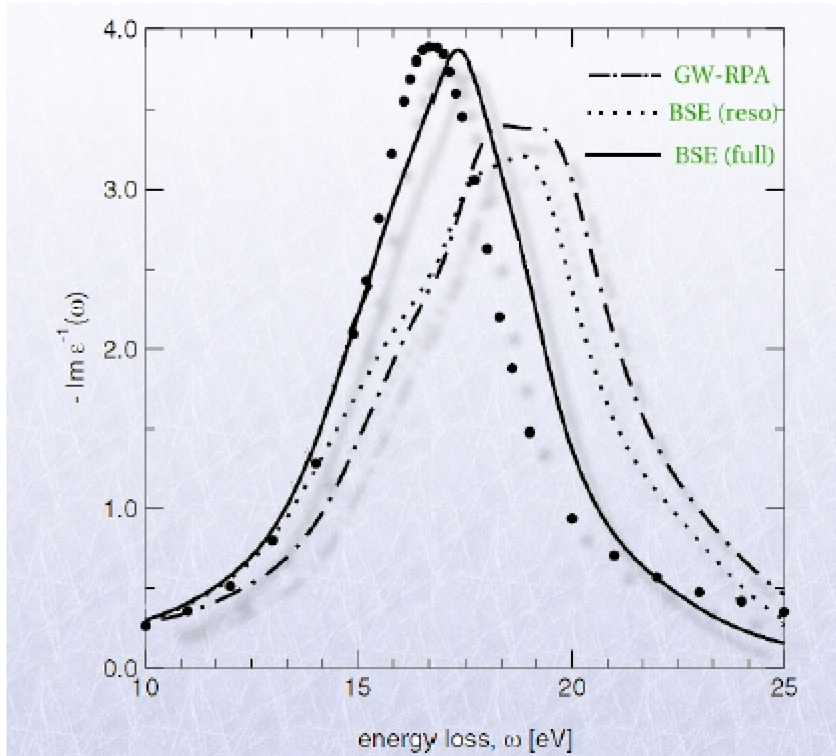
(c) Charge density of the true hole.



Hahn *et al.*, PRL **94**, 37404 (2005)



Bruneval *et al.*, PRL **97**, 267601 (2006)



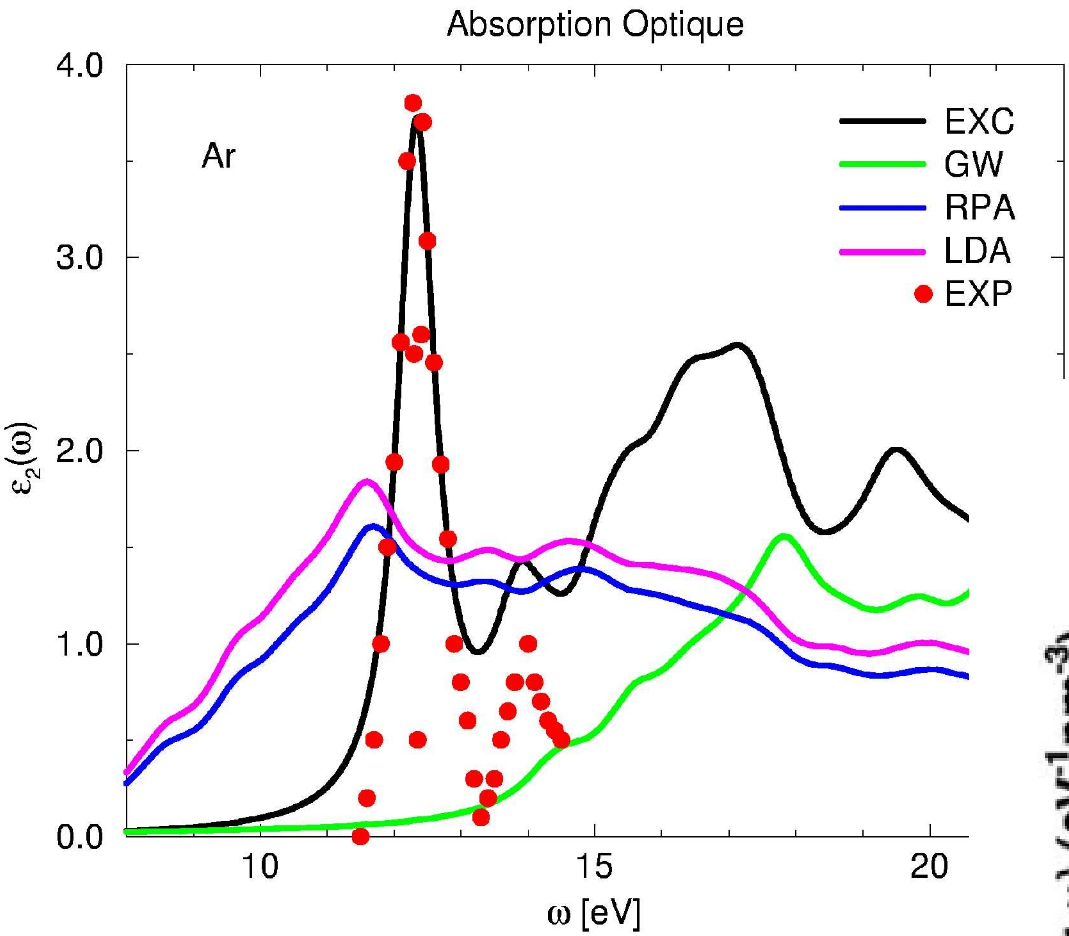
Olevano and Reining, PRL **86**, 5962 (2001)

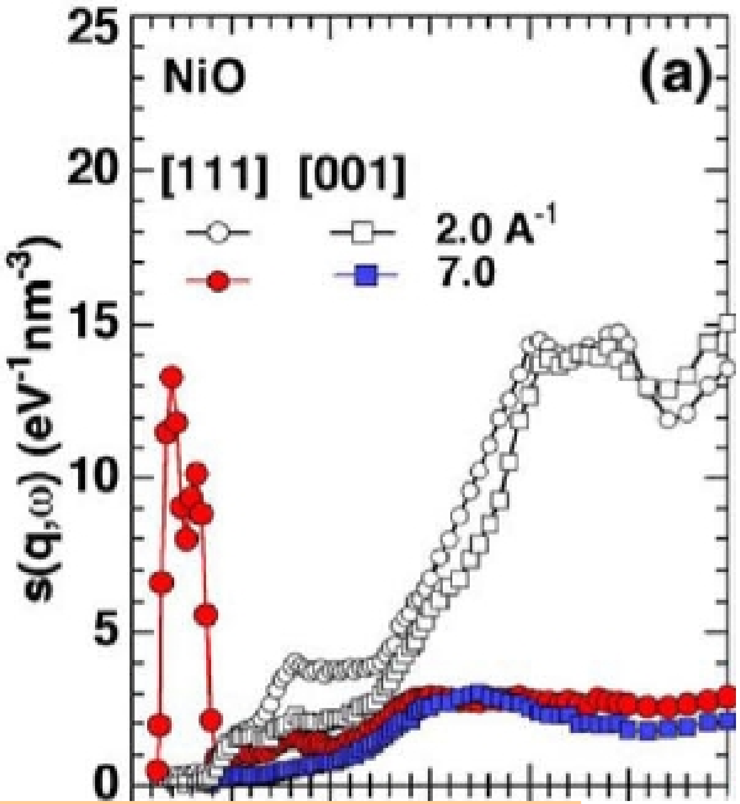
- DFT - ground state
- GW - quasiparticle energies
- BSE - optical and dielectric properties

√ several spectroscopies

√ variety of systems

× Cumbersome Calculations



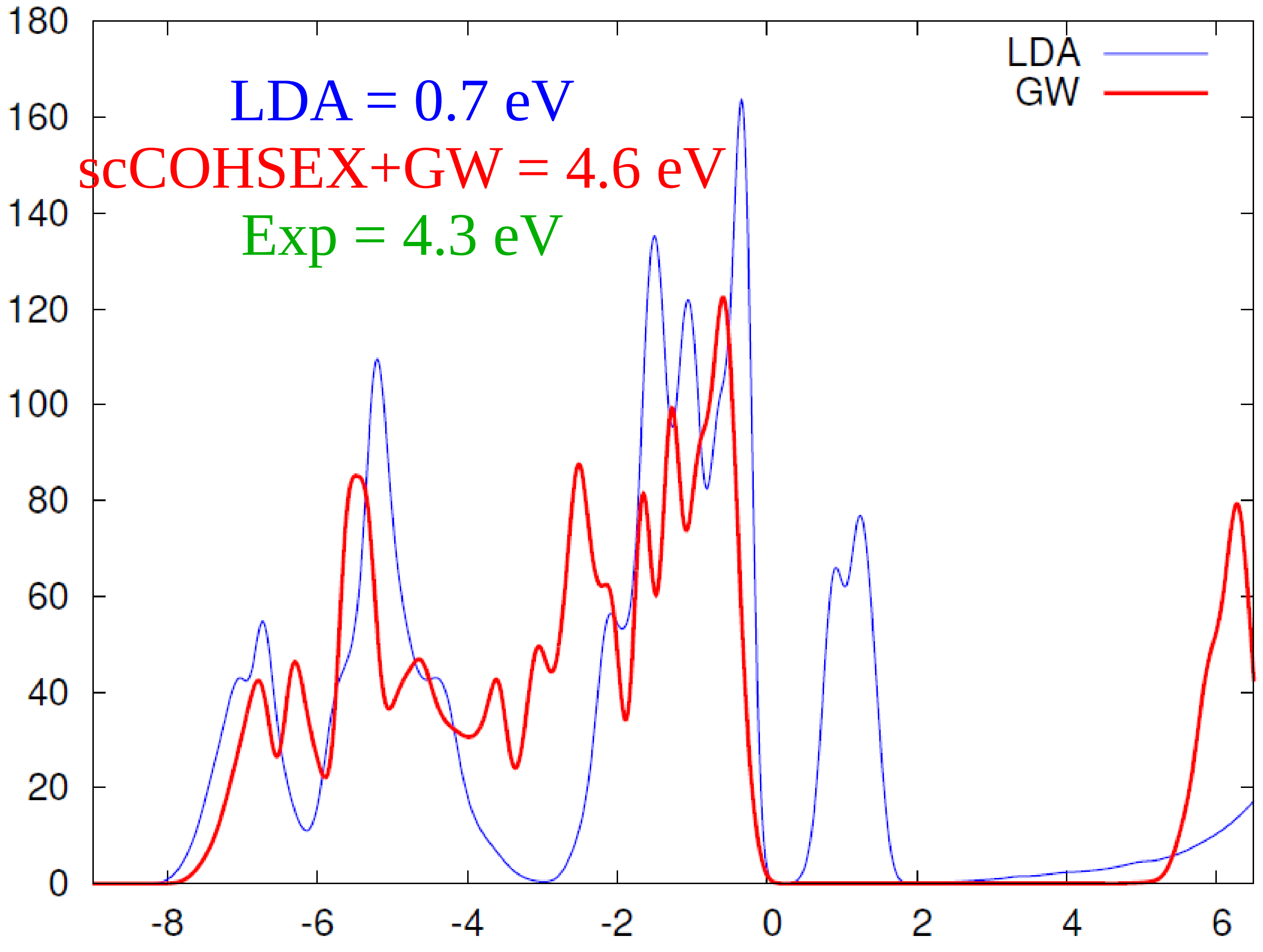


V. Olevano et al. (2000)
(bulk silicon 1998)

Larson et al., PRL 99, 026401 (2007)

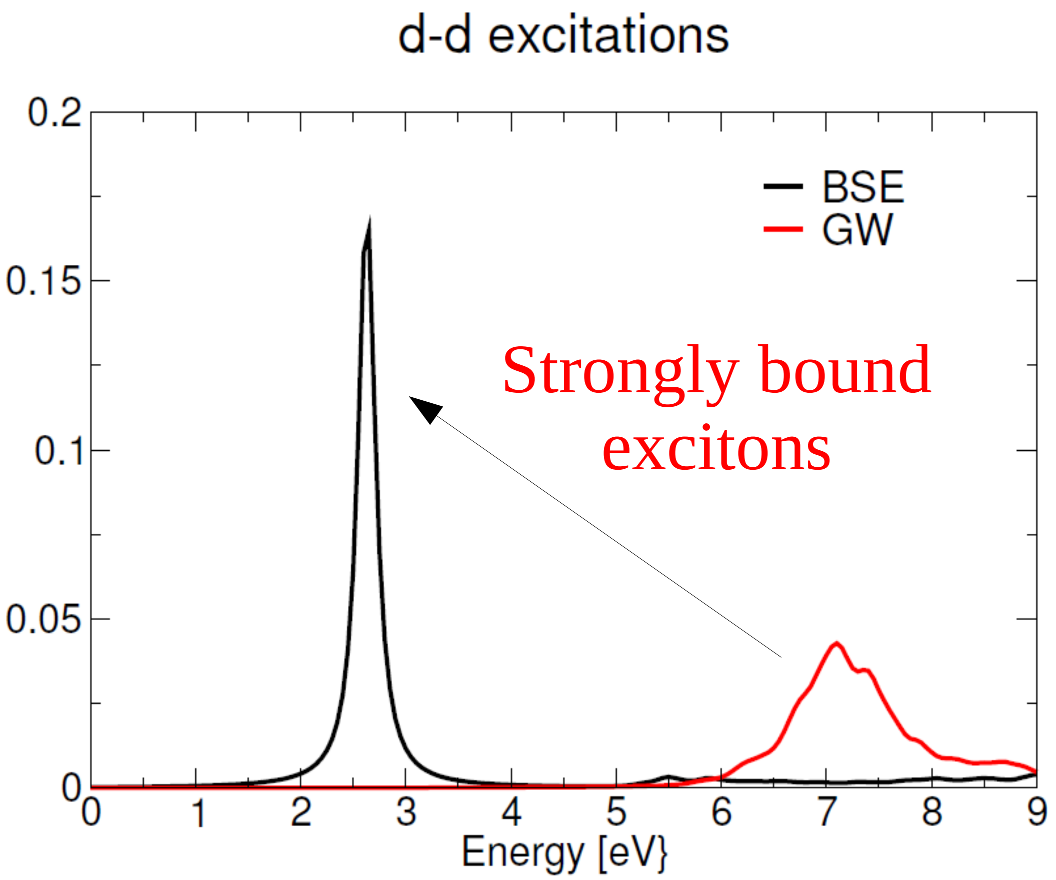
Exciton: Lee, Hsueh, Ku, PRB 82, 081106 (2010)

NiO: density of states



M. Guzzo, Master thesis (2008)

NiO: dd excitations

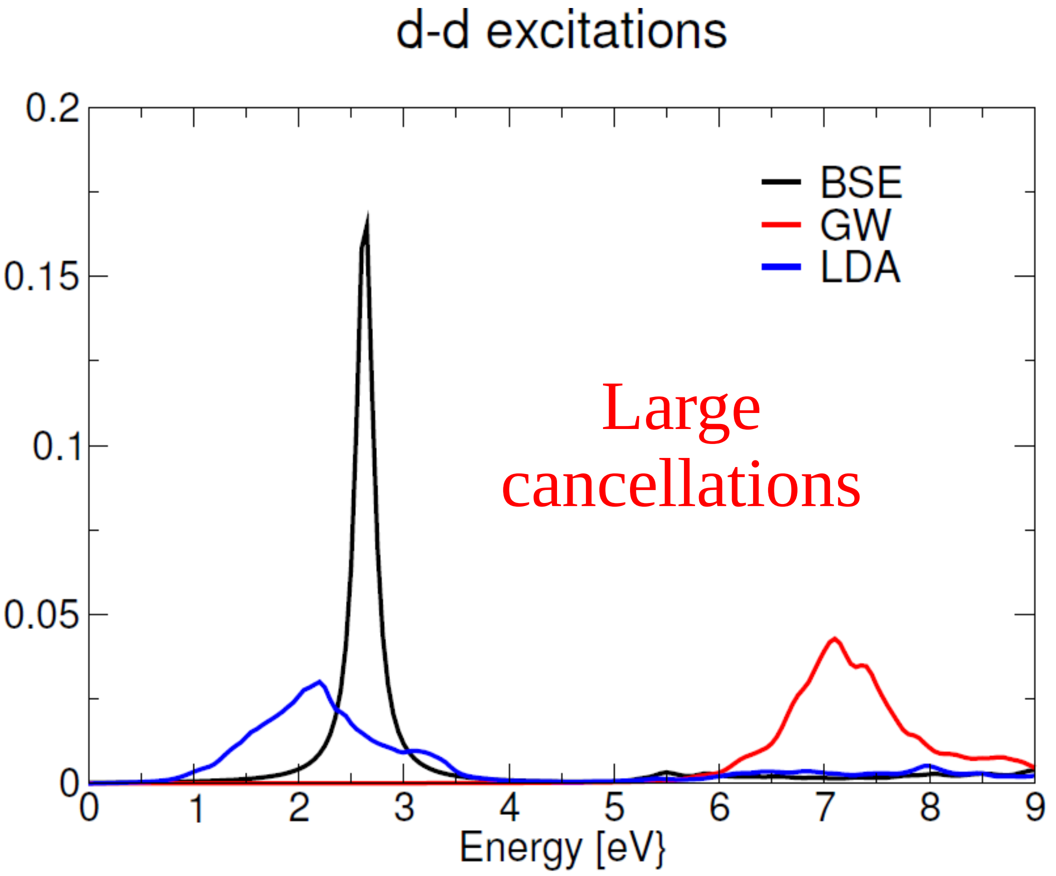


Q ~ 8 Å^{-1} [111]

M. Gatti et al. (2014)

BSE(q): M. Gatti and F. Sottile, Phys. Rev. B 88, 155113 (2014) (LiF)

NiO: dd excitations



Notes:

* Finite systems and correlation

* The “bandgap problem”

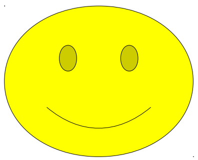
* Excitons are fake!

Notes:

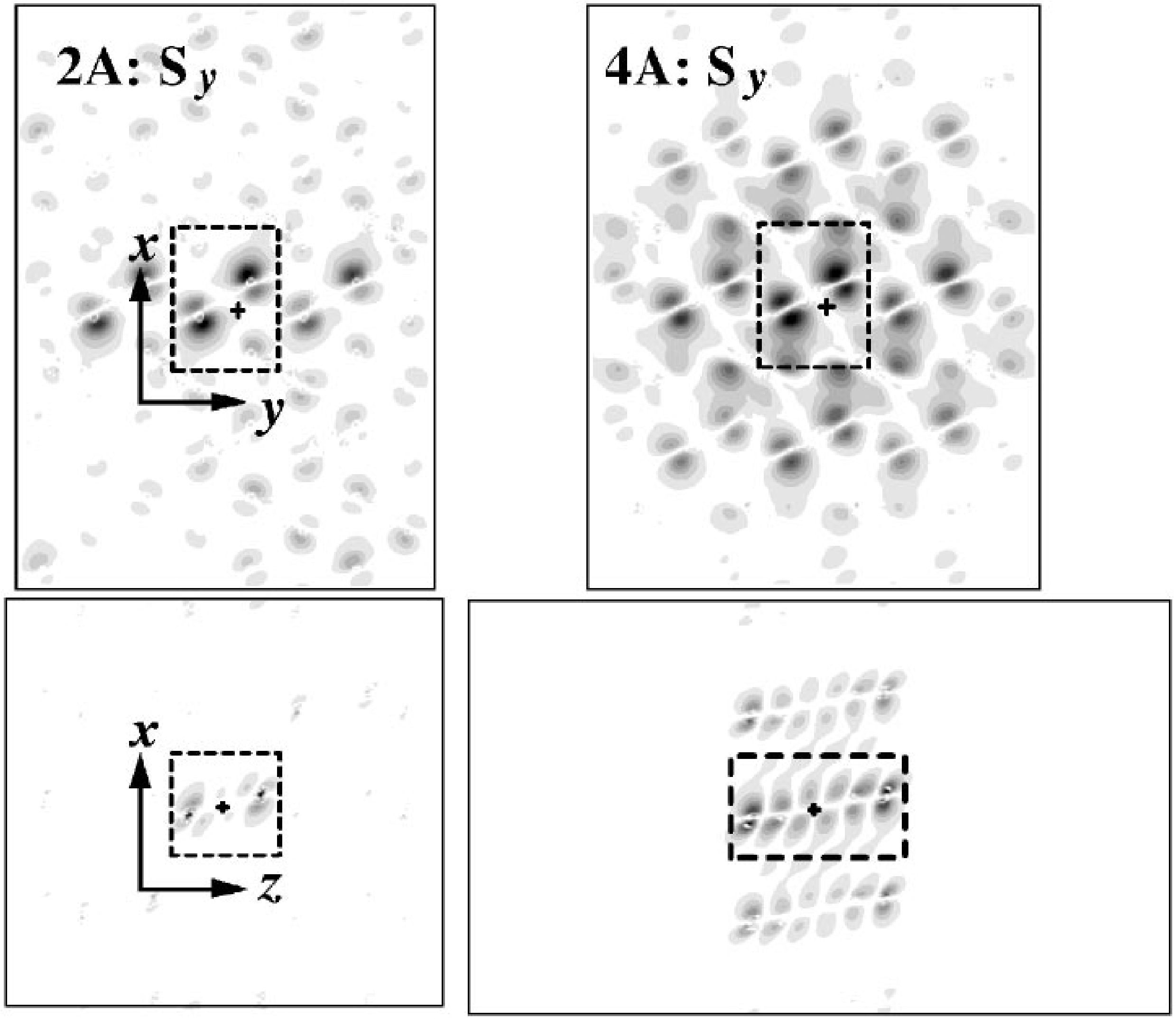
* Finite systems and correlation

* The “bandgap problem”

* Excitons are **NOT** fake!



Oligoacene exciton binding

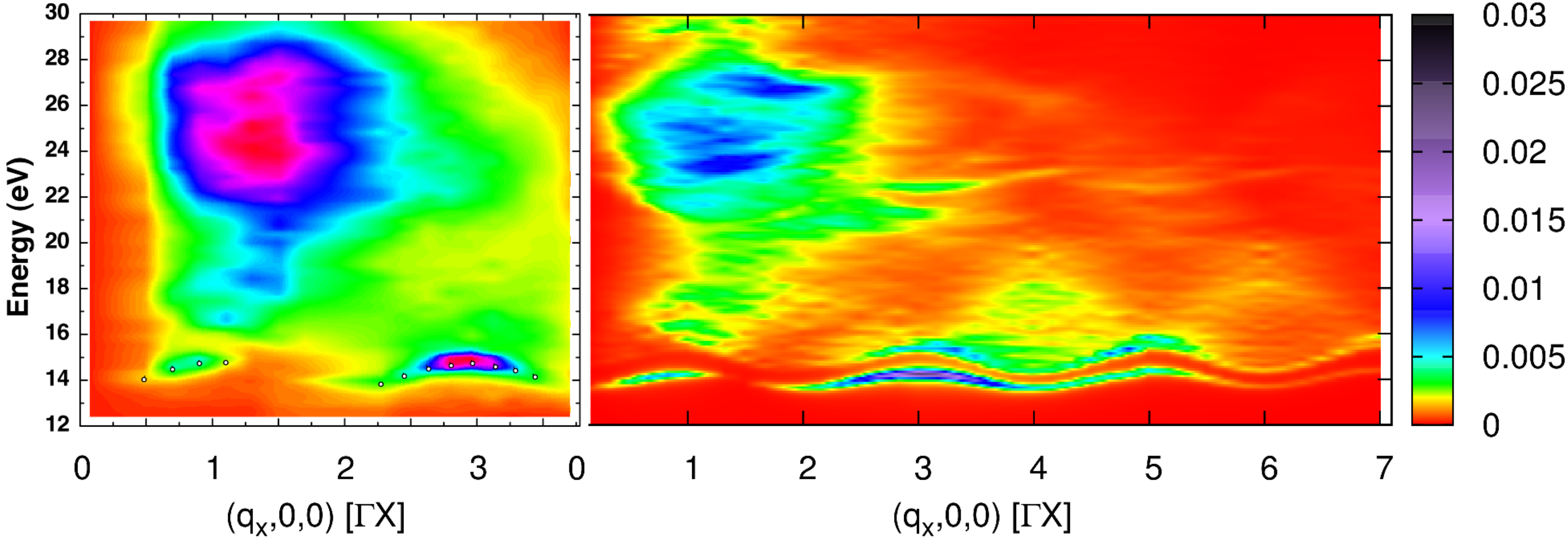


K. Hummer and C. Draxl, PRB 71, 081202(R) (2005)

Some references

- Hanke and Sham, PRB **21**, 4656 (1980)
- Onida, Reining, Rubio, RMP **74**, 601 (2002)
- Strinati, Riv Nuovo Cimento **11**, 1 (1988)

Exciton dispersion in LiF



M. Gatti and F. Sottile, Phys. Rev. B 88, 155113
Exp. P. Abbamonte et al., Proc. Natl. Acad. Sci. USA 105, 12159 (2008).

Notes:

* Finite systems and correlation

* The “bandgap problem”

* Excitons are **NOT** fake!

* dynamical effects

Notes:

* Finite systems and correlation

* The “bandgap problem”

* Excitons are **NOT** fake!

* dynamical effects

* TDDFT from the BSE

BSE Screening equation

$$L = L^0 + L^0(v - W)L$$

TDDFT screening equation

$$\chi = \chi^0 + \chi^0(v + f_{xc})\chi$$

4 point formulation

$$v(\mathbf{r}-\mathbf{r}') \Longrightarrow v(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_3-\mathbf{r}_4)$$

$$f_{xc}(\mathbf{r}-\mathbf{r}') \Longrightarrow f_{xc}(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_3-\mathbf{r}_4)$$

cf. Casida, TD-HF !

BSE

$$v(\mathbf{r}-\mathbf{r}') \Longrightarrow v(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_3-\mathbf{r}_4)$$

$$W(\mathbf{r}-\mathbf{r}') \Longrightarrow W(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4)$$

BSE: unavoidable 4-point formulation, TDDFT *sometimes* convenient!

BSE Screening equation

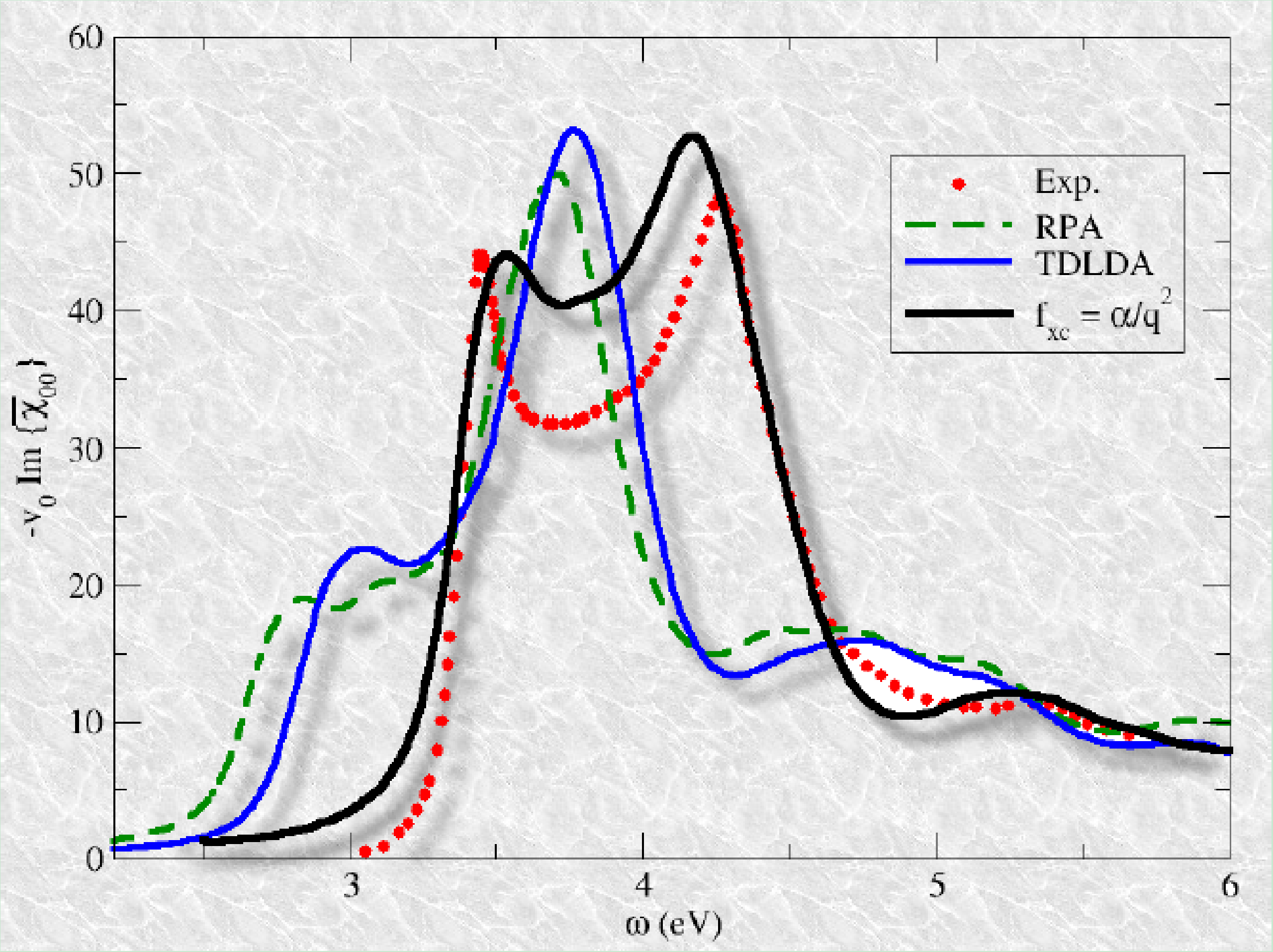
$$L = L^0 + L^0(v - W)L$$

TDDFT screening equation

$$\chi = \chi^0 + \chi^0(v + f_{xc})\chi$$

ALDA: Achievements and Shortcomings

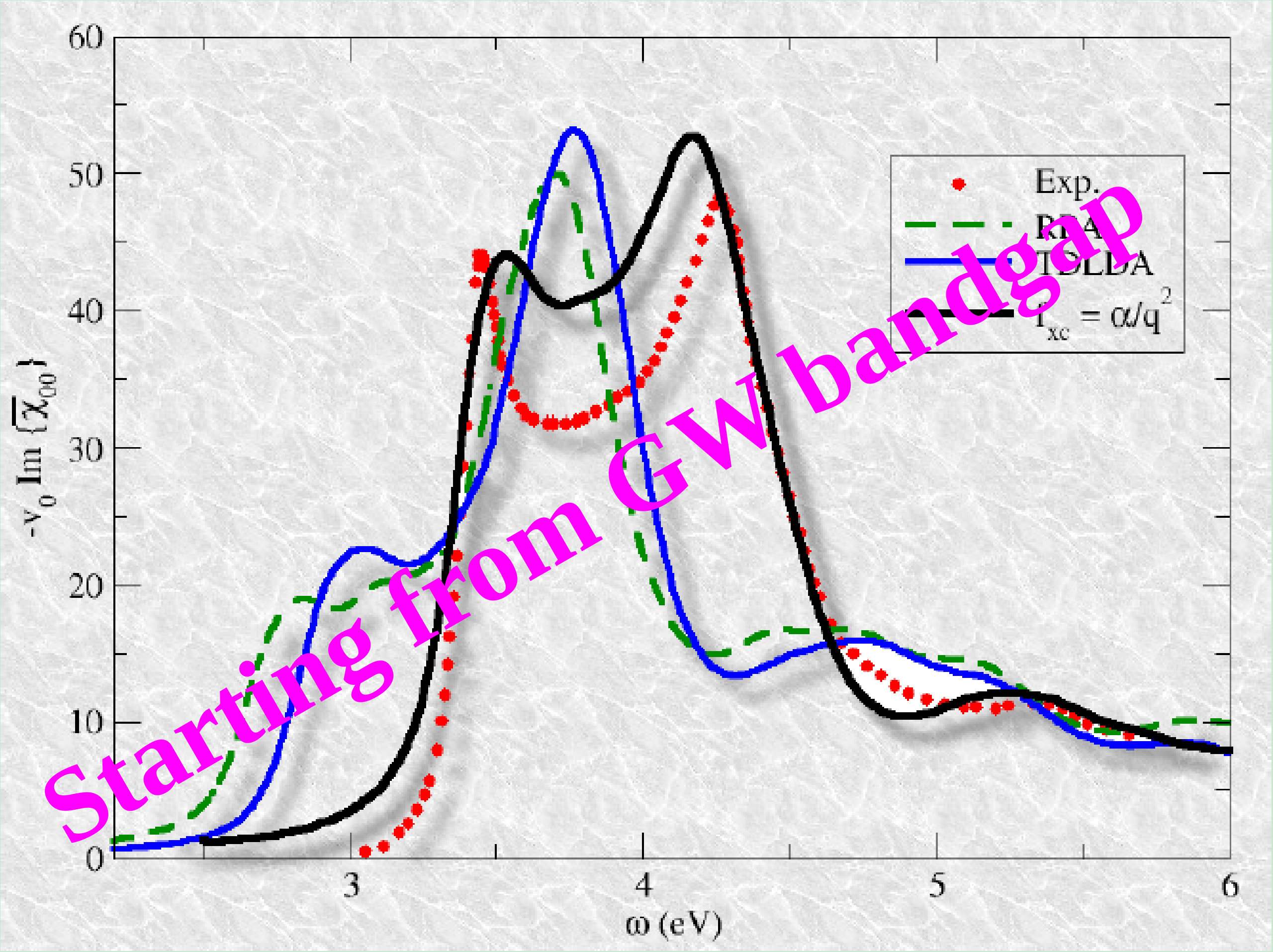
Absorption of Silicon $f_{xc} = \frac{\alpha}{q^2}$



L.Reining *et al.* Phys.Rev.Lett. **88**, 66404 (2002)

ALDA: Achievements and Shortcomings

Absorption of Silicon $f_{xc} = \frac{\alpha}{q^2}$



L.Reining *et al.* Phys.Rev.Lett. **88**, 66404 (2002)

Notes:

* Finite systems and correlation

* The “bandgap problem”

* Excitons are **NOT** fake!

* dynamical effects

* TDDFT from the BSE

* $\Sigma = iGW\Gamma$

$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \\ + \int d(4567)\frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)G(7,5)\tilde{\Gamma}(6,7,3)$$

$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \\ + \int d(4567)\frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)G(7,5)\tilde{\Gamma}(6,7,3)$$

e.g. E. Shirley et al.

1

$V_{xc}(1)$

$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \\ + \int d(4567) \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6) G(7,5) \tilde{\Gamma}(6,7,3)$$

$n(4)$

f_{xc}

e.g. Del Sole, Reining, Godby PRB 1994

The Bethe-Salpeter Equation

→ A reminder

→ TD-GFT

→ The electron-hole problem

→ Approximations

→ Realizations

→ Applications

→ Notes

http://etsf.polytechnique.fr